1. The performance of a complete probe forming instrument is best characterized by the dependence of the obtainable probe current $I$ on the minimum probe size $d$. However, the $I$-$d$ relation itself can only be optimized if the Coulomb effects in the complete system are considered.

2. The miniaturization of electron optical systems was proposed because of the fact that the probe current probe size performance in *micro electron optical columns* is much better than that in *conventional columns* (T.H.P. Chang et al., *J. Vac. Sci. Technol.* **B8**(6), p.1698, 1990).

3. Low-voltage scanning electron microscopes (LVSEM) enjoy wide applications in all areas of development and manufacture of microelectronic and optoelectronic components. However, no further development of the LVSEM would be possible without studying the Coulomb effects in these systems.

4. The *inaccessible area* used for showing the limitations of the performance of a probe forming instrument, representing a balance between different physical and optical effects occurring in the system, is in fact *accessible* if a smarter redesign of the system is made.

5. The *non-crossover imaging mode* is better than the *crossover imaging mode* of a probe forming instrument no matter whether the Coulomb effects are considered or not.

6. The low throughput of focussed particle beam lithography machines is expected to be increased by the development of charged particle projection lithography systems.

7. Considering the achievements in microfabrication up till now, it is more advantageous to develop *particle beam projection systems* than to develop *multiple micro-beam systems* for enhancing the lithographic throughput of wafers.

8. A high brightness source is not always advantageous to improve the performance of charged particle optical instruments such as electron microscopes, electron beam lithography machines, focussed ion beam systems, etc.

9. Learning is much easier than discovering, and designing is much easier than building.

10. The one who achieved something is the one who lost something else.
Stellingen behorende bij het proefschrift:
Coulomb Interacties in Optische Systemen voor Geladen Deeltjes
door Xinrong Jiang

1. Het prestatievermogen van een compleet probe vormend instrument wordt het best gekarakteriseerd door de relatie tussen de haalbare probestroom \( I \) en de minimale probeafmeting \( d \). De \( I-d \) relatie zelf kan echter alleen worden geoptimaliseerd als de Coulombeffecten in het gehele systeem in beschouwing worden genomen.


3. Lage-versnelspanning scanning elektronenmicroscopen (LVSEM) genieten brede toepassingen in alle gebieden van ontwikkeling en fabrikage van microelektronische en optoelektronische onderdelen. Verdere ontwikkeling van de LVSEM zou echter niet mogelijk zijn zonder de Coulombwisselwerking in deze systemen te bestuderen.

4. Het *ontoeogankelijke gebied* dat gebruikt wordt om de beperkingen van het prestatievermogen van een probe vormend instrument te laten zien, en een balans tussen verschillende fysische en optische effecten die in het systeem voorkomen representeert, is eigenlijk *toegankelijk* indien het systeem op slimme wijze wordt herontworpen.

5. De *afbeeldingsmodus zonder asdoorsnijding* van een probevormend instrument is beter dan de *afbeeldingsmodus met asdoorsnijding* onafhankelijk van het feit of Coulombeffecten al dan niet worden beschouwd.


7. In ogenschouw nemend wat tot op heden in de microfabrikage is bereikt, is het beter om een *deeltjes optisch projectiesysteem* dan een *multi microbundelsysteem* te ontwikkelen teneinde de lithografische produktie van wafers op te voeren.

8. Een bron met hoge helderheid is niet altijd voordelig voor het prestatievermogen van geladen deeltjes optische instrumenten zoals electronenmicroscopen, electronenstraal lithografie machines, gefocussedde ionenstraal systemen, etc.

9. Leren is veel gemakkelijker dan ontdekken en ontwerpen is veel gemakkelijker dan bouwen.

10. Degene die iets bereikt heeft, is degene die iets anders verloren heeft.
Coulomb Interactions
in Charged Particle Optical Columns
Coulomb Interactions
in Charged Particle Optical Columns

PROEFSCHRIFT

ter verkrijging van de graad van doctor

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## Contents

1 Introduction to Coulomb Interactions in Charged Particle Optical Columns 1  
1.1 Problem: Coulomb effects in particle optical columns 1  
1.2 Literature overview 3  
1.3 Approaches in this thesis 5  
References 6  

2 Optical models of charged particle instruments 8  
  Abstract 8  
  2.1 Introduction 8  
  2.2 Source model 8  
  2.3 Imaging modes 10  
  2.4 Beam segment model 12  
  2.5 Column model 13  
  2.6 Discussion 14  
References 15  

3 Evaluations of statistical Coulomb effects in charged particle optical columns 16  
  Abstract 16  
  3.1 Introduction 16  
  3.2 Analytical evaluation of Boersch effect in particle beams 17  
  3.3 Analytical evaluation of trajectory displacement effect in particle beams 22  
  3.4 Numerical evaluation of statistical Coulomb effects in particle beams 26  
  3.5 Discussion 28  
  3.6 Conclusions 31  
References 32  

4 Evaluations of space charge aberrations in charged particle optical columns 33  
  Abstract 33  
  4.1 Introduction 33  
  4.2 Particle trajectory under space charge effect 34  
  4.3 Influence of laminar flow on microfocussed beams 36  
  4.4 Expression of space charge aberrations 39  
  4.5 Evaluation of space charge aberrations 41  
  4.6 Space charge effect discs 44  
  4.7 Calculation method of real focal distance 46  
  4.8 Real focal distance analyses 49  
  4.9 Conclusions 51  
References 52  

5 Coulomb aberrations in complete particle optical columns 53  
  Abstract 53  
  5.1 Introduction 53  
  5.2 Description of symbolizations 53  
  5.3 Lens aberrations in different imaging modes 54  
  5.4 Statistical Coulomb interaction aberrations 57  
  5.4.1 Boersch effect disc in a complete particle optical column 57  
  5.4.2 Trajectory displacement effect disc in a complete particle optical column 59  
  5.5 Space charge effect discs in a complete particle optical column 60  
  References 61
5.5.1 Defocussing distance and defocussing aberration 60
5.5.2 Space charge spherical aberration 61
5.6 Total spot size and I-d relations 62
References 63

6 Combined calculation of lens aberrations, space charge aberrations and statistical Coulomb effects in charged particle optical columns 65
   Abstract 65
   6.1 Introduction 65
   6.2 Approach of the combined calculation 66
   6.3 Features and organization of ANALIC 70
   6.4 Calculation example using ANALIC 71
   6.5 Discussion 72
   References 75

7 Influence of Coulomb interactions on choice of magnification, aperture size and source brightness in a two lens focussed ion beam column 76
   Abstract 76
   7.1 Introduction 76
   7.2 Example column 77
   7.3 Optimization without Coulomb interactions 78
   7.4 Influence of Coulomb effects 80
   7.5 Full optimization of the column 82
   7.6 Discussion 83
   7.7 Conclusions 85
   References 86

8 Comparison between different imaging modes in focussed ion beam instruments 87
   Abstract 87
   8.1 Introduction 87
   8.2 I-d relations in different modes 88
   8.3 Conclusions 90
   References 91

9 Intermediate aperture effect in charged particle optical instruments 92
   Abstract 92
   9.1 Introduction 92
   9.2 General column and example columns 93
   9.3 Intermediate aperture effect 94
   9.3.1 Danger area of an optical column 94
   9.3.2 Intermediate aperture range 97
   9.3.3 Definition of the intermediate aperture effect 99
   9.4 Influence of aperture position on intermediate aperture effect 99
   9.5 Essence of the intermediate aperture effect 102
   9.6 Conclusions 103
   References 104

10 Influence of aperture position in focussed ion beam systems on statistical Coulomb interaction effects 105
   Abstract 105
   10.1 Introduction 105
   10.2 Influence of aperture position on column optimization 106
10.3 Discussions
10.3.1 About the column optimization
10.3.2 About the aperture size and position
10.4 Conclusions
References

11 Influence of Coulomb interactions on low-voltage scanning electron microscopes
Abstract
11.1 Introduction
11.2 General column characteristics of VSEM
11.3 Impact of Coulomb effects on 3L-SEM column
11.4 New aperture and imaging modes of 3L-SEM column
11.5 Optimization of 3L-SEM column
11.5.1 Aperture size optimization
11.5.2 Simplified aperture setting
11.5.3 Column length optimization
11.6 Conclusions
References

12 Verifications of ANALIC program
Abstract
12.1 Introduction
12.2 Comparison between ANALIC and INTERAC
12.3 Comparison between ANALIC and MONTEC
12.4 Comparison between ANALIC and experiments
12.4.1 Comparison with mode one
12.4.2 Comparison with mode two
12.4.3 Error analysis
12.5 Conclusions
References

13 Further investigations on Coulomb interactions in charged particle optical columns
Abstract
13.1 Introduction
13.2 Space charge aberrations in accelerating and decelerating fields
13.3 Evaluation of Coulomb effects in high brightness electron sources
13.3.1 Coulomb effects in vicinity of Schottky emitter
13.3.2 Coulomb effects in whole region of electron sources
13.4 Evaluation of Coulomb effects in ion beam projection systems
13.5 Approximate two-particle dynamics
13.6 Conclusion
References
Summary
Samenvatting
Curriculum Vitae
1 Introduction to Coulomb Interactions in Charged Particle Optical Columns

1.1 Problem: Coulomb effects in particle optical columns

Interactions between individual particles may limit the performance of charged particle optical columns. By way of introduction, these limitations will be demonstrated taking the ion beam pattern generator (IBPG) built by Slingerland\textsuperscript{1} as an example.

The original goals developing the Delft IBPG were a shaped square probe with a size variable from 50 to 1000 nm and edge sharpness of typically one fifth of the shape, a variable energy of 30 to 180 keV and a beam current up to 10 nA. This column consists of six lenses including the source lens with total 776.5 mm long (see figure 1.1).

Vijgen calculated the impact of the Coulomb interactions on the whole column in figure 1.1 by using a Monte Carlo simulation\textsuperscript{1,3}. Figure 1.2 presents the results of this simulation for six probe current values. The plot areas in the figure are all 500×500 nm large, and the markers 100 nm. It can been seen that, when the current is lower than 92 pA, the 100×100 nm shaped beam in the target plane expands reasonably, but it becomes unacceptable when the current is greater than 250 pA. However, the former current is really too low for a shaped beam system.

We evaluated the impact of the Coulomb interactions between ions on the resolution of this system by measuring the probe size in the image plane (the crossover plane between the condensor doublet of figure 1.1) of the second lens. The optical column from the tip to the measured image plane can be modelled with several optical parameters. The virtual source diameter $d_0$ is 50 nm, which is already experimentally confirmed. The Full Width Half Maximum (FWHM) source energy spread $\Delta E$ is known to be 5 eV below 2 $\mu$A extraction current. For higher current $\Delta E$ increases rapidly to 10 eV at 30 $\mu$A extraction current\textsuperscript{1}. The distance from the tip to the first lens is 6.5 mm, from the first lens to the second lens 310 mm, and from the second lens to its image plane 37.6 mm\textsuperscript{2}. In all measurements, the considered column operated at 15 keV beam energy. The total magnification of the column $M=M_1 \times M_2$ is 4.4, where $M_1 (=20.5)$ and $M_2 (=0.214)$ are the magnifications of the first (source) and the second lenses of the column. Referred to the object-side and in the infinite magnification

\textbf{Fig.1.1 The Delft IBPG optical set-up.}
Fig. 1.2 Position plot for a shaped beam in the target plane of figure 1.1 for currents (pA): (1) 1.1, (2) 9.1, (3) 92, (4) 250, (5) 565 and (6) 850 (from Vijgen2).}

case, the spherical and chromatic aberration coefficients are $C_{s1}=16$ mm, $C_{c1}=3$ mm, $C_{s2}=3810$ mm and $C_{c2}=105$ mm. With this model and its parameter values, the probe size in the image plane of the second lens can also be calculated.

Figure 1.3 shows the comparison between the designed probe size and the measured probe size based on the previous conditions. In the measurement of the probe size, the emission current from the source tip is varied by changing the extraction voltage, thereby resulting in the variation of the probe current. Most of the tip current is cut by a beam selected aperture in the source, therefore, the probe current is less than 0.1% of the tip current (see figure 1.3). A knife edge scanning method with a 12-88% height measurement of the current wave was used for the probe size in figure 1.3. The designed probe sizes in figure 1.3 were evaluated with FW50 measurement, which is equal to the 12-88% measured probe width if the beam distribution is assumed to be Gaussian.

As can been seen from figure 1.3, the performance of this part of the IBPG is much poorer than designed. The calculated total geometrical aberration disc $d_{\text{geo}}$, which is the addition of the chromatic aberration disc $d_{\text{cha}}$, the spherical aberration disc $d_{\text{sph}}$, and the source image $d_{\text{si}}$, is 6.5-11.6 times smaller than the measured probe size. If both the measurement and the evaluation are correct, the Coulomb interactions in the considered column should be responsible for this big difference. The spot sizes $d_{\text{si}}$ and $d_{\text{sph}}$ do not vary with the probe current, $d_{\text{cha}}$ only changes with the current slightly since the source energy spread $\Delta E$ changes with the tip current, however, the measured probe size increases with the probe current rapidly. This is consistent with the fact that the Coulomb repulsion between the ions increases with the current.
This shows that the Coulomb interactions can greatly limit the performance of a charged particle optical instrument.

1.2 Literature overview

The theoretical analysis of Coulomb interaction effects has been considerably studied by many authors during the last decades. For instance, Boersch noted the induced energy spread in 1954\(^8\), Loeffler noted the induced beam broadening in 1969\(^7\), and Pierce noted the space charge effect in 1954\(^4\), etc. But, the most complete description about the Coulomb interactions so far is the work by Jansen\(^9\). In this section, we do not want to comment in detail on the literature on Coulomb interactions. The reasons are 1) Jansen has summarized more than 250 articles on Coulomb interactions in his book\(^9\), which is a systemic comment on most of the important work on this subject, and 2) our objective is to develop a comprehensive way of performing the combined calculation of the lens aberrations, the statistical Coulomb effects and the space charge aberrations in a practical and complete particle optical column, not in a single beam segment. For these reasons we mainly concentrate ourselves on the contributions which involve the calculation methods of the influence of the Coulomb interactions on a complete optical column after Jansen’s work. From this point of view, the contributions to this subject so far are not very many.

Jansen’s contribution to the study of the Coulomb interactions in particle beams is that he developed the extended two-particle approximation method\(^9,10\) including the two-particle dynamics. With this theory he derived the analytical expressions, by following the approaches of simplification, interpolation and modification, to calculate the Boersch effect, the trajectory displacement effect and the space charge effect in a single crossover beam segment or a single cylindrical beam segment. Jansen did not pay much attention to the calculation of the Coulomb interactions in practical probe forming instruments. He stated that, in the preface of Ref.\(^[9]\), the emphasis of his work is on
fundamentals rather than on applications. Jansen also developed two programs used to calculate the Coulomb interactions in particle beams. One, called INTERAC\textsuperscript{11}, is based on the equations resulting from the analytical model presented in Ref.[9]. The other, called MONTEC\textsuperscript{12}, which is a Monte Carlo simulation program, is based on a direct ray-tracing of the particles through a defined optical column. The main disadvantage of the INTERAC program is that it can not be used to perform the combined calculation of the lens aberrations and the Coulomb interactions in a complete optical column, although its calculation speed is so fast that the operation time can be totally ignored. Oppositely, the main disadvantage of the MONTEC program, and also of other Monte Carlo simulation programs, is that the operation time spent for a single calculation is so long that it can not be used to optimize a complete optical column. Nevertheless, Jansen's work is complete, systemic and correct.

Vijg\textsuperscript{2,3} used Jansen's MONTEC program to carefully calculate the Coulomb interactions in the shaped ion beam column in figure 1.1, and pointed out that there is a serious impact of the Coulomb effects on the resolution of this machine, as shown in figure 1.2. He concluded that, to get rid of the influence of the Coulomb interactions, the column can only operate at a current lower than 0.1 nA.

Brodie\textsuperscript{13} investigated the Coulomb interaction aberration and its impact on the retarding field lens design of a practical system, KLA's SEMSpec\textsuperscript{14}, by using the Monte Carlo program CI5\textsuperscript{15} for computations.

Munro et al\textsuperscript{16} developed a multi-particle Monte Carlo simulation program, called BOERSCH, as a commercially available program. This program can be used to compute the effect of discrete Coulomb interactions in electron and ion beam columns. The program predicts the energy broadening (Boersch effect) and the radial broadening as well as the defocus. Graphical output of energy and radial histograms and spot diagrams is also included in this program.

Shimoyama et al\textsuperscript{17} developed a specialized program to simulate the energetic Boersch effect in the diode region of the field emission (FE) gun. The output of this program is the energy spread in the diode region of the FE gun.

Groves et al\textsuperscript{18} used a Monte Carlo simulation to calculate electron-beam broadening effects caused by the discreteness of space charge for conditions relevant to electron beam lithography. The output of this simulation is the relation between the spot size and the beam current or the column geometry.

The low-energy electron emission from surfaces was simulated with Monte Carlo method by Allen et al\textsuperscript{19}. This calculation was mainly carried out to estimate the spatial distribution of low-energy secondary and back scattered electrons emitted from Si bombarded by low-energy (<4 keV) electron beams.

The aberration properties of a two-lens focussed ion beam column with including the space charge effect were investigated by Hirohata et al\textsuperscript{20} with a Monte Carlo simulation. This evaluation took the lens aberrations into account when the space charge effect in the column was simulated, but the statistical Coulomb effects were not considered.

With the development of the micro-fabrication technology, the micro-columns have been proposed as a route to gaining improved probe currents and probe sizes because of their reduced lens aberrations. Thomson\textsuperscript{21} recently calculated the electron-electron scattering in field-emission electron beam micro-columns with a few millimeters in length by using both Monte Carlo and analytic methods.

Stickel\textsuperscript{22} used both the INTERAC\textsuperscript{11} and the MONTEC\textsuperscript{12} programs evaluated the impact of the Coulomb effects on the well-known electron beam system EL4\textsuperscript{23} and commented some achievements on the research of the Coulomb effects.

It can be found from Ref.[12-22] that the usual approaches of investigating the influence of the Coulomb interactions on particle optical columns are focussed on the Monte Carlo simulation, and
that the Monte Carlo method has been used to calculate the Coulomb interactions in many aspects of particle optics. However, these studies also show that the very expensive CPU time in the simulation process and the unclear quantitative relation between the different parameters of an optical column have been limiting this method to be used in the multi-variable optimization of the column with many continuous calculations.

Besides the Monte Carlo simulations commented previously, Venables et al.\textsuperscript{24} and Barth et al.\textsuperscript{25} analytically calculated the impact of the Coulomb interactions on electron beam instruments several years ago. Kruit et al.\textsuperscript{26} recently considered the impact of the Coulomb interactions on an optimized setting of a probe forming instrument by using an analytical method. These last examples differ from the usual approach because the lens aberrations and the Coulomb interactions in the particle optical column are analytically calculated simultaneously. The characteristic of Ref.\textsuperscript{[24,25,26]} is that they all used the equations derived by Jansen\textsuperscript{9} for the calculations of their problems. These equations are applicable to some determined regimes such as the pencil beam regime, the Lorentzian regime, or the Holtsmark regime and the Gaussian regime. Each regime is totally determined by the beam parameters. From one regime to another, the used equation is different.

The theory on the research of the Coulomb interactions is so far not beyond Jansen's\textsuperscript{9}. The nearest neighbor (N-N) theory, contributed by Mkrtchyan et al.\textsuperscript{27,28,29}, is mainly focussed on the evaluation of the trajectory displacement blur in Holtsmark regime. Mkrtchyan's equation for this special evaluation underestimates 1.22 times compared to Jansen's theory\textsuperscript{9}, and it does not cover the calculations for other beam regimes. However, the N-N theory did demonstrate that Jansen's equations can not be extrapolated towards the regime relevant for projection lithography.

Coulomb effects in particle beam projection systems are being noted during the last years. For instance, Berger et al.\textsuperscript{30} investigated the particle-particle interaction effects in image projection lithography systems (e.g. SCALPEL etc.\textsuperscript{31}). Harriott et al.\textsuperscript{32} and Petillo et al.\textsuperscript{33} looked into the impact of the Coulomb effects on ALPHA5X\textsuperscript{34} and ALG-1000\textsuperscript{35,36} ion beam lithography systems. The Monte Carlo simulation is the main approach of these studies.

1.3 Approaches in this thesis

Approaches in this thesis are different from those in the literature commented previously. We aim at pursuing the combined calculation of lens aberrations, statistical Coulomb effects and space charge aberrations in a complete and practical particle optical system consisting of a number of lenses and apertures. Following the combined evaluation, the full system optimization including the calculation of Coulomb effects is the main topic of this thesis.

In chapter 2, we shall present the optical models of charged particle instruments, with which the lens aberrations, the statistical Coulomb effects and the space charge aberrations in particle beams can be evaluated simultaneously. These optical models will cover the source model, imaging model, beam segment model and system model.

The Coulomb effects including the Boersch effect, the trajectory displacement effect and the space charge effect in our beam segment models will be evaluated by both analytical and numerical approaches in chapters 3 and 4. Based on these calculations for beam segments, chapter 5 will present the combined system evaluation of the lens aberrations, the statistical Coulomb effects and the space charge aberrations. Chapters 2, 3, 4 and 5 constitute the theoretical part of this thesis.

A computer program, named ANALIC, which consists of more than 15000 lines, will be presented in chapter 6 for the full system optimization including the combined calculation of lens aberrations and Coulomb effects in a complete electron or ion beam instrument. All optical models and
theoretical equations from chapter 2 to chapter 5 are included in this program. The program will be used in all evaluations of the studies in chapter 7 to chapter 13, which are our applied investigations of the Coulomb effects for special objectives.

The influence of the Coulomb effects on focussed ion beam (FIB) instruments, including the full optimization of a FIB system and the theory of an "inaccessible area", will be carefully investigated in chapter 7. Based on these studies, we shall give a description of what we think is a good procedure to analyze and optimize any particle optical column.

Chapter 8 intends to answer such a question: in a particle optical column, what type of imaging modes is the best when the lens aberrations and the Coulomb interactions are taken into account simultaneously in the design of the column?

The apertures in a particle optical column play a very important role in limiting the impact of the Coulomb interactions on the image quality. However, the apertures strongly cut the beam current, which is normally a key parameter of a charged particle instrument. To get a balance between the micro-fabrication efficiency (the beam current) and the image quality (the beam spot size in lithography instruments), the "intermediate aperture effect" in focussed particle beams will be investigated in chapter 9. Our further investigation to the "aperture problem" will be presented in chapter 10, in which the influence of aperture position in focussed ion beam systems on statistical Coulomb interaction effects will be studied. This is our observation on the "aperture position effect". The intermediate aperture effect and the aperture position effect constitute the "aperture effect" theory, which is our discovery on the studies of the Coulomb effects in charged particle optical columns.

Low-voltage scanning electron microscopes (LVSEM) are enjoying wide applications in all areas of development and manufacture of microelectronic and optoelectronic components. However, they also suffer strongly from Coulomb interactions due to their low landing energy. Our attention to this area will be presented in chapter 11, in which a novel approach for full system optimization will be given.

Are our models, equations, programs and studies in special applications from chapter 2 to chapter 11 correct and reliable? This will be answered in chapter 12, in which the analytical approach, the Monte Carlo simulation approach and the experimental approach will be used to verify our work.

Finally, some more extended studies on the Coulomb effects in an accelerating or decelerating field, in an electron source and in an ion beam projection system, which are in fact still in progress, will be presented in chapter 13.

References

11. G.H. Jansen, INTERAC Program Package (1989), distributed by Delft Particle Optics Foundation, Delft University of Technology, the Netherlands.
12. G.H. Jansen, MONTEC Program Package (1989), distributed by Delft Particle Optics Foundation, Delft University of Technology, the Netherlands.
2 Optical models of charged particle instruments

Abstract Complete charged particle optical systems are modeled for the combined calculation of the lens aberrations, statistical Coulomb effects and space charge aberrations. First of all, a model is proposed for a virtual source to replace the real source to make it easier to perform the combined evaluation for a practical system. It is then shown that most practical systems can be considered as consisting of a number of rotationally symmetric beam segments between lenses and apertures. Four basic segments can be defined: cylindrical, trapezoidal converging, trapezoidal diverging and crossover.

2.1 Introduction

To evaluate the combined impact of lens aberrations and Coulomb interactions on a practical probe forming instrument, first of all, an appropriate particle optical column model must be developed.

Jansen\(^1\) and other authors\(^2,3\) used a narrow crossover model to calculate the Coulomb interaction effects in a single beam segment between two lenses. When the lens aberrations and the Coulomb interactions in a practical optical column have to be investigated simultaneously, this choice of segmentation is not the most suitable one since lens aberrations are usually calculated for segments in between two crossovers. Furthermore, a particle optical column is normally separated by several apertures and lenses. Some beam segments between the apertures or between an aperture and a lens can not be included in the narrow crossover model since the crossover radius \(r_c\) is no longer "narrow" (\(r_c = 0\)).

This chapter first looks into the source of a complete particle optical system, and a virtual source model is proposed to replace the real source. From the full system design and optimization point of view, the virtual source model greatly simplifies the operation. It then investigates four elementary imaging modes, which are often found in an electron or ion beam instrument. Next, it presents the trapezoidal beam segment and the cylindrical beam segment models for the calculation of the beam in between the apertures or in between an aperture and a lens. Finally, it studies the complete optical system model for the programming of the ANALIC program\(^4\), which is a new software package used to perform the combined calculation of the lens aberrations and the Coulomb effects in a universal particle optical system.

2.2 Source model

Looking into a complete charged particle optical instrument, we first meet the source of the system. To be able to perform the combined calculation of the lens aberrations, the statistical Coulomb interactions and the space charge aberrations in the whole system from the source to the target, first of all, the charged particle gun should be modeled.

Taking a Schottky electron emitter for example, we use a virtual source model to simulate the real source because the former can be conveniently utilized to investigate a whole particle optical system. The tip of the emitter with a radius \(R_e = 0.8 \mu m\) is supposed to be fixed at the position of \(z = -R_e\), as shown in figure 2.1. The electric field at the tip is \(E_e\), which, for a high brightness Schottky emitter, is about \(5 \times 10^8 \) V/m\(^5\). Thus, the electrons which have moved from the tip a short distance \(z_1\) (say,
$z_i \approx R_e = 0.8 \, \mu m$) have an energy $V_i = E_e z_i$ ($\approx E_e R_e = 400 \, \text{V}$). Compared with the distance from the tip to the extractor L (for instance, $L \approx 0.5 \, \text{mm}$ as the usual), the electrons with the energy $V_i$ can still be thought of very close to the tip, which can now be considered as an object of an imaging system with size $d_i$. Suppose that the variation of the potential from $V_i$ at the object $z_i$ to $V_e$ at the extractor is linear, thus, the extractor can be considered as a negative aperture lens with an object distance $(L - z)$ and an image distance $L_v$. Accordingly, the virtual source, which is in fact the image of the extractor lens, is located in $z = L - L_v$ with a virtual size $d_0$ (≈ 20 nm as the usual) and a half opening angle $\alpha_0$.

Our objective is to evaluate the Coulomb effects in the source region. In other words, we want to calculate the energy spread due to the Boersch effect in the emission system of figure 2.1 and the trajectory displacement blur referred to the image plane of the extractor lens. To do these, first of all, we have to determine the real beam shape $r(z)$, which is given by solving the ray equation

$$\frac{d^2 r(z)}{dz^2} + \frac{V'(z)}{2V(z)} \frac{dr(z)}{dz} = 0$$ (2.1)

where $V'(z)$ is the derivative of the potential distribution $V(z)$ in respect of $z$. The initial conditions of the equation is $r(z)_{z = z_i} = d_i / 2$ and $(dr(z)/dz)_{z = z_i} = \alpha_i$. Suppose that the linear potential is defined as $V(z) = V_i [1 + (\rho - 1)(z - z_i)/(L - z_i)]$, where $\rho = V_e/V_i$, the solution of Eq.(2.1) is determined by

$$r(z) = \frac{d_i}{2} - \frac{2 \alpha_i (L - z_i)}{\rho - 1} + \frac{2 \alpha_i (L - z_i)}{\rho - 1} \left[ 1 + \frac{\rho - 1}{L - z_i} (z - z_i) \right]^{1/2}$$ (2.2)

The initial conditions $d_i$ and $\alpha_i$ can be evaluated with the image relation of the negative extractor lens. According to Ref.[5], the magnification $M$, the image distance $L_v$ and the focal distance $f$ of the lens are calculated by

Fig. 2.1 Modeling of a high brightness Schottky emitter: using a virtual source model to replace the real source.

Fig.2.2 The source is modeled as several beam segments separated by several apertures.
\[ M = \frac{2^{1/2}}{3^{1/2} - 1}, \quad |L_v| = \frac{4 \rho (L - z)}{3 \rho + 2 \rho^{1/2}} - 1, \quad f = \frac{1}{4 \rho (L - z)} \left( 1 - \frac{1}{\rho} \right), \quad \rho = \frac{V_e}{V_1} \] (2.3)

The total emission current \( I \) and the angular current density \( J_\theta \) can be experimentally measured. For a normal Schottky emitter, \( I \) can be varied from 50 to 300 \( \mu \)A, and \( J_\theta \) from 0.2 to 1 mA/sr. Thus, the half opening angle at the virtual source is given by

\[ \alpha_0 = \left( \frac{I}{\pi J_\theta} \right)^{1/2} \] (2.4)

and, finally, the initial conditions \( d_i \) and \( \alpha_i \) are determined by

\[ d_i = \frac{d_0}{M}, \quad \alpha_i = M^{1/2} \alpha_0 \] (2.5)

Based on this modeling, the Coulomb interactions in the emission system of figure 2.1 will be evaluated in chapter 13. Figure 2.2 shows a complete source model of a practical electron beam system, in which the real source is replaced by the virtual source with the size \( d_0 \), angle \( \alpha_0 \) and position \( L_v \).

\[ \text{Fig. 2.3 The four imaging relations of a lens system.} \]

Since the thickness of the extractor can not always be ignored compared to the distance \( L \) in figure 2.1, the extractor is modeled as two apertures \( D_1 \) and \( D_2 \). \( D_3 \) in figure 2.2 is the real aperture used to select the beam current, and \( D_4 \) is the electrode of the source lens, which is also modeled as an aperture. It is seen that the emission current is greatly limited by different apertures.

With the source model of figure 2.2, the Coulomb interactions in the whole source region can be evaluated by using our numerical approach presented in chapter 3. This model will be used in the studies of chapters 11, 12 and 13.

2.3 Imaging modes

A complete particle optical instrument consists of at least two lenses, one of which may be the source lens. The particle beam transported in between the lenses can be modeled: with a crossover
Tab. 2.1 Properties of the different imaging modes in figure 2.3. \( u = \frac{f_{12}}{f_{12}} = (V_0/N)^{1/2} \) and \( v = \frac{f_{22}}{f_{22}} = (V/V)^{1/2} \).

<table>
<thead>
<tr>
<th>crossover mode</th>
<th>divergent mode</th>
<th>cylindrical mode</th>
<th>convergent mode</th>
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</thead>
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<tr>
<td>focal distance ( f_{12} )</td>
<td>LPMv ( \frac{L}{P} )</td>
<td>( f_{12} )</td>
<td>LMPv ( \frac{L}{P} )</td>
</tr>
<tr>
<td>( u_{f_{12}} )</td>
<td>( u_{f_{12}} )</td>
<td>( u )</td>
<td>( u_{f_{12}} )</td>
</tr>
<tr>
<td>focal distance ( f_{11} )</td>
<td>LQqv ( \frac{L}{Q} )</td>
<td>( f_{12} )</td>
<td>Q</td>
</tr>
<tr>
<td>( v_{f_{12}} )</td>
<td>( v )</td>
<td>( v )</td>
<td>( v )</td>
</tr>
<tr>
<td>range of magnification ( M )</td>
<td>( 0 &lt; M &lt; \infty )</td>
<td>( Qu &lt; \frac{L}{Q} )</td>
<td>( Qu )</td>
</tr>
<tr>
<td>range of focal distance ( f_{11} )</td>
<td>( 0 &lt; f_{11} &lt; \infty )</td>
<td>( P &lt; f_{11} &lt; \infty )</td>
<td>( P_{u(L+Q)} )</td>
</tr>
<tr>
<td>range of focal distance ( f_{12} )</td>
<td>( 0 &lt; f_{12} &lt; \infty )</td>
<td>( u &lt; f_{12} &lt; \infty )</td>
<td>( u )</td>
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<tr>
<td>range of focal distance ( f_{11} )</td>
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<td>( Q(L+Q) &lt; \frac{L}{Q} )</td>
<td>( Q )</td>
</tr>
<tr>
<td>range of focal distance ( f_{12} )</td>
<td>( 0 &lt; f_{12} &lt; \infty )</td>
<td>( Lq + Q )</td>
<td>( Q &lt; f_{12} )</td>
</tr>
</tbody>
</table>

that \( f_{11} \) and \( f_{12} \) are the focal distances in the object-side and image-side of the first (second) lens, \( M (=M_{12}) \) the total magnification of the two lenses, \( P \) the object distance of the first lens, \( Q \) the image distance of the second lens, \( L \) the distance between the lenses, \( D \) the aperture size at the center of the first lens, and \( V_0 \) the beam potential in the object-side of the first lens, \( V_1 \) in the image-side of the second lens and \( V \) in between the lenses. It is seen from table 2.1 that the different imaging modes can be obtained by varying the magnification \( M \) when the column parameters \( P, Q \) and \( L \) are fixed. For the crossover mode in figure 2.3(1), when the crossover position moves in between the lenses, the total magnification of the column \( M \) changes, in principle, from zero to infinite, but for the non-crossover modes in figures 2.3 (2), (3) and (4), the magnification \( M \) is limited in the range of

\[
\frac{Qu}{Lv + PV} < M < \frac{Luv + Qu}{Pv} \quad ; \quad u = \frac{f_{11}}{f_{12}} = (\frac{V_0}{V})^{1/2} \quad \text{and} \quad v = \frac{f_{22}}{f_{21}} = (\frac{V_1}{V})^{1/2} \quad \text{(2.6)}
\]

A combination of the elementary imaging modes in figure 2.3 constitutes a complete optical column of a probe forming instrument. As a typical example of a combined calculation of the lens aberrations, the statistical Coulomb effects and the space charge aberrations, the two lens column model
in figure 2.3 will be repeatedly used in this thesis.

The imaging mode with a crossover in between two lenses has been widely used in an electron or ion beam instrument. However, it is not the best mode, particularly in the case of a focussed ion beam instrument. It can be found from the literature, for instance in Ref.[7,8,9], that the non-crossover imaging modes were calculated or used in their different ways, but the complete analysis including the combined evaluation of the lens aberrations and the Coulomb interactions was not presented.

2.4 Beam segment model

A particle optical column can be considered as consisting of a number of rotationally symmetric cylindrical or trapezoidal beam segments as shown in figure 2.4 no matter how many lenses and apertures the column has. These segments transport the beam between two lenses or apertures, or between an aperture and a lens. Figures 2.4(1) and (2) indicate the divergent and convergent trapezoidal beam segments with beam current I and beam potential V respectively. One can find the trapezoidal beam segment in every practical particle optical column. A combined beam section in an imaging lens with an object distance P, an image distance Q, a beam spot disc in the object plane 2r_o and in the image plane 2r_o consists of a divergent trapezoidal beam segment and a convergent trapezoidal beam segment shown in figures 2.4(1) and (2). A crossover beam segment in between two lenses with a crossover diameter 2r_c, a segment length L=P+Q and a half opening
angle $\alpha$ also consists of two trapezoidal beam segments, as shown in figure 2.4(3). However, the more elementary beam segment is the cylindrical beam segment in figure 2.4(4). The trapezoidal beam segment can be considered as a pile-up of a series of very thin cylindrical beam segments with different radii $r_0$ along the z-axis. If the beam potential changes with the position $z$, one has to use a series of slices to simulate the real beam segment\textsuperscript{1}, however, one slice is in fact a very thin cylindrical beam.

2.5 Column model

Figure 2.5 shows a general charged particle optical system model. A complete optical system consists of the particle gun, the optical column and the target. Suppose that the general optical column consists of $n$ lenses and $m$ apertures, and that the particle beam in between the first lens and the last lens is transported in four imaging modes shown in figure 2.3. The apertures can be placed at any position along the axis, and the beam energy from the tip to the target can be distributed in any function. In this case, the beam shape $r(z)$ and the beam current $I(z)$ are all the functions of $z$. The input of the system model in figure 2.5 is the parameters of the virtual source described in figure 2.1 and figure 2.2, where $Rm$ is the relative particle mass to the electron, $\Delta E$ the energy spread of the virtual source and $B$ the source reduced brightness. The output of the system is the total probe size $d_{\text{tot}}$ with a determined current $I$, which is a summation\textsuperscript{4,10,11} of the different individual contributions: the source image $d_{\text{img}}$, the chromatic aberration $d_{\text{chr}}$, the spherical aberration $d_{\text{sph}}$, the diffraction aberration $d_{\text{dif}}$, the Boersch effect blur $d_{\text{Boe}}$, the trajectory displacement effect blur $d_{\text{tra}}$, the space charge defocussing blur $d_{\text{loc}}$ and the space charge spherical aberration $d_{\text{sca}}$. Accordingly, $d_{\text{tot}}$ in fact characterizes the combined measurement of the lens aberrations and the Coulomb interactions in a particle optical system. In addition, in our model, the measurement of the combined lens aberrations is characterized by the total geometrical aberration disc $d_{\text{ger}}$, and the measurement of the combined Coulomb effects by the total Coulomb interaction disc $d_{\text{coul}}$, as shown in figure 2.5.

The general system model in figure 2.5 includes many practical optical systems. Accordingly, we use this model as an imaginary universal optical system in the design of ANALIC program\textsuperscript{8}, which will be described in chapter 6.

An example of a practical system is shown in figure 2.6, which is considered as a typical probe forming instrument with all characteristics mentioned in the previous models. It is equipped with a Schottky emitter as analyzed in figure 2.1 and figure 2.2, and with three lenses and three apertures which are used for the imaging of the beam and the limiting of the current. The first aperture in figure 2.6 stands for the aperture $D_1$ in figure 2.2. Using the first and second lens, the four imaging modes described in figure 2.3 and table 2.1 are selected. The four basic beam segments in figure 2.4

![Figure 2.6 A focused electron beam system with three lenses and three apertures.](image-url)
can be found in the system, for instance, the beam in between the first lens and the second aperture is the convergent, in between the second lens and the third lens the crossover. A cylindrical beam or a divergent beam in between the first and second lens can be formed when the focal distances of the lenses are selected in accordance with the definition of table 2.1. The beam potential varies in different beam sections. In the beam segment before the first lens, the potential is the same as that in extractor since the virtual source model is used, in the section from the first lens to the second lens, the potential is high to limit Coulomb interactions. As a typical low-voltage scanning electron microscope (LVSEM), the influence of the Coulomb interactions on this practical system will be carefully investigated in chapter 11.

The charged particle projection instruments are very different from the ones shown in figure 2.5 or figure 2.6. Figure 2.7 presents a typical projection system, which is modeled based on the practical system of ALG-1000\textsuperscript{12,13,14}. Other practical projection systems, for instance ALPHA5\textsuperscript{15,16} and SCALPEL\textsuperscript{17}, have a similar configuration to ALG-1000. The ALG-1000 ion beam lithography prototype is being built for the goal of a resolution at and below 0.18 \textmu m with the current higher than 1 \textmu A. The main ion optical column of the system can be modeled as four beam segments $S_1$, $S_2$, $S_3$, and $S_4$. The investigation of the Coulomb interactions in the projection system in figure 2.7 is presented in chapter 13.

2.6 Discussion

The presented modelling of particle optical columns, which covers the source to the universal system, is for the design of ANALIC program and for all applied studies in this thesis with the program. The idea of ANALIC is to calculate the lens aberrations from crossover to crossover and to evaluate the Coulomb effects in the beam segments in between the crossovers. Each type of the segments has its own equations for the estimations of both lens effects and Coulomb effects. Effects in individual segments are added. Rules of addition will be discussed in chapter 6 and chapter 12.

The being considered beam segments can have two energy modes: a constant energy and a continuously varying energy. Accordingly, the ANALIC program will have two operation modes: the segments and the slice, which can be simply set in an input file of the program (chapter 6). In the mode of the segments that constitute a complete particle optical column, the beam energy from the virtual source to the target can change in a step function but can not vary in a segment. For instance, there are seven segments in the focussed electron beam system of figure 2.6. The beam energies in
the two segments from the virtual source to the first lens are 5 keV, in the two segments from the first lens to the second lens are 10.5 keV and in the three segments from the second lens to the target are 0.5 keV. The ANALIC computes the Coulomb effects for these segments independently. If the beam energy in one of the segments of a complete column changes continuously, for instance the ion energy varies from 10 keV in the mask plane through 200 keV in the crossover plane to 150 keV in the wafer plane of the ALG-1000 projection system of figure 2.7, the ANALIC program will use the slice operation mode for the evaluation of the Coulomb effects in the column. A slice is in fact a very thin cylindrical beam segment defined in figure 2.4(4), in which the beam is considered to be equipotential. Consequently, in an accelerating or decelerating field, a particle beam can not be modeled as one of basic beam segments shown in figure 2.4 since the beam shape, which is determined by Eq.(2.1), will change with the field. In this case, the particle optical column should be sliced and can be calculated numerically for the studies of the Coulomb effects. This will be presented in chapters 3, 6 and 13.

References

5. J.E. Barth, Simple model of a high brightness gun, Private communication, 1996.
3 Evaluations of statistical Coulomb effects in charged particle optical columns

Abstract The analytical and numerical expressions for evaluating the energy spread due to the Boersch effect and the blur due to the trajectory displacement effect are presented in this chapter. The expressions take into account different current distributions and different characteristic values for the spread and blur. The numerical result of the evaluation of the Coulomb effects approximates the analytical result, but it has not been proven yet which evaluation is more accurate. However, the numerical method is more flexible and useful than the analytical method for the evaluation of the Coulomb effects in practical optical systems because the former can be used in the case in which the beam shape, energy and current of the systems can all be taken as functions of the position z.

3.1 Introduction

The influence of the Coulomb interaction effects on charged particle optical systems are normally investigated from two approaches: Monte Carlo simulation\textsuperscript{1,2,3,4,5} and analytical evaluation\textsuperscript{6,7,8,9}. From the full system optimization point of view, the Monte Carlo simulation is too time-consuming to be used to calculate the Coulomb effects in a multi-variable optical system. The most complete description of using analytical equations to evaluate the Coulomb effects so far is the work by Jansen\textsuperscript{6}. He used the approximations of simplification, interpolation and modification in the evaluations of the statistical Coulomb effects in a crossover or a cylindrical beam segment. The equations derived by Jansen are enough to be used to perform a fundamental calculation of the Coulomb effects in a single beam segment. However, these equations are limited to the evaluation of a narrow crossover beam segment with a determined beam shape, a constant beam energy and a constant beam current. A practical optical instrument often does not fit these requirements.

For the combined calculation of the lens aberrations and the Coulomb effects, the beam segment model in between the object plane and the image plane of a lens is better than the crossover beam model in between two lenses, because the former can be directly used to calculate the lens aberrations and the Coulomb effects in an imaging system simultaneously.

Based on the previous considerations, first of all, this chapter presents the analytical expressions of evaluating the statistical Coulomb effects in single beam segments: a divergent segment, or a convergent segment, or a cylindrical segment, which are modeled in figure 2.4. They are considered as the basic beam segments that constitute a practical optical column. For the derivation of the expressions, we follow the approaches of the simplification, interpolation and modification used in Ref.[6]. We then derive the integral expressions for evaluating the Coulomb effects in a general beam segment, which is characterized by an arbitrary beam shape, an arbitrary beam energy distribution and an arbitrary current distribution. The derivation of these expressions is based on a limit operation of the Coulomb effects in a cylindrical beam segment. A practical optical column can be regarded as a combination of a series of the general beam segments. This general segment model is used in the design of the ANALIC program\textsuperscript{10}, which is described in chapter 6. Finally, this chapter presents several typical calculation results for investigating the statistical Coulomb effects in different beam potentials and currents with different measurements.
3.2 Analytical evaluation of Boersch effect in particle beams

The energy spread effect in a charged particle beam segment due to the statistical Coulomb interactions between the particles is referred to as Boersch effect. The evaluation of the Boersch effect depends on the estimation of the statistical distribution of the axial velocity shift $\rho(\Delta v_z)$. If we can evaluate the energy spread produced by the Boersch effect for the elementary beam segments shown in figure 3.1, we can do the same for a complete optical column that usually consists of a number of these beam segments if we know how to add these contributions: linearly, quadratically, etc.

Based on this idea, our task is to evaluate the energy spread functions $\Delta E_{Boe_a}(m,I,V_a,r_a,\alpha_0,P)$ and $\Delta E_{Boe_c}(m,I,V_0,r_0,L)$. Here $m$ is the mass of a particle, $I$ the current in a beam segment, $V_a$ the potential of a beam segment, $r_a$ the minimum original radius of the divergent beam segment in figure 3.1(1), $\alpha_0$ the half opening angle, and $P$ the length of the divergent beam segment. For the cylindrical beam segment, $V$ denotes the beam potential, $r_0$ the beam segment radius, and $L$ the beam segment length. \{m,I,V_a(\text{or} V),r_a(\text{or} r_0),\alpha_0 \text{ and } P(\text{or} L)\} are referred to as macroscopic experimental parameters. $\Delta E_{Boe_a}$ expresses the energy spread function in the divergent beam segment or in the object-side beam segment of an imaging lens, and $\Delta E_{Boe_c}$ the energy spread function in the cylindrical beam segment. For the convergent beam segment or the image-side beam segment of a lens shown in figure 2.4(2), the energy spread function is expressed as $\Delta E_{Boe_b}(m,I,V_0,r_0,\beta_0,Q)$. Here $V_0$ is the potential, $r_0$ the original radius in the minimum convergent plane $b$, $\beta_0$ the half opening angle, and $Q$ the length of the convergent beam segment.

The statistical part of evaluating the distribution of the axial velocity shift in the divergent beam segment in figure 3.1(1) consists of

$$
\rho_z(\Delta v_z) = \frac{2 v_d v}{V_0^2} \left( \frac{2 \pi}{2} \right) \int_0^r \int_0^{2 \pi} \frac{2 r_z dr_z}{r_a^2} \int_0^p \delta(\Delta v_z - \Delta v_z(r_z, b_z, \Phi)) db_z
$$

$$
(3.1)
$$

$$
\rho(k) = \frac{4}{\sqrt{2}} \rho_z(\Delta v_z) \sin(k \frac{\Delta v_z}{2}) d\Delta v_z
$$

$$
(3.2)
$$

Fig.3.1 Two elementary beam segments. (1) a divergent beam segment, and (2) a cylindrical beam segment.
\[
\rho(\Delta v_z) = \frac{1}{\pi} \int_{0}^{\infty} \cos(k\Delta v_z) \exp[-\lambda p(k)] dk \tag{3.3}
\]

In the case of the cylindrical beam segment in figure 3.1(2), Eq.(3.1) can be simplified into

\[
\rho_z(\Delta v_z) = \int_{0}^{r_c} \frac{2r_\perp dr_\perp}{r_0^2} \int_{0}^{L} \delta[\Delta v_z - \Delta v_z(r_\perp, b_z)] db_z \tag{3.4}
\]

where \( r_\perp \) is the modulus of the projection of the relative position vector \( r \) between a test particle and a field particle on x-y plane, \( b_z \) the projection of the vector \( r \) on the z-axis, \( v \) the modulus of the relative velocity vector \( v \) between the test particle and the field particle, and \( \delta(.) \) the \( \delta \)-function. Eq.(3.1) and Eq.(3.4) can be only used in the case that the distributions of the angular current density and the spatial current density are all uniform. If not so, Eq.(3.1) and Eq.(3.4) should be modified. In general, they can be written as \(^6\)

\[
\rho_z(\Delta v_z) = \int_{0}^{\infty} f_z(v) dv \int_{0}^{2\pi} \frac{d\Phi}{2\pi} \int_{0}^{r_c} f_r(r_\perp) dr_\perp \int_{0}^{L} \delta[\Delta v_z - \Delta v_z(r_\perp, b_z, v, \Phi)] db_z \tag{3.5}
\]

and

\[
\rho_z(\Delta v_z) = \int_{0}^{\infty} f_z(r_\perp) dr_\perp \int_{0}^{L} \delta[\Delta v_z - \Delta v_z(r_\perp, b_z)] db_z \tag{3.6}
\]

in which \( f_z(r_\perp) \) and \( f_z(v) \) represent the spatial and angular distribution functions respectively. The Gaussian distribution and the uniform distribution are normally used in practical evaluations. In the case of uniform distributions, \( f_z(r_\perp) \) and \( f_z(v) \) are defined as

\[
f_z(r_\perp) = \frac{2r_\perp}{r_0^2} \text{step}(r_a - r_\perp), \quad f_z(v) = \frac{2v}{v_0^2} \text{step}(v_0 - v) \tag{3.7}
\]

where \( \text{step}(.) \) is a step function. Because of the small angle \( \alpha_0 \) in usual beam segments, we take \( \tan\alpha_0 = \alpha_0 \). Therefore, \( v_0 \) in Eq.(3.7) is \( v_0 \approx v_z\alpha_0 \), where \( v_z \) is the identical axial velocity of the particles moving along the z-axis. However, for the Gaussian distributions, \( f_z(r_\perp) \) and \( f_z(v) \) are determined by

\[
f_z(r_\perp) = \frac{2r_\perp}{r_a^2} \exp[-(\frac{r_\perp}{r_a})^2], \quad r_a = \sqrt{2} \sigma_r, \quad f_z(v) = \frac{2v}{v_0^2} \exp[-(\frac{v}{v_0})^2], \quad v_0 = \sqrt{2} v_z \sigma_v \tag{3.8}
\]

in which \( \sigma_r \) and \( \sigma_v \) are the \( \sigma \)-values of the spatial Gaussian distribution and the angular Gaussian distribution. Accordingly, in the case of the divergent (or convergent) beam segment, there are four usual combinations of the distribution of the axial velocity shift \( \rho(\Delta v_z) \). For our convenience, we use parameter KK to define these combinations, as shown in table 3.1. In the ANALIC program \(^8\), which is described in chapter 6, KK is an important input data. There are only two usual combinations in the case of the cylindrical beam segment since the angular distribution is absent in this situation.
The dynamical part of evaluating the distribution of the axial velocity shift in the divergent beam segment in figure 3.1(1) is determined by

\[ \Delta v_z = \frac{mv^2b_z}{2C_0(1+q_c)}, \quad q_c = \left( \frac{mbv^2}{2C_0} \right)^2, \quad b = (b_z^2 + b_\perp^2 + r_\perp^2 \sin^2 \Phi)^{1/2} \]  

(3.9)

where \( C_0 = e^2/(4\pi\varepsilon_0) \). It is clear that \( \Delta v_z \) in Eq. (3.9) is a function of the integral variables \( r_\perp, b_z, v \) and \( \Phi \) in Eq. (3.1) or Eq. (3.5). Eq. (3.9) can be used in the case in which the nearly complete collision between the particles dominates. If the weak interactions dominate the collision between the particles, Eq. (3.9) should be replaced by

\[ \Delta v_z(r_\perp, b_z, v, \Phi) = \frac{2C_0b_z}{mv(b_z^2 + b_\perp^2 + r_\perp^2 \sin^2 \Phi)} \]  

(3.10)

In the case of the cylindrical beam segment, the dynamical part of evaluating the distribution of the axial velocity shift is determined by

\[ \Delta v_z(r_\perp, b_z) = \frac{Ab_z}{(b_z^2 + r_\perp^2)^{3/4}}, \quad A = \frac{C_0}{m} = \frac{e^2}{4\pi\varepsilon_0\hbar} \]  

(3.11)

Eq. (3.11) describes the situation in which the half-complete collision between the particles dominates. However, if the weak interactions dominate the collision, Eq. (3.11) should be replaced by

\[ \Delta v_z(r_\perp, b_z) = \frac{4TA^2b_z}{7(b_z^2 + r_\perp^2)^{3/2}} \]  

(3.12)

We shall use the nearly complete collision model and the half-complete collision model to calculate the distributions of the axial velocity shift for the divergent beam (including the convergent beam) segment and the cylindrical beam segment respectively.

The calculated result from Eq. (3.3) is a statistical distribution function of the axial velocity shift, as shown in figure 3.2. Normally, there are two manners to evaluate the width of the statistical distribution, that is the Full Width at the Half Maximum (FWHM) measurement and the median Full Width (FW50) measurement, the latter indicates the smallest width containing 50% of the particles. Figure 3.2 shows the two measurements.

Our aim is to evaluate the energy spread, not the velocity shift, in a charged particle beam segment. Accordingly, we are forced to transform the velocity shift to the energy spread. This transformation is determined by

<table>
<thead>
<tr>
<th>KK</th>
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<th>angular distribution</th>
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<td>uniform</td>
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</tr>
<tr>
<td>10</td>
<td>Gaussian</td>
<td>uniform</td>
</tr>
<tr>
<td>11</td>
<td>Gaussian</td>
<td>Gaussian</td>
</tr>
</tbody>
</table>

Tab. 3.1 The usual combinations of the distribution of the beam current density.
\[ \text{FWHM} \Delta E_{\text{Boc}_a}(m, I, V, r_o, \alpha_0, P) = \sqrt{2emV_a \text{FWHM} \Delta v_x(m, I, V, r_o, \alpha_0, P)} \] (3.13)

or

\[ \text{FWHM} \Delta E_{\text{Boc}_c}(m, I, V, r_o, L) = \sqrt{2emV \text{FWHM} \Delta v_x(m, I, V, r_o, L)} \] (3.14)

Eq. (3.13) and Eq. (3.14) can be respectively used to evaluate the energy spread functions in a divergent beam segment and a cylindrical beam segment. For the FW50 energy spread measurement, i.e. FW50ΔE_{Boc_a} or FW50ΔE_{Boc_c}, FWHMΔv_x in Eq. (3.13) and Eq. (3.14) is substituted by FW50Δv_x.

So far, we only considered the physical aspects of determining the energy spread function caused by the Boersch effect. The residual problem is how to calculate the energy spread function practically by using a mathematical method. We are able to compute the energy spread function by means of the numerical calculation methods. The disadvantage of this way is that it can not be conveniently used to compute the energy spread in a complete optical column consisting of many different beam segments. However, to calculate this energy spread function analytically is also very difficult.

Ref. [6] evaluates the statistical distributions of the axial velocity shift in a crossover beam segment and a cylindrical beam segment by using the methods of simplification, interpolation and modification. First of all, Ref. [6] divides the distribution of the axial velocity shift into several regimes such as the pencil beam regime, the Lorentzian regime, the Holtsmark regime and the Gaussian regime. Ref. [6] then calculates the distribution of the axial velocity shift in these regimes independently. Next, the distribution expressions in these regimes are linked together by interpolating each distribution expression in these regimes. And finally, the results that are calculated by means of the simplification and interpolation are modified for fitting the different situations described in table 3.1. This approach is also used in the evaluation of the trajectory displacement effect in a crossover beam segment and a cylindrical beam segment. Although

<table>
<thead>
<tr>
<th>ΔE_{Boc_a}</th>
<th>B_1</th>
<th>B_2</th>
<th>B_3</th>
<th>B_4</th>
</tr>
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<td>FW50</td>
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<tr>
<td>KK</td>
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<td>B_6</td>
<td>B_7</td>
<td>B_8</td>
</tr>
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<td>1.037</td>
</tr>
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</table>

**Tab. 3.2** A set of constants used to distinguish the different measurements and different distributions for the calculation of the energy spread in a trapezoidal beam segment.

![Fig. 3.2 Two usual manners of measuring a statistical distribution.](image-url)
this approach is very complicated, this is the only way, so far, to analytically evaluate the statistical distributions of the displacements of the test particle. We now follow this approach to evaluate the energy spread and the trajectory displacement effect in the divergent (or convergent) beam segment and in the cylindrical beam segment. Accordingly, in the following discussions, we shall directly give the final results, omitting all detailed derivations described in Ref.[6]. When reading this chapter the reader is advised to refer to chapter 7, 8 and 9 of Ref.[6].

For the divergent beam segment in figure 3.1(1), the energy spread function $\Delta E_{\text{Boe}_{a}}$ due to the Boersch effect is expressed as

$$\Delta E_{\text{Boe}_{a}} = \Delta E_{\text{Boe}_{a}}(m, I, V_{a}, r_{a}, \alpha_{0}, P) \tag{3.15}$$

From Eq.(3.5), Eq.(3.7), Eq.(3.8), Eq.(3.9), Eq.(3.2), Eq.(3.3) and Eq.(3.13), this energy spread function is determined by

$$\Delta E_{\text{Boe}_{a}} = \left\{ \frac{B_{1}X^{4}V_{a}^{4}}{B_{5} + B_{2}X^{2}f(\bar{r}_{a}) + B_{3}(\bar{X}, \bar{r}_{a}, \bar{\alpha}_{0})^{2}f(\bar{\alpha}_{0}) + B_{4}(\bar{X}, \bar{r}_{a}, \bar{\alpha}_{0})^{4}} \right\}^{0.25} \tag{3.16}(eV)$$

where

$$f(\bar{r}_{a}) = \left\{ 1 + B_{8}\bar{r}_{a} \ln(B_{6} + B_{7}\bar{r}_{a}) \right\}^{2} \tag{3.17}$$

$$f(\bar{\alpha}_{0}) = (\bar{\alpha}_{0}^{-2/3} + 9\bar{\alpha}_{0}^{-8/3} + 2\bar{\alpha}_{0}^{-1})^{2} \quad \bar{\alpha}_{0} = \alpha_{0}P/r_{a} \tag{3.18}$$

$$X = \frac{m^{1/2}}{\pi \varepsilon_{0}^{2/3} e^{1/2} \alpha_{0}^{2} V_{a}^{2/3}} \tag{3.19}$$

$$\bar{r}_{a} = \frac{8\pi \varepsilon_{0}}{e} \alpha_{0} r_{a} V_{a} \tag{3.20}$$

We use coefficients $B_{1}$, $B_{2}$, $B_{3}$ and $B_{4}$ to distinguish FW50 from FWHM. On the other hand, the charge density distribution of a beam segment may be uniform or Gaussian in the spatial or angular region, these differences are determined by the coefficients $B_{5}$, $B_{6}$, $B_{7}$ and $B_{8}$. $B_{i} (i=1,2,\ldots,8)$ are listed in table 3.2, in which KK denotes the charge density distribution of a beam segment. 0 and 1 express the uniform and Gaussian distributions, and the first K and second K represent the spatial and angular distributions, respectively. The four usual combinations have been listed in table 3.1. For the Gaussian distribution, $r_{a}$ and $\alpha_{0}$ should be substituted with 1.21$r_{a}$ and 1.21$\alpha_{0}$ in the previous equations. Eq.(3.15), Eq.(3.16), Eq.(3.17), Eq.(3.18), Eq.(3.19) and Eq.(3.20) can all be used to determine the energy spread function $\Delta E_{\text{Boe}_{b}}$ in the convergent beam segment shown in figure 2.4(2). The form of the function $\Delta E_{\text{Boe}_{b}}$ is exactly the same as function $\Delta E_{\text{Boe}_{a}}$. What one should do for determining the function $\Delta E_{\text{Boe}_{b}}$ is to simply substitute $V_{b}$ for $V_{a}$, $r_{b}$ for $r_{a}$, $\beta_{0}$ for $\alpha_{0}$ and Q for P from Eq.(3.15) to Eq.(3.20), i.e.
\[ \Delta E_{Boe_b} = \Delta E_{Boe_b}(m, I, V_{b}, r_{b}, \beta_0, Q) = \Delta E_{Boe_a}(m, I, V_{b}, r_{b}, \beta_0, Q) \text{ (eV)} \]  \hspace{1cm} (3.21)

For the same reason, from Eq.(3.6), Eq.(3.7), Eq.(3.8), Eq.(3.11), Eq.(3.2), Eq.(3.3) and Eq.(3.14), the energy spread function \( \Delta E_{Boe_c} \) in the cylindrical beam segment in figure 3.1(2) can be determined by

\[ \Delta E_{Boe_c} = \Delta E_{Boe_c}(m, I, V, r_0, L) \]  \hspace{1cm} (3.22)

\[ \Delta E_{Boe_c} = \left[ \frac{B_1 \lambda^* r_0^6 V L^{-0.5}}{1 + [B_2(\lambda^* r_0^3)^8 + B_3 \lambda^* (r_0^4 4.51 + 0.24 r_0^3 3.4205 5.250.25)]} \right]^{2/3} \text{ (eV)} \]  \hspace{1cm} (3.23)

where

\[ \lambda^* = \frac{m^{1/2} IL^2}{\pi \varepsilon_0^{1/2} e^{1/2} r_0^2 V^{3/2}} \]  \hspace{1cm} (3.24)

\[ r_0^* = \left[ \frac{2 \pi \varepsilon_0}{e} \right]^{1/3} \frac{r_0 V^{1/3}}{L^{2/3}} \]  \hspace{1cm} (3.25)

The FW50 and FWHM measurements for the energy spread function \( \Delta E_{Boe_c} \) are distinguished by the coefficients \( B_1, B_2 \) and \( B_3 \) listed in Table 3.3. When the spatial Gaussian distribution is considered, the radius \( r_0 \) should be substituted with \( 1.21 r_0 \).

### Tab. 3.3 A group of constants for the calculations of the Boersch effect and the trajectory displacement effect in a cylindrical beam segment.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Coefficient</th>
<th>Unit</th>
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</thead>
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<td>( \Delta E_{Boe_c} )</td>
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<td>B_2</td>
</tr>
<tr>
<td>FW50</td>
<td>7.861e-2</td>
<td>6.828e+9</td>
</tr>
<tr>
<td>FWHM</td>
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<td>1.776e+4</td>
</tr>
<tr>
<td>( d_{\text{usc}} )</td>
<td>T_1</td>
<td>T_2</td>
</tr>
<tr>
<td>FW50</td>
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<td>2.041e+5</td>
</tr>
<tr>
<td>FWHM</td>
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</tr>
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<td>( r_0 )</td>
</tr>
<tr>
<td>10 or 11</td>
<td>5.10e-2</td>
<td>1.21r_0</td>
</tr>
</tbody>
</table>

3.3 Analytical evaluation of trajectory displacement effect in particle beams

The distribution of the virtual lateral displacement \( \rho(\Delta r) \) generated in a rotationally symmetric beam segment is directly related to the trajectory displacement effect in the beam segment. The lateral displacements \( \Delta r \) result from the stochastic fluctuations in the charge density.

The evaluation of the distribution of the virtual lateral displacement \( \rho(\Delta r) \) depends on the determination of the reference plane or the image plane. The location of the reference plane is specified by the parameter \( S_i \) described in Ref.[6]. In the case of the crossover beam segment, the crossover location is defined by parameter \( S_c \), which
is also described in Ref.[6].

Our final objective is to evaluate the different spot discs including the trajectory displacement effect disc in the object plane or image plane of a charged particle optical column such as figure 2.5 or figure 2.6. This implies that we are interested in the evaluation of the distribution of the lateral displacement \( \rho(\Delta r) \) in the minimum radial plane of a divergent beam segment in figure 3.1(1), or a convergent beam segment in figure 2.4(2), or in the terminal plane of a cylindrical beam segment in figure 3.1(2). In this case it is obvious that \( S_z=S_0=0 \) for the divergent beam segment, and \( S_z=S_1=1 \) for the convergent beam segment. This situation should lead to simplify the evaluation of the distribution of the lateral displacements \( \rho(\Delta r) \) induced by the trajectory displacement effect.

The statistical part of evaluating the distribution of the lateral displacement in a divergent beam segment is determined by

\[
\rho_2(\Delta r) = \int_0^\infty f_2(v) dv \int_0^{2\pi} \frac{d\Phi}{2\pi} \int_0^\infty \int_0^L \delta[\Delta r-\Delta r(r_z,b_z,v,\Phi)]db_z
\]

(3.26)

\[
p(k) = \int_0^\infty \rho_2(\Delta r)[1-J_0(k\Delta r)]d\Delta r
\]

(3.27)

\[
\rho(\Delta r) = \frac{1}{2\pi} \int_0^\infty kJ_0(k\Delta r)\exp[-\lambda p(k)]dk
\]

(3.28)

In Eq.(3.26), the definition of functions \( f_2(r_z) \) and \( f_2(v) \) are the same as Eq.(3.7) and Eq.(3.8). Accordingly, the four usual combinations defined in table 3.1 are again used in the evaluation of the trajectory displacement effect. In the case of the cylindrical beam segment, Eq.(3.26) is simplified into

\[
\rho_2(\Delta r) = \int_0^\infty f_2(r_z)dr_z \int_0^L \delta[\Delta r-\Delta r(r_z,b_z)]db_z
\]

(3.29)

When the crossover plane \( S_z \) coincides with the reference plane \( S_0 \), the dynamical part of evaluating the distribution of the lateral displacement in a divergent beam segment is determined by

\[
\Delta r(r_z,b_z,v,\Phi) = \frac{1}{1+q_c} \left[ \frac{b^2}{q_c} + \frac{r_z^2}{b} - \frac{2br_z}{q_c} \cos\Phi + \frac{q_c^4}{4b^2} \sin^2 2\Phi + 2br_z \sqrt{q_c (\frac{r_z^2 \sin^2 \Phi}{b})^2} \right]^{1/2}
\]

(3.30)

in which \( b \) and \( q_c \) are defined by Eq.(3.9). Eq.(3.30) is derived in the case of the nearly complete collision. Although Eq.(3.30) is defined in the special case of \( S_z=S_0 \), it is very complicated. In the case of a narrow half-crossover beam segment, we can further suppose that the original minimum spot radius of a divergent beam segment \( r_s \) (or a convergent beam segment \( r_s \)) approaches the limit zero, thereby, taking \( r_z=0 \) in Eq.(3.30) yields
\[
\Delta r(x,v) = \frac{2C_0}{mv^2 \left\{ 1 + [mb^2v^2/(2C_0)]^2 \right\}} \tag{3.31}
\]

For the weak interactions, the lateral displacement is evaluated by\(^6\),

\[
\Delta r(x,v) = \frac{C_0}{mv^2} \left[ \ln \frac{vT_f + [(vT_f)^2 + b_x^2]^{1/2}}{b_x} - \frac{vT_f}{[(vT_f)^2 + b_x^2]^{1/2}} \right] \tag{3.32}
\]

For the cylindrical beam segment in figure 3.1(2), the distribution of the lateral displacement in the terminal plane of the beam segment is the most important. When the reference plane coincides with the terminal plane, \(S_1 = 1\). In the case of the half-complete collision, the dynamical part of the problem is determined by\(^6\)

\[
\Delta r(r_\perp,v_\parallel) = \left| -\frac{7}{8} T_\perp^\prime \frac{(C_0/m)^{1/2}}{(b^2 + r_\perp^2)^{3/4}} \right| \tag{3.33}
\]

However, in the case of the weak interactions, Eq. (3.33) should be replaced by\(^6\)

\[
\Delta r(r_\perp,v_\parallel) = \frac{2T_\perp C_0}{7m(b^2 + r_\perp^2)^{3/2}} \tag{3.34}
\]

It should be noted that the flight time \(T_f\) is different in the different beam segments. For the divergent beam segment, \(T_f = \sqrt{m/(2eV_\perp)}\), and for the cylindrical beam segment, \(T_f = L(m/(2eV))\).

We shall use the model of weak interactions to calculate the distribution of the lateral displacement \(\rho(\Delta r)\) by following the mathematical derivations in chapters 8 and 9 of Ref.[6], thereby omitting the detailed procedure of these derivations as declared previously.

The evaluated results based on Eq.(3.28) are directly related to the macroscopic experimental parameters \(\{m, I, V_a, r_a, \alpha_0, P, K_0\}\). On the other hand, \(\rho(\Delta r)\) is a statistical distribution function of the lateral displacement \(\Delta r\), which is similar to the distribution in figure 3.2. Accordingly, the two usual measurements, FWHM and FW50, can be again used to evaluate the trajectory displacement effect in a particle beam segment. For this reason, we use FWHM\(\Delta r\) and FW50\(\Delta r\) to indicate the Full Width at Half Maximum and the median Full Width of the statistical distribution of the lateral displacement \(\rho(\Delta r)\) respectively.

FWHM\(\Delta r\) (or FW50\(\Delta r\)) is in fact a direct measure for the beam expansion in radial direction due to the trajectory displacement effect. It results in a blurred spot in the object plane or in the image plane of a lens system. In order to create the convenience of evaluating a practical particle optical column with different spot sizes in the object plane or in the image plane, we directly define FWHM\(\Delta r\) (or FW50\(\Delta r\)) as the trajectory displacement effect disc FWHM\(d_{ua}\) (or FW50\(d_{ua}\)), i.e.

\[
\text{FWHM}d_{ua}(m,I,V_a,r_a,\alpha_0,P,K_0) = \text{FWHM}\Delta r(m,I,V_a,r_a,\alpha_0,P,K_0) \tag{3.35}
\]

or

\[
\text{FWHM}d_{ua}(m,I,V_a,r_a,\alpha_0,P,K_0) = \text{FWHM}d_{ua}(m,I,V_a,r_a,\alpha_0,P,K_0)
\]

\[
24
\]

\[
\text{FWHM}d_{ua}(m,I,V_a,r_a,\alpha_0,P,K_0) = \text{FWHM}d_{ua}(m,I,V_a,r_a,\alpha_0,P,K_0)
\]

\[
\text{FWHM}d_{ua}(m,I,V_a,r_a,\alpha_0,P,K_0) = \text{FWHM}d_{ua}(m,I,V_a,r_a,\alpha_0,P,K_0)
\]
\[ \text{FW50d}_{\text{na}}(m,I,V_a,r_a,\alpha_0,P,K_d) = \text{FW50}\Delta r_d(m,I,V_a,r_a,\alpha_0,P,K_d) \]  
(3.36)

This definition is also suited to the cases of the convergent beam segment and the cylindrical beam segment.

In the original minimum spot plane \( a \) of the divergent beam segment in figure 3.1(1), the blurred spot diameter \( d_{\text{na}} \) produced by the trajectory displacement effect in this beam segment is expressed as

\[ d_{\text{na}} = d_{\text{na}}(m,I,V_a,r_a,\alpha_0,P,K_d) \]  
(3.37)

where the trajectory displacement effect disc is determined by

\[ d_{\text{na}} = \left\{ \frac{\chi^{18/7} P^{4/7} V_a^{-2/7}}{T_1 T_4 v_0^{-6} (1 + T_5 \bar{\alpha}_0^{-1})^{-6/7} + [T_2 \chi^{14} f(\bar{\alpha}_0) + T_3 \chi^{15} f(v_0^*)]^{1/7}} \right\}^{7/6} \]  
(3.38)

in which

\[ f(\bar{\alpha}_0) = (0.794 + 2.38 \bar{\alpha}_0^{-1} - 2.38 \bar{\alpha}_0^{-2/3}) \cdot 10^{-6} \quad \bar{\alpha}_0 = \alpha_0 P/r_a \]  
(3.39)

\[ f(v_0^*) = K_v v_0^{-11.97} (1.395 + v_0^{1.14})^{10.5} \]  
(3.40)

\[ v_0^* = (2 \pi \varepsilon_0 V_a P \alpha_0^3/e)^{1/3} \]  
(3.41)

For the same reason as the Boersch effect, the measurement of \( d_{\text{na}} \) is performed with FW50 and FWHM in the case of the uniform distribution or Gaussian distribution. All combinations of these cases are distinguished with the coefficients \( T_i \) (i=1,2,3,4,5) listed in table 3.4. The calculation of the trajectory displacement effect disc \( d_{\text{na}} \) in the original minimum spot plane \( b \) of a convergent beam segment is determined by simply substituting \( V_b \) for \( V_a \), \( r_b \) for \( r_a \), \( \beta_0 \) for \( \alpha_0 \), \( Q \) for \( P \) and \( K_c \) for \( K_d \) in equation (3.37), (3.38), (3.39), (3.40), (3.41) and (3.19), i.e.

\[ d_{\text{na}} = d_{\text{na}}(m,I,V_b,r_b,\beta_0,Q,K_c) \]  
(3.42)

It can be found that there are some differences between the cases of the divergent beam segment and the convergent beam segment, or between Eq.(3.37) and Eq.(3.42), except for the difference of the experimental parameters. For the divergent beam segment the coefficient \( K_d \) in Eq.(3.37) is taken as 9.346, and for the convergent beam segment the coefficient \( K_c \) in Eq.(3.42) is 0.647. This fact implies that the trajectory displacement in the minimum spot plane of a convergent beam segment is heavier than that of a divergent beam segment when the experimental parameters in both beam segments are taken the same. By contrast to the trajectory displacement effect, the energy spread caused by the Boersch effect in the divergent beam segment is totally equal to that in the convergent beam segment when the experimental parameters in both beam segments are identical.

For the cylindrical beam segment in figure 3.1(2), the statistical trajectory displacement in the terminal plane is evaluated by
\[ d_{na,c} = d_{na,c}(m, I, V, r_0, L) \]  

where the function \( d_{na,c} \) is determined by

\[ d_{na,c} = \left( \frac{T_1 L^{4/7} V^{-2/7} \lambda^{*18/7} r_0^{*6}}{T_4 + [T_2 r_0^{*42} \lambda^{*14} + T_3 \lambda^{*15} (r_0^{*4} + 0.185 r_0^{*20/7})^{21/21}]^{1/7}} \right)^{7/16} \]  

The FW50 or FWHM measurement of the trajectory displacement \( d_{na,c} \) is determined by the coefficients \( T_1, T_2, T_3 \) and \( T_4 \) listed in table 3.3. It must be noted that the meaning of 0.5 \( d_{na,c} \) should be understood as the statistical radial shift of the cylindrical beam in the terminal plane of the segment. In other words, the statistical angular deflection \( \Delta \alpha \) of the cylindrical beam segment is \( 0.5d_{na,c}/L \).

### 3.4 Numerical evaluation of statistical Coulomb effects in particle beams

The previous analytical evaluation of the statistical Coulomb effects is in fact considerably limited from the investigation of a practical optical system point of view. First of all, it requires a determined beam shape characterized by \( \alpha_0 \) or \( r_0 \), a constant beam current \( I \) and a constant beam energy \( V \). It then requires a narrow crossover radius \( r_a \) or \( r_b \), since Eqs. (3.16) and (3.38) are the results from the interpolation around the zero crossover radius \( (r_a \text{ or } r_b = 0)^9 \). Normally, a practical optical system is difficult to meet these needs. For the example of the focussed electron beam system in figure 2.6, the beam segment in between the first lens and the second aperture is not a narrow crossover beam segment, and the beam shape in the source region (see figure 2.1) can not be characterized by a constant angle.

To meet the needs of the evaluation of the statistical Coulomb interactions in a practical optical system, this section discusses an integral method for the calculation of the Coulomb effects in a general beam segment. Figure 3.3 shows the general beam segment with an arbitrary beam shape \( r(z) \), an arbitrary beam energy distribution \( V(z) \) and an arbitrary beam current distribution \( I(z) \).

The length of the segment is \( (z_b-z_a) \). \( z_{refa} \) or \( z_{refb} \) is the position of a reference plane, for instance the object plane or

<table>
<thead>
<tr>
<th>( d_{na,c} )</th>
<th>( T_1 )</th>
<th>( T_2 )</th>
<th>( T_3 )</th>
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</thead>
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<tr>
<td>FW50</td>
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<td>1.916e+13</td>
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</tr>
<tr>
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<td>4.341e+15</td>
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<td>KK</td>
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</tr>
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<td>11</td>
<td>0.2487</td>
<td>1.500</td>
<td>1.21( r_a )</td>
</tr>
</tbody>
</table>

**Fig.3.3** A general beam segment with an arbitrary beam shape, an arbitrary energy distribution and an arbitrary current distribution.
the image plane of an imaging lens. The shadowed area is a very thin cylindrical beam segment in figure 3.1(2) with a length of $\Delta z \rightarrow 0$. A practical charged particle optical column can be considered as a combination of a series of the beam segments in figure 3.3.

The total energy spread due to the Boersch effect in the general beam segment is calculated by

$$\Delta E_{\text{Boe total}} = \left\{ \lim_{L \to \Delta z \to 0} \left( \frac{\Delta E_{\text{Boe}}}{\Delta z} \right) \right\}_{\Delta z}^{z_f} \int_{z_i}^{z_f} \frac{dz}{F_{\text{Boe}}[r(z),V(z),I(z)]dz}$$

(3.45)

where $\Delta E_{\text{Boe}}$ is the energy spread due to the Boersch effect in a cylindrical beam segment, which is calculated by Eq.(3.23). $F_{\text{Boe}}[r(z),V(z),I(z)]$ is defined as an energy spread function caused by the Boersch effect, i.e.

$$F_{\text{Boe}}[r(z),V(z),I(z)] = \lim_{L \to \Delta z \to 0} \left\{ \frac{\Delta E_{\text{Boe}}}{\Delta z} \right\}$$

$$= \lim_{L \to \Delta z \to 0} \frac{1}{\Delta z} \left\{ \frac{B_1 \lambda^* r_0^* 6 V L^{-1/2}}{1 + \left( B_2 (\lambda^* r_0^* 3)^8 + B_3 \lambda^* 9 (r_0^* 327 + 0.24 r_0^* 2475) 1/4 \right) 1/4} \right\}^{2/3}$$

(3.46)

Rewriting Eqs.(3.24) and (3.25) yields

$$\lambda^* = C_\lambda L^2 \quad C_\lambda = D_\lambda \frac{I(z)}{r(z)^3 V(z)^{3/2}} \quad D_\lambda = \frac{m^{1/2}}{\pi^{1/2} e_0 e^{1/2}}$$

(3.47)

$$r_0^* = C_r \frac{L}{2^{3/3}} \quad C_r = D_r r(z) V(z)^{1/3} \quad D_r = \left( \frac{2 \pi e_0}{e} \right)^{1/3}$$

(3.48)

Substituting Eqs.(3.47) and (3.48) into Eq. (3.46) and performing the limit operation results in

$$F_{\text{Boe}}[r(z),V(z),I(z)] = \left( \frac{B_1 C_\lambda^3 C_r^6 V(z)}{1 + B_2^{1/4} C_\lambda^2 C_r^6} \right)^{2/3}$$

(3.49)

Substituting $C_\lambda$ and $C_r$ in Eqs.(3.47) and (3.48) into Eq.(3.49) gives

$$F_{\text{Boe}}[r(z),V(z),I(z)] = \left\{ \frac{B_1 D_\lambda^3 D_r^6 I(z)^3 V(z)^{-3/2}}{1 + B_2^{1/4} D_\lambda^2 D_r^6 r(z)^2 V(z)^{-1}} \right\}^{2/3} (eV.m^{-1})$$

(3.50)

The SI-unit of the energy spread function $F_{\text{Boe}}$ is eV/m. In the limit operation of Eq.(3.46), the Gaussian regime term characterized by the coefficient $B_3$ disappears. This means that there is no
Gaussian regime in a slice beam segment.

The total trajectory displacement effect disc \( d_{tra\ total} \) referred to the \( z_{ref} \) plane can be calculated by

\[
d_{tra\ total} = \left( z - z_{ref} \right) \lim_{L \to z - 0} \left( \frac{d_{tra\ c}}{L \Delta z} \right) dz = \left( z - z_{ref} \right) F_{tra}(r(z), V(z), I(z))dz
\] (3.51)

where \( d_{tra\ c} \) characterizes the trajectory displacement effect in a cylindrical beam segment, which is calculated by Eq.(3.44). \( F_{tra}(r(z), V(z), I(z)) \) represents the angular deflection function due to the trajectory displacement effect in the general beam segment of figure 3.3, which is defined as

\[
F_{tra}(r(z), V(z), I(z)) = \lim_{L \to z - 0} \left( \frac{d_{tra\ c}}{L \Delta z} \right)
\] (3.52)

Substituting Eqs.(3.47), (3.48) and (3.44) into Eq.(3.52) and evaluating the limit of Eq. (3.52) yields

\[
F_{tra}(r(z), V(z), I(z)) = \left( \frac{T_1 V(z)^{-2/7} C_r^{1/87} C^6}{T_4 + T_2^{1/7} C_r^{1/2} C^2} \right)^{7/6} = \left( \frac{T_1 D_{187}^{1/87} D_{187}^{1/6} I(z)^{187} r(z)^{6/7} V(z)^{-15/7}}{T_4 + T_2^{1/7} D_{187}^{1/2} D_{187}^{1/2} I(z)^{2} r(z)^{2} V(z)^{-1}} \right)^{7/6} \quad (m^{-1})
\] (3.53)

For the same reason, the total trajectory displacement effect disc referred to the \( z_{ref} \) plane is determined by

\[
d_{tra\ total} = \left( z_{ref} - z \right) F_{tra}(r(z), V(z), I(z))dz
\] (3.54)

where the angular deflection function \( F_{tra}(.) \) is the same as that in Eq.(3.53). In Eq.(3.53), the Gaussian regime term characterized by the coefficient \( T_1 \) in Eq.(3.44) disappears for the same reason as in the evaluation of the Boersch effect. The coefficients \( B_1, B_2, T_2 \) and \( T_4 \) in previous equations are still defined in table 3.3. Normally, Eq.(3.45) or Eq.(3.51) can not be calculated analytically, but it can be easily computed by using normal numerical integration methods.

It should be emphasized that the numerical evaluation of the statistical Coulomb effects, which is expressed as Eqs.(3.45) and (3.50) for the energy spread and Eqs.(3.51) and (3.53) for the trajectory displacement effect disc, is now not limited anymore to a narrow crossover beam segment. It is in fact applicable to a beam segment with arbitrary distributions of the beam shape \( r(z) \), beam potential \( V(z) \) and beam current \( I(z) \). We shall find in the later applications that such a beam segment is very flexible to be used to simulate a practical charged particle optical column.

3.5 Discussion

The statistical Coulomb interactions are observed with two usual measurements: FWHM and FW50. For the divergent beam segment in figure 3.1(1), figure 3.4 shows that the energy spread due to the Boersch effect \( \Delta E_{Boers} \) increases with the beam current \( I \) at the condition of a Ga\(^+\) beam potential \( V_s=15 \text{ kV} \), \( r_s=25 \text{ nm} \), \( \alpha_0=0.1 \text{ mrad} \) and \( P=100 \text{ mm} \). For the lower currents, the energy spread
with a FW50 measurement is larger than that with a FWHM measurement. In this case, the statistical distribution of the axial velocity shift shown in figure 3.2 has a long tail. Oppositely, for the higher current, the energy spread with a FW50 measurement is smaller than that with a FWHM measurement. This means that the shape of the distribution of the axial velocity shift is sharp around the original point $\Delta v_z = 0$ in figure 3.2. However, the different distributions (different KK) of the beam current in the spatial or angular region do not greatly alter the curves of the energy spread versus the current.

The dependence of the trajectory displacement effect disc $d_{\text{tra}}$ on the beam current $I$ in a divergent beam segment in figure 3.1(1) is shown in figure 3.5. The calculation conditions of figure 3.5 are the same as those of figure 3.4. It is found that in the case of a higher current range the trajectory displacement effect discs in different current distributions and with different measurements are going to be close to each other. However, in the lower currents the trajectory displacement effect discs with FW50 measurement are much larger than those with FWHM measurement.

The use of the analytical expressions is limited from investigating a complete practical system point of view. However, the numerical evaluation method is flexible to be used to simulate a practical system. How about the accuracy of the numerical evaluation? Figure 3.6 and figure 3.7 show that the numerical evaluation approximates the analytical evaluation reasonably. For a Ga$^+$ divergent beam segment with a potential $V = 30$ kV, length $L = 100$ mm, half opening angle $\alpha_0 = 2$ mrad and crossover radius $r_c = 0.1$ $\mu$m, the Boersch effect energy spread $\Delta E_{\text{Boes}}$ and the trajectory displacement effect disc $d_{\text{tra}}$ are calculated in a large current range by using both the analytical expressions in Eqs. (3.16) and (3.38) and the integral expressions in Eqs. (3.45) and (3.51). The two evaluations fit
reasonably. The limited difference between the two calculations is because the evaluations are based on different models of the collisions between charged particles. The analytical estimation for the Boersch effect is based on the nearly complete collision (Eq. (3.9)), but the integral estimation on the half-complete collision (Eq. (3.11)). For the trajectory displacement effect, however, the analytical estimation is based on the weak collision (Eq. (3.32)), but the integral estimation on the half-complete collision (Eq. (3.33)).

Figures 3.8, 3.9 and 3.10 present the demonstrations to observe the energy effect in the statistical Coulomb interactions. Four typical energy functions, the constant (a), linear (b), exponential (c) and logarithmic (d) relations, are used to simulate the beam energy distributions in a divergent Ga⁺ beam segment, as shown in figure 3.8. In order to obtain a understanding how the beam energy influences the statistical Coulomb effects, we suppose that the beam shape (which is in practice not possible) and the beam current do not vary with the beam energy. The calculations are performed in a large current range by using the integral methods in Eqs. (3.45) and (3.51).

Figure 3.9 shows that 1) there exists a bigger energy spread difference between the different beam energy distributions in the lower current range, 2) the energy spread in the non-constant energy distributions is much larger than that in the constant energy distribution in the intermediate beam current range, and 3) the beam energy distribution does not obviously alter the energy spread caused by the Boersch effect in the higher current range. However, it is found from figure 3.10 that the dependence of the trajectory displacement effect on the beam energy distribution is very different from that of the Boersch effect. In the lower current range, the trajectory displacement effect disc in the non-constant energy distribution is smaller than that in the constant distribution no matter what...
kind of beam energy distributions are taken into account. However, in the higher current range, this conclusion is totally opposite. Of the non-constant energy distributions, the logarithmic distribution is the best from decreasing the statistical Coulomb effects point of view, especially, in the lower current range, as seen from figure 3.9 and figure 3.10. This observation means that, in order to decrease the statistical Coulomb effects in a particle optical column, it is always advantageous to accelerate the beam as early as possible.

3.6 Conclusions

The analytical and numerical expressions of evaluating the energy spread caused by the Boersch effect and the trajectory displacement effect are directly related to all experimental parameters of particle beam segments which constitute the optical column of a charged particle instrument. Together with the calculation of lens aberrations, these expressions can be directly used to design a particle optical column.

It is not necessary to distinguish the pencil beam regime, Lorentzian regime or Holtsmark regime and Gaussian regime in the calculation of the statistical Coulomb effects when using the presented expressions in this chapter. In practice, which regime dominates a particle beam segment depends on the given experimental parameters, however, these parameters are already included in the presented expressions.

The numerical evaluation of the statistical Coulomb effects can be flexibly used to meet the needs of the real configuration of a complete charged

Fig.3.8 Four typical beam energy distributions used to compare the energy effect in the statistical Coulomb interactions.

Fig.3.9 Comparison of the energy spread due to the Boersch effect at different beam energy distributions, relative to the spread at constant beam energy.
particle optical instrument. The calculation accuracy of the numerical method approximates that of the analytical method, but it has not been proven yet that one is better than the other in accuracy. The numerical evaluation is in fact based on a linear addition to the contributions from different slices. This is different from the gamma-rule summation proposed by Jansen. The discussion about this difference will be presented in chapter 12, in which more considerations will be included.

Both the analytical expression and the numerical expression are suggested to be limited in the use of the beam segments with a low or moderate particle density because they are essentially based on the first order perturbation dynamics.

References

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4 Evaluations of space charge aberrations in charged particle optical columns

Abstract The particle ray equation in a uniform accelerating or decelerating field is derived with taking into account the impact of the space charge effect. The analytical equations of evaluating the space charge aberrations are then presented for a divergent or convergent beam segment. These expressions are different from those based on a crossover beam segment model since not only they are simpler but also they can be directly used to calculate the space charge aberrations in the object or image plane of an imaging lens, in which the lens aberrations are also defined. Finally, the variation of the focal distance due to the space charge effect is calculated for the imaging lenses in charged particle optical columns. The trapezoidal beam segment is again used as a unified model for the combined evaluation of the space charge aberrations, the lens aberrations and the statistical Coulomb effects in a charged particle optical column simultaneously.

4.1 Introduction

The earlier studies on the space charge effect were concentrated on the region of a charged particle source or on the beam segment with a high beam current density. With the development of the particle beam microfabrication technology, one learns that the resolution of the microfabrication is also severely degraded by the space charge effect with a medium or even a low beam current density and with a low or even a medium energy in a beam segment\(^{1-6}\). One hopes to make use of higher beam currents in order to improve the low efficiency of the fabrication with focussed particle beams. Unfortunately, the lateral expansion of the focussed beam induced by the space charge effect is directly proportional to the beam current. Besides, the space charge effect is highly sensitive to the particle energy, the particle mass and the shape of a beam segment.

Some calculations for the impact of the space charge effect on a charged particle beam were limited by using a Monte Carlo simulation method\(^{1-6}\). The disadvantages of this kind of computation are too expensive CPU time and unclear relation between the different parameters.

Jansen\(^7\) presented the complete analytical equations for the evaluation of the space charge effect in a crossover beam segment. However, when the lens aberrations and the space charge aberrations have to be calculated simultaneously for designing an imaging system, the crossover beam segment does not stand for every imaging beam section in an imaging system.

This chapter is to first derive the general particle ray equation in a uniform accelerating or decelerating field including the impact of the space charge effect. The particle beam between the laminar flow and non-laminar flow is differentiated by defining the continuum condition\(^7,8\). It then researches into the impact of the space charge on the image quality and presents the analytical expressions for the evaluation of the space charge aberrations in the object or image plane of an imaging lens. This is based on the fact that most of charged particle optical columns run in the lower current range. In this case the continuum condition breaks down. The image quality of a charged particle optical column is not only severely degraded by the lens aberrations, but can be also heavily deteriorated by the space charge aberrations if the current density is not homogeneous. The trapezoidal beam segment model is again used for the investigation of the space charge aberrations. The advantage of this model is that it can be used to represent the imaging relation of a lens. Finally, it will look into the variation of the focal distance due to the space charge effect in the imaging
system of a lens. When the space charge effect occurs, the original imaging relation (i.e. the geometrical relation without the impact of the space charge effect) of an lens is broken, and a new imaging relation is established. The calculation of the focal distance of an electromagnetic lens is usually performed in terms of the paraxial trajectory equation and the definition of the focal distance. Unfortunately, it is impossible to obtain a standard paraxial trajectory equation (i.e. the second order linear and homogeneous differential equation) when the influence of the space charge effect is taken into account. Accordingly, the calculation of the focal distance of a lens under the influence of the space charge effect discussed in this chapter is an approximate evaluation.

The further investigations on the space charge aberrations in a slice and in an accelerating or decelerating field will be presented in chapter 6 and chapter 13.

4.2 Particle trajectory under space charge effect

Consider a rotationally symmetric charged particle beam segment shown in figure 4.1, in which \( \phi(r,z) \) expresses the potential distribution of the beam segment, \( E \) the electric field, \( \rho(r,z) \) the density distribution of the space charge, \( r_0(z) \) a characteristic radius of the beam segment at position \( z \), \( r(z) \) the trajectories of particles. \( r_0(z) \) or \( r(z) \) is regarded as a measurement of the beam radius under the influence of the space charge effect.

Because at this point we are not interested in the statistical nature of particle-particle interactions, we assume that the space charge density of the beam segment is stable within a time long enough for an observation. We also assume that the beam segment is in a uniform accelerating or decelerating field, i.e. the beam potential distribution along the \( z \)-axis \( V(z) \) is linear from \( V_1 \) in \( z_1 \) plane to \( V_2 \) in \( z_b \) plane in figure 4.1.

If \( \rho(r,z) \) is expressed as the average value of the space charge density within an enough long time of an observation \( \tau \), i.e.

\[
\rho(r,z) = <\rho(r,z,t)> = \lim_{\tau \to \infty} \frac{1}{\tau} \int_0^\tau \rho(r,z,t) dt
\]  \hspace{1cm} (4.1)

one can expand Eq.(4.1) into a power series in terms of the first assumption:

\[
\rho(r,z) = \rho_0(z) + \rho_2(z)r^2 + \rho_4(z)r^4 + \ldots
\]  \hspace{1cm} (4.2)

No odd powers of \( r \) appear in Eq.(4.2) because of the rotationally symmetric segment being considered. The coefficients \( \rho_{2i}(z) \) \((i=0,1,2,\ldots)\) can be determined according to the practical distribution of the space charge density. The Gaussian distribution, parabolic distribution and uniform distribution are usually considered as three typical distributions of the density. In these distributions \( r_m(z) \) denotes the maximum beam radius at position \( z \) under the impact of the space charge effect on the beam. In the case of Gaussian distribution, one defines the characteristic radius \( r_0(z) = 2^{1/2} \sigma(z) \) and \( r_m(z) = \infty \).
Here \( \sigma(z) \) is the sigma-value of the Gaussian distribution at the axial position \( z \). For the parabolic distribution or uniform distribution, \( r_0(z) \) or \( r_m(z) \) are defined as the outer beam radius, and \( r_0(z)=r_m(z) \). The representations of these distributions are respectively defined as:

\[
\rho_0(r,z)=\frac{\rho_m(z)}{\sqrt{2\pi} \sigma(z)} \exp\left[-\frac{r^2}{2\sigma(z)^2}\right] \quad r_0(z)=\sqrt{2\pi} \sigma(z) \quad |r| < \infty
\]

(4.3)

\[
\rho_p(r,z)=\rho_m(z)\left[1-(\frac{r}{r_0(z)})^2\right] \quad |r| \leq r_m(z)
\]

(4.4)

\[
\rho_u(r,z)=\rho_m(z) \quad |r| \leq r_m(z)
\]

(4.5)

The maximum density \( \rho_m(z) \) at the axial position \( z \) is determined by the normalization of \( \rho(r,z) \):

\[
\int_0^{r_m(z)} 2\pi r \rho(r,z) dr = \frac{I}{v_z} = \frac{I}{\sqrt{2\eta V(z)}}
\]

(4.6)

in which \( I \) is the current of the beam segment, \( v_z \) the average axial velocity of the particles (\( v_z=(2\eta V(z))^{1/2} \)), \( \eta \) the ratio of the charge to the mass of a particle (\( \eta=e/m \)), \( V(z) \) the axial potential at position \( z \). Respectively substituting Eq.(4.3), (4.4) and (4.5) into Eq.(4.6), one obtains

\[
\rho_0(r,z)=\frac{I}{\pi r_0(z)^3\sqrt{2\eta V(z)}} \exp\left[-\frac{r^2}{r_0(z)^2}\right] \quad |r| < \infty
\]

(4.7)

\[
\rho_p(r,z)=\frac{2I}{\pi r_0(z)^3\sqrt{2\eta V(z)}} \left[1-(\frac{r}{r_0(z)})^2\right] \quad |r| \leq r_m(z)
\]

(4.8)

\[
\rho_u(r,z)=\frac{I}{\pi r_0(z)^3\sqrt{2\eta V(z)}} \quad |r| \leq r_m(z)
\]

(4.9)

Expanding Eq.(4.7), Eq.(4.8) and Eq.(4.9) into a power series respectively leads to

\[
\rho(r,z)=\frac{I}{\pi r_0(z)^3\sqrt{2\eta V(z)}} [c_0(z)+c_2(z)(\frac{r}{r_0(z)})^2+c_4(z)(\frac{r}{r_0(z)})^4+...]
\]

(4.10)

If the distribution shapes of the space charge density at different axial position \( z \) are variant, the coefficients \( c_i(z) \) (\( i=0,1,2,\ldots \)) in Eq.(4.10) are the functions of \( z \). If the shapes are similar, \( c_i(z) \) (\( i=0,1,2,\ldots \)) are a set of constants. The latter means that the space charge effect may cause the expansion of the beam segment in radial direction, but it does not alter its shape, i.e. the shape at any position \( z \) is similar to that of its initial state. For instance, in the case of Gaussian distribution, \( c_0(z)=1, c_2(z)=-1, c_4(z)=1/6, \ldots, \) in the case of the parabolic distribution, \( c_0(z)=2, c_2(z)=-2, c_4(z)=0 \) (\( i=2,3,4,\ldots, \)), and in the case of the uniform distribution, \( c_0(z)=-1, c_2(z)=0 \) (\( i=1,2,3,\ldots, \)).

The series expansion of the potential distribution \( \phi(r,z) \) in figure 4.1 results in
\[ \phi(r,z) = V(z) + V_2(z)r^2 + V_4(z)r^4 + V_6(z)r^6 + \ldots \]  

(4.11)

Substituting Eq. (4.10) and Eq. (4.11) into Poisson equation yields

\[ V_2(z) = -\frac{I_{C_0}(z)}{4\pi\varepsilon_0 f_0(z)\sqrt{2\eta V(z)}}, \quad V_4(z) = -\frac{I_{C_2}(z)}{16\pi\varepsilon_0 f_0(z)^4\sqrt{2\eta V(z)}}, \quad V_6(z) = -\frac{I_{C_4}(z)}{36\pi\varepsilon_0 f_0(z)^6\sqrt{2\eta V(z)}} \]  

(4.12)

Newton's motion law in the radial direction is expressed as

\[ \frac{d^2r}{dt^2} = -\eta \frac{\partial \phi(r,z)}{\partial r} = -\eta (2V_2r + 4V_4r^3 + 6V_6r^5 + \ldots) \]  

(4.13)

where

\[ \frac{d^2r}{dt^2} = \frac{d}{dt} \left( \frac{dz}{dt} \right) = \frac{d^2z}{dt^2} + \left( \frac{dz}{dt} \right)^2 \frac{d^2r}{dz^2} \]  

(4.14)

in which \( \frac{dz}{dt} = v_e = \left[ 2\eta V(z) \right]^{1/2} \). According to the second assumption, one gets \( (d^2z/dt^2) = -(\eta \partial \phi/\partial z) = E \). Substituting Eq. (4.12) and (4.13) into Eq. (4.14) results in the general particle trajectory equation under the influence of the space charge effect on a beam segment

\[ \frac{d^2r}{dz^2} + \frac{E}{2V(z)} \frac{dr}{dz} = \mu(z) [c_0(z) \frac{r}{r_0(z)^2} + c_2(z) \frac{r^3}{2r_0(z)^4} + c_4(z) \frac{r^5}{3r_0(z)^6} + \ldots] \]  

(4.15)

where

\[ \mu(z) = \frac{I}{4\pi\sqrt{2\eta \varepsilon_0 V(z)^{3/2}}} \]  

(4.16)

Eq. (4.15) shows that the particle ray is determined by not only the electric field but also the space charge. Accordingly, the investigation of the space charge aberrations determined by Eq. (4.15) is very complicated since the combined impact of the field and the space charge have to be taken into account simultaneously. Chapter 13 of this thesis will look into this problem. In order to simplify the following discussion, this chapter only considers the space charge aberrations in a drift space. In this case, Eq. (4.15) is simplified into

\[ \frac{d^2r}{dz^2} = \mu [c_0(z) \frac{r}{r_0(z)^2} + c_2(z) \frac{r^3}{2r_0(z)^4} + c_4(z) \frac{r^5}{3r_0(z)^6} + \ldots], \quad \mu = \frac{I}{4\pi\sqrt{2\eta \varepsilon_0 V^{3/2}}} \]  

(4.17)

4.3 Influence of laminar flow on microfocussed beams

Eq. (4.17) is a general equation about the particle trajectory in a drift space. This equation can be solved by different approaches in terms of different practical situations, for the examples of the laminar flow beam or the non-laminar flow beam. If in a particle beam segment the following equation is fulfilled
at any position of \( z \geq z_0 \), it is referred to as a beam segment with a laminar flow, and Eq. (4.18) is named the continuum condition \(^7^8\). Eq. (4.18) means that the total number of the particles which are simultaneously present in a cylindrical volume in the segment with some characteristic length \( \Delta z \) (let \( \Delta z \) take the order of \( r_w(z) \)) is large compared to unity. It is indispensable that the continuum condition in Eq. (4.18) should be fulfilled in order to get a laminar flow. Kruit et al \(^9\) recently further considered that to obtain a laminar flow requires a second condition: focus size condition.

When the laminar flow occurs in a beam segment, each particle trajectory does not intersect with the optical axis, and these trajectories do not cross each other, either. Based on these conditions, it is sufficient to determine the characteristic trajectory \( \tau_0(z) \) of the beam segment in figure 4.1. Substituting \( \tau(z) = \tau_0(z) \) into Eq. (4.17) gives

\[
\frac{d^2 \tau_0(z)}{dz^2} = \frac{c(z) \mu}{\tau_0(z)}
\]

(4.19)

where

\[
c(z) = c_0(z) + c_2(z)/2 + c_4(z)/3 + \ldots
\]

(4.20)

Suppose that the distribution shape of the space charge density at any axial position \( z \) (\( z \geq z_0 \)) is similar to its initial state (\( z = z_0 \)), thus, \( c(z) \) is independent of \( z \). Usually this type of laminar flow is referred to as a congruent flow \(^7^8\). For instance, in the case of the Gaussian distribution, \( c = 1 - 1/4 + 1/18 - \ldots \approx 0.795 \), for the parabolic distribution and the uniform distribution, \( c = 1 \).

The solution of Eq. (4.19) is determined by

\[
\int \frac{dR}{\sqrt{\xi + lnR}} = +\sqrt{2\mu c} (z_f - z)/\tau_f = 0
\]

(4.21)

in which \( x = \tau_0(z)/\tau_f \). \( \xi \) in Eq. (4.21) is referred to as the diffusion coefficient of a laminar flow \(^7^8\), it includes all parameters of a beam segment.

In the case of the laminar flow, Eq. (4.21) exactly specifies the characteristic trajectory \( \tau_0(z) \) at any position for a determined beam segment. In order to look into how the laminar flow influences a practical charged particle optical column, we take the focussed ion beam system shown in figure 1.1
for example. Here, we only consider a single beam segment in the image-side of the first lens in figure 1.1, which is a convergent beam segment as shown in figure 2.4(2), in which the diffusion coefficient is determined by

$$\xi = \frac{\beta_0^2}{2\mu c} = \frac{2\pi \sqrt{2\eta}}{e\beta_0^2 V_b^{3/2}}$$

(4.22)

where $\beta_0$ is the half opening angle and $V_b$ the potential of the beam segment.

For the uniform distribution and the parabolic distribution ($c=1$) of the space charge density, numerically calculating Eq.(4.21) yields the characteristic trajectory curves shown in figure 4.2 and figure 4.3 respectively. In figure 4.2, the initial Ga$^+$ beam with $r_i=50$ $\mu$m, $r_b=0$, $z_b=0$ and $z_b=150$ mm belongs to a convergent beam segment with a smaller diffusion coefficient.

In figure 4.2 and figure 4.3, every characteristic trajectory has a minimum radius $r_c$ at the minimum section position $z_c$. The minimum radius is evaluated by

$$r_c = r_0 e^{-g}$$

(4.23)

and, the minimum section position is determined by

$$z_c - z_b = \frac{r_i}{\sqrt{2\mu c}} \int_0^1 \frac{dR}{\sqrt{1 + R^2}}$$

(4.24)

Figure 4.2 shows that the higher the beam current I (or the smaller the diffusion coefficient $\xi$), the severer the lateral expansion of the beam occurs. Figure 4.3 is another case. In which $r_i$ equals 200 $\mu$m, and the beam current I (or the diffusion coefficient $\xi$) is larger than that of figure 4.2, but the lateral expansion of the beam is smaller than that of figure 4.2. Accordingly, the larger the diffusion coefficient $\xi$, the smaller the space charge effect influences a beam segment. When $\xi > 6$, one finds $r_i/r_c < 0.25\%$ for a convergent beam with $r_b=0$ (see figure 4.3). The continuum condition may break down, or the particle trajectory may intersect with the optical axis in this case.

In general, the continuum condition in Eq.(4.18) may be easily fulfilled in an ion beam column because of the large mass of ion, and the ion trajectory can be evaluated by the laminar flow theory. For the electron beam column or the ion beam column with lower currents, the continuum condition may break down. In this case the calculation of the particle trajectory should be performed by a non-laminar flow theory.
4.4 Expression of space charge aberrations

The particle beam segment in the imaging system of a lens usually consists of two trapezoidal beam segments, as shown in figure 2.4(1) and figure 2.4(2) or figure 4.4. P and Q express the object distance and the image distance of the imaging system, and $f_a$ and $f_b$ the focal length in the object-side and in the image-side, respectively. Usually the trapezoidal beam segment in the object-side is a divergent beam segment, in the image-side a convergent beam segment. We shall take the trapezoidal beam segment in the object-side for example to derive the equations of the space charge aberrations.

An arbitrary particle trajectory $r=r(z)$ in a beam segment under the influence of the space charge effect on it is determined by Eq.(4.17). Suppose that the arbitrary trajectory $r(z)$ and the characteristic trajectory $r_0(z)$ in figure 4.1 and in Eq.(4.17) can be expressed as

$$r(z)=r_p(z) + \delta r_p(z), \quad r_0(z)=r_{0p}(z) + \delta r_{0p}(z)\tag{4.25}$$

Eq.(4.25) should come true when the continuum condition is not fulfilled in a beam segment. In this case the expansion of the beam segment in radial direction is relatively small. $r_p(z)$ and $r_{0p}(z)$ in Eq.(4.25) represent the arbitrary trajectory and the characteristic trajectory in a beam segment before the space charge effect occurs, $\delta r_p(z)$ and $\delta r_{0p}(z)$ are the spatial displacements of $r_p(z)$ and $r_{0p}(z)$ which are induced by the space charge effect.

As shown in figure 4.2 and figure 4.3, it is possible that an arbitrary trajectory intersects the optical axis when the continuum condition (or focus size condition) is not fulfilled in a beam segment. For the trapezoidal beam segment in figure 4.4, the characteristic trajectory $r_{0p}(z)$ is a straight line before the space charge effect is taken into account, i.e. $r_{0p}(z)=r_s + \alpha_0 z$ ($\alpha_0=(r_r-r_s)/P$). For the same reason, the arbitrary trajectory $r_p(z)$ in this beam segment, before the space charge effect is included, may be considered as a straight line, i.e. $r_p(z)=r_1 + \alpha z$. Here $r_s$ or $r_1$ express the initial beam radius of $r_{0p}(z)$ or $r_p(z)$, $\alpha_0$ or $\alpha$ the angle included between $r_{0p}(z)$ or $r_p(z)$ and the z-axis, respectively. $r_s$, $r_1$, $\alpha_0$ and $\alpha$ may be taken both positive and negative.

The space charge aberration is defined as the total shift of a trajectory, in a plane perpendicular to the z-axis, due to the space charge effect, compared with the same trajectory upon which no space charge effect is supposed to work. The space charge aberrations in the object-side of a lens is usually defined at the object plane, but the aberrations in the image-side at the image plane.

The total differential of the equation $r_1=r_p(z) - \alpha z$ is determined by

$$dr_1 = \frac{\partial r_1}{\partial r_p(z)} dr_p(z) + \frac{\partial r_1}{\partial \alpha(z)} d\alpha(z) = dr_p(z) - \alpha dz\tag{4.26}$$

or
\[ \delta r_i = \delta r_p(z) - z \delta \alpha(z) \] (4.27)

where \( \delta r_i \) means the total shift of the initial radius \( r_i \) of the arbitrary trajectory \( r_p(z) \) at the object plane. \( \delta r_p(z) \) and \( \delta \alpha(z) \), induced by the space charge effect, respectively express the spatial displacement and the angular displacement of the trajectory \( r_p(z) \).

Usually the spatial displacement \( \delta r_p(z) \) and \( \delta r_{op}(z) \) are much smaller than \( r_p(z) \) and \( r_{op}(z) \). On the other hand, for the trapezoidal beam segment model shown in figure 4.4, it is clear that \( (d^2 r_p/dz^2) = 0 \) and \( (d^2 r_{op}/dz^2) = 0 \). Accordingly, substituting \( r_p(z) \) for \( r(z) \) and \( r_{op}(z) \) for \( r_0(z) \) in Eq.(4.17) results in the approximate equation of the spatial displacement \( \delta r_p(r) \) of an arbitrary trajectory \( r_p(z) \):

\[ \frac{d^2 \delta r_p(z)}{dz^2} \approx \mu f(z) \] (4.28a)

where

\[ f(z) = c_0 - \frac{r_p(z)}{r_{op}(z)^2} + c_2 z \frac{r_p(z)^3}{2 r_{op}(z)^3} + c_4 z \frac{r_p(z)^5}{3 r_{op}(z)^6} + \ldots \] (4.28b)

Integrating Eq.(4.28) gives

\[ \delta r_p(z) \approx \mu \int_0^z f(\xi) d\xi dZ = \mu \left[ (z-Z)f(Z)dZ \right] \] (4.29)

On the other hand, the angular displacement \( \delta \alpha(z) \) induced by the space charge effect can also be determined by integrating Eq.(4.28)

\[ \delta \alpha(z) \approx \frac{d \delta r_p(z)}{dz} = \mu \int_0^z f(Z) dZ \] (4.30)

Substituting Eq.(4.29) and Eq.(4.30) into Eq.(4.27) results in

\[ \delta r_i(z) \approx -\mu \int_0^z Z f(Z) dZ = \delta r_{1i}(z) + \delta r_{13}(z) + \delta r_{15}(z) + \ldots \] (4.31)

where \( \delta r_{1i}(z), \delta r_{13}(z), \delta r_{15}(z), \ldots \) are defined as the first, the third, the fifth, ..., order space charge aberrations respectively, and they can be evaluated by

\[ \delta r_{1i}(z) = -\mu \int_0^z Z c_0(z) \frac{r_p(Z)}{r_{op}(Z)^2} dZ \] (4.32)

\[ \delta r_{13}(z) = -\mu \int_0^z Z c_2(z) \frac{r_p(Z)^3}{2 r_{op}(Z)^4} dZ \] (4.33)
\[
\delta r_{11}(z) = -\mu c_0 \int_{0}^{z} Zc_0(Z) \frac{r_f(Z)^3}{3r_0(Z)^3} dZ 
\]  
(4.34)

If the distribution shape of the space charge density at any axial position \( z \) is similar to its initial state, \( c_{2i} \) (\( i=0,1,2,\ldots \)) are independent of \( z \). There is only the first order space charge aberration \( \delta r_{11} \) in the beam segment of a uniform density distribution because of \( c_{2i}(i=1,2,3,\ldots) \) equaling zero. However, all space charge aberrations \( \delta r_{11}, \delta r_{13}, \delta r_{15}, \ldots \) exist in the beam segment of a Gaussian density distribution.

### 4.5 Evaluation of space charge aberrations

Substituting \( r_s(z) = r_1 + \alpha z \) and \( r_0(z) = r_0 + \alpha_0 z \) into Eq. (4.32) and assuming \( c_0 \) being independent of \( z \) gives the expression of the first order space charge aberrations:

\[
\delta r_{11}(z) = -\mu c_0 \int_{0}^{z} \frac{Z}{(r_a + \alpha_0 Z)^2} dZ = r_1 m(z) + \alpha \Delta z(z) 
\]
(4.35a)

or

\[
\delta r_{11}(P) = r_1 m(P) + \alpha \Delta z(P) 
\]
(4.35b)

where

\[
m(P) = -\mu c_0 \int_{0}^{P} \frac{ZdZ}{(r_a + \alpha_0 Z)^2} 
\]
(4.36)

\[
\Delta z(P) = -\mu c_0 \int_{0}^{P} \frac{Z^2 dZ}{(r_a + \alpha_0 Z)^2} 
\]
(4.37)

Eq. (4.35b) means that the particle beam segment under the influence of the space charge effect may be considered as a divergent lens. \( m(P) \) and \( \Delta z(P) \) in Eq. (4.35b) indicate the lateral magnification and the longitudinal defocussing distance. Integrating Eq. (4.36) and Eq. (4.37) respectively gives

\[
m(P) = \frac{\mu c_0}{\alpha_0} \left[ 1 - \ln \frac{r_f}{r_a} - \frac{r_a}{r_f} \right] 
\]
(4.38a)

\[
\Delta z(P) = \frac{\mu c_0 r_a^2}{\alpha_0} \left[ \frac{r_a}{r_f} - \frac{r_f}{r_a} + 2 \ln \frac{r_f}{r_a} \right] 
\]
(4.38b)

Substituting \( r_s \) for \( r_1 \) and \( \alpha_0 \) for \( \alpha \) in Eq. (4.35b) results in a maximum value of the first order space
charge aberration. Consequently, the total first order space charge aberration can be expressed as

$$\delta r_{1m} = \sqrt{(r_m^2) + (\alpha_0^2 \Delta z)^2} = \sqrt{e_{1m}^2 + e_{1\Delta z}^2}$$  \hspace{1cm} (4.39)$$

where

$$e_{1m} = r_m m(P) , \hspace{1cm} e_{1\Delta z} = \alpha_0 \Delta z(P)$$  \hspace{1cm} (4.40)$$

e_{1m} and e_{1\Delta z} respectively represent the component of the magnification and the component of the defocusing induced by the space charge effect in the object plane of figure 4.4.

Substituting \( r_\phi(z) = r_1 + \alpha z \) and \( r_\theta(z) = r_\alpha + \alpha_0 z \) into Eq.(4.33) and assuming \( c_2 \) being independent of \( z \) result in the expression of the third order space charge aberrations:

$$\delta r_{13}(z) = -\frac{\mu c_2}{2} \int_0^z \frac{Z (r_1 + \alpha Z)^3}{(r_\alpha + \alpha_0 Z)^4} dZ$$  \hspace{1cm} (4.41a)$$

or

$$\delta r_{13}(z) = D(z) r_1^3 + F(z) r_1^2 \alpha + C(z) r_1 \alpha^2 + S(z) \alpha^3$$  \hspace{1cm} (4.41b)$$

or

$$\delta r_{13}(P) = D(P) r_1^3 + F(P) r_1^2 \alpha + C(P) r_1 \alpha^2 + S(P) \alpha^3$$  \hspace{1cm} (4.41c)$$

where

$$D(P) = -\frac{c_2 \mu}{2} \int_0^P \frac{Z dZ}{(r_\alpha + \alpha_0 Z)^4}$$  \hspace{1cm} (4.42)$$

$$F(P) = -\frac{3c_2 \mu}{2} \int_0^P \frac{Z^2 dZ}{(r_\alpha + \alpha_0 Z)^4}$$  \hspace{1cm} (4.43)$$

$$C(P) = -\frac{3c_2 \mu}{2} \int_0^P \frac{Z^3 dZ}{(r_\alpha + \alpha_0 Z)^4}$$  \hspace{1cm} (4.44)$$

$$S(P) = -\frac{c_2 \mu}{2} \int_0^P \frac{Z^4 dZ}{(r_\alpha + \alpha_0 Z)^4}$$  \hspace{1cm} (4.45)$$

Because the function of a particle beam segment under the influence of the space charge effect may be considered as a divergent lens, Eq.(4.41) represents the relation of the third order space charge aberrations of the lens. \( Dr_1^3(D) \), \( Fr_1^2 \alpha (F) \), \( Cr_1 \alpha^2 (C) \) and \( Sr_1^3 (S) \) express the components (the coefficients) of the distortion, the field curvature and astigmatism, the coma and the spherical
aberration, respectively. Integrating Eq.(4.42), (4.43), (4.44) and (4.45) yields

\[
D(P) = \frac{c_2 \mu}{2 \alpha_0 r_a} \left( \frac{r_a^2 - \frac{r_a^3}{3}}{2r_f - \frac{3}{r_f^2}} - \frac{1}{6} \right) \tag{4.46a}
\]

\[
F(P) = \frac{3c_2 \mu}{2 \alpha_0 r_a} \left( \frac{r_a^2}{r_f} - \frac{r_a^3}{3r_f^2} - \frac{1}{3} \right) \tag{4.46b}
\]

\[
C(P) = \frac{3c_2 \mu}{2 \alpha_0} \left( \frac{3r_a^2}{2r_f^2} - \frac{3r_a^3}{r_f} - \frac{r_a^3}{3r_f^3} - \frac{\ln r_f}{r_a} + \frac{11}{6} \right) \tag{4.46c}
\]

\[
S(P) = \frac{c_2 \mu r_a}{2 \alpha_0^5} \left( \frac{6r_a - \frac{r_f^2}{r_a} - \frac{2r_a^2}{r_f} + \frac{r_a^3}{3r_f^3} + 4\ln r_f - \frac{10}{3} \right) \tag{4.46d}
\]

Substituting \(r_a\) for \(r_1\) and \(\alpha_0\) for \(\alpha\) in Eq.(4.41) results in a maximum value of the third order space charge aberration. The total third order space charge aberration is determined by

\[
\delta r_{13m} = \sqrt{(Dr_a^3)^2 + (Fr_a^3 + Cr_a^2)^2 + (S\alpha_0^5)^2} \tag{4.47a}
\]

or

\[
\delta r_{13m} = \sqrt{e_{3d}^2 + e_{3f}^2 + e_{3c}^2 + e_{3s}^2} \tag{4.47b}
\]

where

\[
e_{3d} = D(P)r_a^3 \quad e_{3f} = F(P)r_a^3 \quad e_{3c} = C(P)r_a^3 \quad e_{3s} = S(P)\alpha_0^5 \tag{4.48}
\]

\(e_{3d}, e_{3f}, e_{3c},\) and \(e_{3s}\) denote the components of the distortion, the field curvature and astigmatism, the coma and the spherical aberration in the object plane of figure 4.4, respectively.

All equations presented previously are suited to calculate the space charge aberrations of the divergent beam segment in the object-side space of figure 4.4. For the convergent beam segment in the image-side space of figure 4.4, the investigation shows that these equations are also suited to calculate the space charge aberrations in the image plane, as long as one simply substitutes \(\beta_0\) for \(\alpha_0\), \(r_b\) for \(r_a\), \(V_b\) for \(V_a\) and \(Q\) for \(P\) and so on in all concerned equations.

According to Eq.(4.39) and Eq.(4.47a), there only exist the component of the magnification of the first order aberration and the component of the distortion of the third order aberration for the cylindrical beam segment in figure 2.4(4) because of the half opening angle \(\alpha_0\) equalling zero, i.e.

\[
\delta r_{13m} = r_0 m(L) = e_{1m}, \quad \delta r_{13m} = D(L) r_0^3 = e_{3d} \tag{4.49}
\]

The coefficients of the magnification and the distortion can be derived directly from Eq.(4.38a) and Eq.(4.42):
In this case the ratio of $e_{3d}$ to $e_{1m}$ is $0.5c_0/c_0$. This ratio is only dependent on the distribution of the space charge density, but independent of the beam current, the beam energy, the beam radius and the mass of a particle.

In previous derivations, we followed Jansen’s approach, but presented the equations for the evaluation of the space charge aberrations in divergent and convergent beam segments, which constitute the imaging section of a lens.

4.6 Space charge effect discs

In this section, we first look into which space charge aberration plays a major role in an imaging system, then, we shall define the space charge effect discs for the combined calculation of a practical optical system, which will be presented in chapters 5 and 6.

Figure 4.5 and figure 4.6 respectively show that the first and third order space charge aberrations vary with the ratio $r_1/r_f$ and $r_1/r_b$ of the beam radii of the imaging system in figure 4.4. The calculation conditions of figure 4.5 and figure 4.6 are supposed to be the beam length $P=Q =150 \text{ mm}$, the beam potential $V_x = V_y =15 \text{ kV}$, the lens aperture radius $r_1 =30 \text{ \mu m}$, the Ga⁺ beam current $I=5$ nA and the Gaussian charge density distribution. One learns from figure 4.5 that the larger the ratio of the beam radii, the more severe the defocussing will be, or that the smaller the ratio, the larger the magnification. In a practical imaging system, the ratio $r_1/r_f$ (or $r_1/r_b$) is usually much less than 1 (for instance less than 50). This means, from figure 4.5, that we can neglect the magnification component instead of only taking the defocussing into account in the calculation of the first order space charge aberrations. For the same reason, one may conclude, from figure 4.6, that the spherical aberration is much larger than the distortion, the field curvature and astigmatism or the coma for the divergent beam or for the convergent beam with a larger half opening angle $\alpha_0$ or $\beta_0$. Therefore, the
spherical aberration dominates the third order space charge aberrations.

Based on the facts of figure 4.5 and figure 4.6 as well as the discussion above, from now on we shall restrict ourselves to only evaluate the space charge spherical aberration and the space charge defocussing aberration for a divergent or convergent beam segment, ignoring the other space charge aberrations. In the case of the cylindrical beam segment, in terms of Eq.(4.49), we shall be only interested in the evaluations of the component of the magnification of the first order aberration and the component of the distortion of the third order aberration.

The space charge defocussing disc \( d_{\text{foc}} \) in the minimum spot plane \( a \) (see figure 3.1(1)) of a divergent beam segment is defined as

\[
d_{\text{foc}} = d_{\text{foc}}(m, I, V_a, r_a, r_f, \alpha_0) = 2\alpha_0 \ast \text{defoc\%} \ast \Delta z_{\text{foc}}(m, I, V_a, r_a, r_f, \alpha_0) \tag{4.51}
\]

in which the factor defoc\% is the fraction of the defocussing used in the addition of the total spot size. The reason of introducing this parameter is that most of the defocussing can be corrected by adjusting the potentials on the electrodes of lenses in a particle optical column. \( \Delta z_{\text{foc}} \) in Eq.(4.51) is a defocussing distance departing from the minimum spot plane \( a \), from now on it is expressed as

\[
\Delta z_{\text{foc}} = \Delta z_{\text{foc}}(m, I, V_a, r_a, r_f, \alpha_0) = \mu_a \frac{r_a}{\alpha_0} \left( \frac{r_a - r_f + 2\ln r_f}{r_a} \right) \tag{4.52}
\]

where

\[
\mu_a = \frac{I m^{1/2}}{\pi \varepsilon_0 2^{5/2} e^{41/2} V_a^{3/2}} \tag{4.53}
\]

The space charge spherical aberration disc \( d_{\text{sch}}a \) in the minimum spot plane \( a \) of a divergent beam segment is defined as

\[
d_{\text{sch}}a = d_{\text{sch}}a(m, I, V_a, r_f, \alpha_0) = K_{sa} \alpha_0^3 C_{sa}(m, I, V_a, r_a, r_f, \alpha_0) \tag{4.54}
\]

where the coefficient \( K_{sa} \) will be explained in chapter 5. \( C_{sa} \) is the space charge spherical aberration coefficient in the divergent beam segment, and it is evaluated by

\[
C_{sa} = C_{sa}(m, I, V_a, r_a, r_f, \alpha_0) = \frac{\mu_a r_a C_2}{2 \alpha_0} \left( \frac{6r_a - r_f - 2r_a^2}{r_f} - \frac{r_a^3}{r_f} + \frac{4\ln r_f}{r_f} - \frac{10}{3} \right) \tag{4.55}
\]

In the case of a convergent beam segment shown in figure 2.4(2), the space charge defocussing disc \( d_{\text{foc}}b \) and the space charge spherical aberration disc \( d_{\text{sch}}b \) in the minimum spot plane \( b \) are respectively calculated by

\[
d_{\text{foc}}b(m, I, V_b, r_b, r_f, \beta_0) = d_{\text{foc}}a(m, I, V_b, r_a, r_f, \beta_0) \tag{4.56}
\]

and

\[
d_{\text{sch}}b(m, I, V_b, r_b, r_f, \beta_0) = d_{\text{sch}}a(m, I, V_b, r_a, r_f, \beta_0) \tag{4.57}
\]

In the case of the cylindrical beam segment shown in figure 3.1(2), we respectively define the
first order lateral displacement $\Delta r_{sch 1}$ and the third order lateral displacement $\Delta r_{sch 3}$ in the terminal plane of the beam segment as

$$\Delta r_{sch 1} = \Delta r_{sch 1}(m, I, V, r_0, L) = -\frac{\mu c L^2}{2r_0}$$ (4.58)

and

$$\Delta r_{sch 3} = \Delta r_{sch 3}(m, I, V, r_0, L) = -\frac{\mu c L^2}{4r_0}$$ (4.59)

For the same reason as the evaluations of the Boersch effect and the trajectory displacement effect, we use parameter KK to characterize the distribution of the space charge density, as shown in table 4.1. The choice of the coefficients $c_0$, $c_2$ and the beam parameters at different distributions of the space charge density are all defined in table 4.1.

If the angular distribution of a particle beam is uniform, the space charge spherical aberration is absent because of $c_2=0$. However, the space charge defocussing aberration is always present and serious although most of the defocussing can be corrected in a practical system. The investigations show that the defocussing aberration can be as heavy as the statistical Coulomb interaction aberrations even though only taking fifteen percent of defocussing (defoc% = 0.15) into account10,11. We believe that it is impossible to totally correct the defocussing aberration in a complete optical system, accordingly, it should be considered as one of important factors of influencing the image quality of an optical system.

### Tab.4.1 A number of coefficients and parameters used to determine the space charge effect discs at different distributions of the space charge density.

<table>
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<th>KK</th>
<th>$c_0$</th>
<th>$c_2$</th>
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<th>$r_0$</th>
<th>$\alpha_0$</th>
<th>$1.21\alpha_0$</th>
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<td>$\alpha_0$</td>
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<tr>
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<td>$1.21r_0$</td>
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</tbody>
</table>

### Fig.4.7 The imaging relation of a lens under the impact of the space charge effect.

4.7 Calculation method of real focal distance

Figure 4.7(1) and figure 4.7(2) show the situations in which the particle beam segment fulfills and does not fulfill the continuum condition respectively. P, Q and f express the object distance, the image distance and the focal distance of the lens before the space charge effect occurs, and $\Delta P$, $\Delta Q$ and $\Delta f$ represent the shift of P, Q and f after the space charge effect is taken into account.
The particle beam in the object-side or in the image-side of figure 4.7 will expand in radial direction under the impact of the space charge effect. The particle trajectory will not intersect with the z-axis and the laminar flow will occur when the space charge effect is relatively serious and the continuum condition is fulfilled in the beam segment.

The universal paraxial trajectory equation in a combined electromagnetic field under the impact of the space charge effect can be determined by following the derivation of section 4.2, i.e.

\[
\frac{d^2r}{dz^2} + \frac{V'(z)}{2V(z)} \frac{dr}{dz} + \left\{ \frac{V''(z)}{4V(z)} + \frac{\rho_0(z)}{4\epsilon_0V(z)} + \frac{\eta B^2(z)}{8V(z)} \right\} = 0 \tag{4.60}
\]

\[
\frac{d\varphi}{dz} = \frac{\eta}{8V(z)} B(z) \tag{4.61}
\]

where \( B(z) \) denotes the magnetic induction distribution on the z-axis, \( \varphi(z) \) the rotational angle of the trajectory and \( \eta \) the ratio of the particle charge to mass. \( V(z) \) in Eq.(4.60) and Eq.(4.61) is the axial potential distribution before the space charge effect is taken into account. The additional magnetic field induced by the motional space charge is neglected in the derivation of Eqs.(4.60) and (4.61). Note that Eq.(4.60) is a more general ray equation than Eq.(4.15) since it includes not only the magnetic field but also the arbitrary potential distribution. The space charge density distribution on the z-axis \( \rho_0(z) \) in Eq.(4.60) is defined by Eq.(4.2) and Eq.(4.10), that is

\[
\rho_0(z) = \frac{\rho_0(r(z))}{\pi r_0(r)^2 \sqrt{2\eta V(z)}} \tag{4.62}
\]

In Eq.(4.60) and Eq.(4.62), \( r = r(z) \) and \( r_0 = r_0(z) \) are the arbitrary trajectory and the characteristic trajectory, as shown in figure 4.8. Substituting Eq.(4.62) into Eq.(4.60), one learns that Eq.(4.60) is not a standard paraxial trajectory equation (i.e. the second order linear and homogeneous differential equation). Consequently, it is impossible to obtain an ideal image in the image plane \( b \) with the trajectory of Eq.(4.60). Rewriting Eq.(4.60) and performing the integration results in

\[
\sqrt{V(z)} r'(z) = \sqrt{V(\infty)} r'(\infty) = \frac{1}{4 \sqrt{V}} \int_{\infty}^{z} r dz \tag{4.63}
\]

\[
- \int_{\infty}^{z} \frac{c_0(\mu(z) r}{r_0(z)^2} dz - \frac{\eta}{8} \int_{\infty}^{z} \frac{B^2(z)}{V(z)} rdz
\]
where $\mu(z)$ is defined in Eq.(4.16).

Without losing generality, one may only consider the calculation of the focal distance in an electrostatic thin lens, ignoring the influence of the magnetic field.

For the incident parallel particle trajectory from the object-side to the field of the thin lens in figure 4.8, we assume that the lateral expansion of the trajectory induced by the space charge effect is so small compared with the expansion of the same trajectory in the image-side that the trajectory always fulfills the condition of $r(z)\approx 0$ in the range from $z=-\infty$ to $z=0$. Accordingly, from Eq.(4.63) we can obtain

$$\frac{r'(z_o)}{r_s} = \frac{1}{4r_s^N/V(z_o)} \left( \frac{\int_{-\infty}^{z} V''r dz}{\int_{-\infty}^{z} V'} \right) + \frac{\int_{-\infty}^{z} c_0(z)\sqrt{V(z)} \mu(z) \frac{r}{r_0(z)^2} dz}{r_s^N/V(z_o)} \tag{4.64}$$

where $r_s$ is the radius of the characteristic trajectory of the parallel incidence. Because the trajectory only alters its direction, but does not alter its radius in the field region $(z_1, z_2)$ of the thin lens, Eq.(4.64) can be expressed as

$$\frac{1}{f_b'} = \frac{1}{f_b} + \frac{1}{f_s} \tag{4.65}$$

where

$$\frac{1}{f_b} = \frac{1}{4r_b^N/V(z_o)} \left( \frac{\int_{-\infty}^{z} V''r dz}{\int_{-\infty}^{z} \sqrt{V'}} \right) \tag{4.66}$$

and

$$\frac{1}{f_s} = \frac{1}{r_s^N/V(z_o)} \left( \int_{-\infty}^{z} c_0(z)\sqrt{V(z)} \mu(z) \frac{r}{r_0(z)^2} dz \right) \tag{4.67}$$

It is obvious that $f_b$ stands for the image-side focal distance of the lens in figure 4.8 before the space charge effect occurs, and that $f_s$ denotes the additional focal distance induced by the space charge effect. From Eq.(4.67) one learns that the additional focal distance $f_s$ is related to the trajectory. Consequently, it is impossible to obtain an ideal image in the image-side space, and there always exist space charge aberrations in the imaging system.

The approximate evaluation of Eq.(4.67) may be performed. Suppose that the distribution shape of the space charge density in any plane perpendicular to the z-axis is similar to its initial state, this results in $c_0(z)$ to be independent of $z$, i.e. $c_0(z)=c_0$. Further suppose that the field region $(z_1, z_2)$ is relatively small, and that within the range from $z=-\infty$ to $z=0$ $V(z)$ equals a constant, say, $V(-\infty)$, but within the range from $z=0$ to $z=z_o$, $V(z)=V(z_o)$. Thus, Eq.(4.67) becomes

$$\frac{1}{f_s} = \frac{c_0\mu(-\infty)}{r_f} \int_{-\infty}^{0} V(-\infty) \left( \int_{-\infty}^{z} \frac{r}{r_f^2} dz + \int_{-\infty}^{z} \frac{r}{r_0(z)^2} dz \right) \tag{4.68}$$

The first and second terms in the right-side of Eq.(4.68) respectively gives the additional focal
distances due to the space charge effect in the object-side and image-side of the lens system. We here only simply consider the additional focal distance caused by the space charge effect in the image-side, i.e. ignoring the first term of Eq.(4.68), which requires the knowledge of a practical system for evaluation. This leads to

$$\frac{1}{f_0^*} = \frac{c_o \mu(z_b)}{r_f} \int_{r_o(z)^2}^{r} \frac{r}{r_o(z)^2} dz \quad (4.69)$$

![Fig.4.9 The relation between the relative change of the focal distance $F$ and the diffusion coefficient $\xi$.](image)

4.8 Real focal distance analyses

The evaluation of Eq.(4.69) should be divided into two cases, i.e. the beam segment fulfills or does not fulfill the continuum condition respectively.

When the beam segment does not fulfill the continuum condition, the particle trajectory intersects with the z-axis even though it expands in radial direction. For the characteristic trajectory $r_0(z)$, suppose that the point of the intersection is at $z = z_b$. Because of the small expansion in radial direction, the characteristic trajectory after the expansion can be assumed to be a straight line, i.e., $r_o(z) = r_i(1-z/z_b)$. For the same reason, the arbitrary trajectory $r = r(z)$ is also assumed to be a straight line, i.e. $r(z) = e^{-\gamma z}$. Substituting $r_0(z)$ and $r(z)$ into Eq.(4.69) and performing the integration operation results in

$$\frac{1}{f_0^*} = \frac{c_o \mu(z_b)}{r_f} \left[ e \cdot \frac{f_b}{f_b'} - \gamma f_b' \left( \frac{f_b}{f_b' - f_b} - \frac{f_b'}{f_b'} \right) \right] \quad (4.70)$$

Eq.(4.70) represents a general expression of the additional focal distance. As a special example, one can suppose $e = r_i$ and $\gamma = r_i/r_b'$, thus, Eq.(4.70) is simplified into

$$\frac{1}{f_0} = -\frac{c_o \mu(z_b)}{r_f} \ln \frac{f_b}{f_b'} = -\frac{f_b'}{2 \xi f_b^2} \ln (1 - \frac{f_b}{f_b'}) \quad (4.71)$$

From point of view of the analysis of the focal distance sign, the right-side sign of Eq.(4.71) should be taken as positive. In Eq.(4.71), $\xi$ is the diffusion coefficient, which is defined by

$$\xi = \frac{\beta_0^3}{2c_o \mu(z_b)} = \frac{1}{2c_o \mu(z_b)} \left( \frac{r_f}{f_b} \right)^2 \quad (4.72)$$

Substituting Eq.(4.71) into Eq.(4.65) results in

49
\[
\ln \left( \frac{F}{1+F} \right) + 2\xi = \frac{F}{(1+F)^2} = 0
\]

where \( F = \Delta f_b/f_b \), \( \Delta f_b = f'_b - f_b \).

Figure 4.9 shows the relation between the relative change of the focal distance \( F \) and the diffusion coefficient \( \xi \). In the logarithm coordinate system, this relation is almost a straight line. The curve shown in figure 4.9 is a universal one since the diffusion coefficient \( \xi \) includes all parameters of a charged particle beam segment. As seen from figure 4.9, in order to keep the focal distance shift less than 10\%, one has to choose a combination of the parameters in a beam segment with the diffusion coefficient \( \xi \) larger than 10.

Figure 4.10 shows the real changes of the focal distance in the case of different beam currents \( I \). \( f_b \) and \( f'_b \) express the focal distance before and after the space charge effect is included. This figure provides a clear relation to correct the defocusing of a lens. Taking the current \( I \) equalling 7 nA and the focal distance \( f_b \) equalling 150 mm for example, one finds that the real focal distance \( f'_b \) equals 250 mm. In order to keep the real focal distance to be 150 mm, the focal distance \( f_b \) should be decreased to 110 mm by adjusting the potential on the electrode of the lens.

The relation between the varied focal distance \( f_b \) and the beam current \( I \) for different \( f_b \) is shown in figure 4.11. It can be concluded from this figure that the real focal distance \( f'_b \) increases with the beam current \( I \) and the focal distance \( f_b \).

When the beam segment in figure 4.8 fulfills the continuum condition, the additional focal distance should be evaluated in another way. Because the particle beam in this case is a laminar flow, one can only pay attention to the calculation of the characteristic trajectory \( r_0(z) \). Accordingly, Eq.(4.69) becomes

\[
1 = c_0 \mu(z) \int_{0}^{z} \frac{dz}{r_0^2(z)}
\]

Suppose that the field region \((z_1,z_2)\) of the thin lens is relatively small, but the axial equipotential region \((z_2,z_0)\) is relatively large. In other words, suppose \( V'(z) \approx 0 \) and \( V''(z) \approx 0 \) within the range from \( z = 0 \) to \( z = z_0 \). Thus, Eq.(4.60) is simplified into
\[
\frac{d^2 r_0}{dz^2} + \frac{\rho_0(z)r_0(z)}{4\varepsilon_0 V(z)} = \frac{d^2 r_0}{dz^2} + \frac{c_0 \mu(z_0)}{r_0(z)} = 0
\] (4.75)

Substituting Eq. (4.75) into Eq. (4.74) results in
\[
\frac{1}{f_s} = -\frac{1}{r_f} \int_0^{z_f} \frac{d^2 r_0}{dz^2} + \frac{1}{f_s} \frac{r_0'(z_f)}{r_f}
\] (4.76)

Substituting Eq. (4.76) into Eq. (4.65) yields
\[
\frac{1}{f_s'} = -\frac{r_0'(z_f)}{r_f}
\] (4.77)

From Eq. (4.75) and the definition of figure 4.8, one finds
\[
r_0'(z_f) = -\beta_0 \sqrt{1 + \frac{1}{\xi} \ln \frac{r_0(f_s)}{r_f}}
\] (4.78)

Finally, substituting Eq. (4.78) into Eq. (4.77) gives
\[
F = [1 + \frac{1}{\xi} \ln \frac{r_0(f_s)}{r_f}]^{-1} - 1
\] (4.79)

where \(F = \Delta f_s / f_s\). The diffusion coefficient \(\xi\) is determined by Eq. (4.72). \(F\) in Eq. (4.79) is only a function of \(\xi\) since \(r_0(f_s) / r_f\) is still only a function of \(\xi\). This conclusion can be proved by using Eq. (4.75). By solving Eq. (4.57) one learns
\[
\int_{r_0(r_f)} \frac{dx}{\sqrt{1 + (\ln(x)/\xi)}} = 1
\] (4.80)

The approach and formulas presented previously are also applicable to the calculation of the real focal distance in the object-side of a lens.

### 4.9 Conclusions

The presented analytical equations of evaluating the space charge aberrations are not only simpler but also applicable to more systems that one encounters in reality from simulating a complete particle optical system point of view. Based on the trapezoidal beam segment model in an imaging system (figure 4.4), these equations can be directly used to evaluate the image quality of a lens as the calculation of the lens aberrations as one usually does.

The space charge effect strongly influences the image quality of a lens even if the continuum condition is not fulfilled in the beam segment of an imaging system. Fifteen percent of defocussing aberrations could be possible to reach the level of the statistical Coulomb interaction aberrations\(^9,10\). The continuum condition can be easily fulfilled in a gallium ion beam optical column, and the
lateral expansion of the column can reach several microns, as can been seen from a practical focussed ion beam system described in figure 4.2 and figure 4.3.

The space charge effect causes not only the deterioration of the image quality but also the variation of the imaging relation of an imaging system. This variation is investigated in this chapter by evaluating the shift of the focal distance of an imaging lens. This shift is related to the distribution of the space charge density, the beam shape, the beam energy and the beam current as well as whether the considered beam segment fulfills the continuum condition or not. The calculation approach has been developed for searching the influence of the space charge effect on the imaging relation.

References

5 Coulomb aberrations in complete particle optical columns

Abstract  Based on the presentations of chapters 3 and 4, which deal with the evaluations of the Boersch effect blur, the trajectory displacement blur and the space charge aberrations in our beam segment model of chapter 2, this chapter researches into the combined calculation of lens aberrations, statistical Coulomb effects and space charge aberrations in complete particle optical columns. Eleven spot discs are defined and calculated for four imaging modes, which should meet the general needs of evaluating probe forming instruments suffering both from lens aberrations and from Coulomb effects. All equations are derived for the design of the ANALIC program described in chapter 6 and used for the applied studies from chapter 7 to chapter 13. This shows that this chapter becomes a center, which connects all studies from the optical models, programs to applications in this thesis.

5.1 Introduction

Looking into complete charged particle optical instruments, for the typical cases of focussed ion beam systems\(^1\),\(^2\), low-voltage scanning electron microscopes\(^3\),\(^4\) and ion beam projection columns\(^5\),\(^6\), one realizes that the practical systems suffer not only from lens aberrations but also from Coulomb effects. A full system optimization including a combined evaluation of both lens aberrations and Coulomb effects can greatly improve the performance of these machines. Unfortunately, the contributions dealing with this problem are so far very limited\(^7\),\(^8\),\(^9\). It is important, but difficult, to analytically calculate the combined influence of the lens aberrations, the statistical Coulomb effects and the space charge aberrations on a complete particle optical column. Equations derived by Jansen\(^10\) are complete for the evaluation of Coulomb effects in beam segments, but it is still a lot of work to use Jansen's equations for the full system optimization.

This chapter presents the expressions of the lens aberrations and Coulomb aberrations in complete charged particle optical columns. The detailed derivation for these expressions is omitted, which results in a chapter that looks like a equation list. It is our purpose to use these expressions to design a computer program and to use this for studies of Coulomb effects in charged particle instruments, which will be presented in the thesis from chapter 6 to chapter 13.

In line with the term lens aberrations, we use the term Coulomb aberrations to describe the impact of the Coulomb effects on the probe size. A linear-rule summation method is used to add different Coulomb aberrations from different beam sections. This is different from the gamma-rule summation in Ref.[10]. Both the linear-rule and the gamma-rule are checked in chapter 12, from which we learn that there are situations in which the former seems better than the latter.

5.2 Description of symbolizations

As described in chapter 2, the rotationally symmetric trapezoidal or cylindrical beam segment can be usually considered as a basic beam segment model. With these beam segments, one is able to build up four elementary imaging modes normally met in a charged particle optical column. Figure 5.1(1) shows the most elementary imaging relation, it consists of two trapezoidal beam segments separated by one thin lens. In which, \(\alpha_0\) and \(\beta_0\) are the half opening angles, \(V_s\) and \(V_b\) the beam potentials, \(f_a\) and \(f_b\) the focal distances of the lens in object-side and image-side, respectively. \(P\) and \(Q\) the object distance and the image distance of the lens. Figures 5.1(2), (3) and (4) show three elementary imaging modes in which three rotationally symmetric beam segments are separated by two thin lenses. \(L\) is the distance between the lenses. \(f, V, \alpha\) and \(l\) still express the focal distance, the beam potential, the half opening angle and the beam current in the corresponding beam segment. In figure 5.1, suppose that the object plane and the image plane are located in \(a\) and \(b\) respectively. Before the lens
aberrations and the Coulomb interactions are taken into account, the spot size in plane \( a \) or \( b \) is assumed as \( 2r_a \) or \( 2r_b \). In the presentations of this chapter, we shall consider the imaging relation with one lens in figure 5.1(1) as an independent imaging unit, and the imaging relation with two lenses in figure 5.1(2) or figure 5.1(3) or figure 5.1(4) as an independent imaging unit, too. It is important to evaluate the spot discs in plane \( a \) or \( b \) when the lens aberrations, the statistical Coulomb effects and the space charge aberrations are included in the design of a probe forming instrument. It is extremely useful to offer the analytical equations for conveniently calculating the relation between the different spot discs in the image plane \( b \) and all experimental parameters such as the beam current \( I \), the particle mass \( m \), the beam potential \( V \), the magnification \( M \), the source brightness \( B \) and the source virtual radius \( r_s \) and so on. The connection between the source parameters and the column parameters is realized by

\[
\alpha_0 = \left( \frac{I}{\pi r_a^2 BV_a} \right)^{1/2} \quad (5.1)
\]

in which we assume that the imaging lens in figure 5.1(1) is the source lens, as shown in figure 2.2, and that the virtual source is located in the plane \( a \). Eq.(5.1) is also applicable to figures 5.1(2), (3) and (4). In this case \( \alpha_0 \) is substituted with \( \alpha_{11} \) and \( V_a \) with \( V_{11} \) in Eq.(5.1) according to the symbolizations in the figures. From the practical optical system point of view, we suppose \( V_{12} = V_{21} = V \) in figures 5.1(2), (3) and (4).

Figures 5.1(2), 5.1(3) and 5.1(4) belong to the non-crossover modes, the optical dependencies of which are presented in table 2.1. Eleven spot discs for different imaging modes will be evaluated in the following, the definition of them is given in figure 2.5.

### 5.3 Lens aberrations in different imaging modes

Lens aberrations include the geometrical spherical aberration, the chromatic aberration and the diffraction aberration. Without taking into account the Coulomb interaction effects described in chapters 3 and 4, one usually finds four spot discs in the image plane \( b \) of figure 5.1. For figure 5.1(1), the source image disc \( d_{gau} \), the spherical aberration disc \( d_{sph} \), the chromatic aberration disc \( d_{chr} \) and the diffraction aberration disc \( d_{dif} \) are respectively calculated by

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54
\[ d_{Gau} = K_{Gg} 2r_b = 2MK_{Gg} r_a \]
\[ M = \frac{\alpha_0}{V_a} \left( \frac{V_a}{V_b} \right)^{\frac{Qf_a}{Pf_b}} \]  \hspace{1cm} (5.2)

\[ d_{sph} = K_{Gg} C_{s0}(\infty, f_a) \left[ 1 + \frac{1}{M} \left( \frac{V_a}{V_b} \right) \right]^{\frac{1}{4}} \alpha_0 M \]  \hspace{1cm} (5.3)

\[ d_{chr} = K_{Gg} C_{c0}(\infty, f_a) \left[ 1 + \frac{1}{M} \left( \frac{V_a}{V_b} \right) \right]^{\frac{1}{4}} \Delta V \frac{V_a}{V_a} \alpha_0 M \]  \hspace{1cm} (5.4)

\[ d_{y} = \frac{K_{Gg} \lambda_b}{B_0}, \quad \lambda_b = \frac{h}{\sqrt{2meV_b}} \]  \hspace{1cm} (5.5)

where \( M \) is the magnification of the imaging system, and \( \Delta V \) the source energy spread, which is usually measured with FWHM or FW50. \( K_{Gg}, K_{ag}, K_{cg} \) and \( K_{f} \) are the prefactors used to evaluate how the different spot discs are measured, which are listed in table 5.1\textsuperscript{11,12,13}. As described in chapters 3 and 4, the spot size can be evaluated with the FWHM or FW50 measurement, however, the measured beam can be in different spatial and angular distributions. These distributions are characterized by the parameter KK, which is defined in table 3.1. Besides, for the evaluation of the chromatic aberration, the source energy spread \( \Delta V \) (or \( \Delta E \)) can also be measured with the FW50 or FWHM, accordingly, the number of the prefactors for the evaluation of the chromatic aberration is two times of that of the spherical aberration. The prefactor \( K_{cg} \) in table 5.1 is defined in the Gaussian image plane. If in the plane of best focus, it is taken four times smaller.

In our combined calculations, including in the ANALIC program\textsuperscript{14}, the spherical and chromatic aberration coefficients are defined at the object-side of an imaging lens and in the infinite magnification case, i.e. \( C_{s0}(\infty, f_a) = C_{s0}(M_0|\infty, f_a) \) and \( C_{c0}(\infty, f_a) = C_{c0}(M_0|\infty, f_a) \). If the lens aberration coefficients are defined in the image-side, the following transformations are required before using both the equations in this chapter and the ANALIC program.

<table>
<thead>
<tr>
<th>Input energy distribution</th>
<th>KK</th>
<th>FWHM</th>
<th>FW50</th>
</tr>
</thead>
<tbody>
<tr>
<td>( K_{Gg} )</td>
<td>00</td>
<td>1.0</td>
<td>( \sqrt{2}/2 )</td>
</tr>
<tr>
<td>11</td>
<td>1.0</td>
<td>1.0</td>
<td></td>
</tr>
<tr>
<td>( K_{ag} )</td>
<td>00</td>
<td>( \sqrt{2}/2 )</td>
<td>( \sqrt{2}/2 )</td>
</tr>
<tr>
<td>11</td>
<td>1.0</td>
<td>1.0</td>
<td></td>
</tr>
<tr>
<td>( \Delta V ) (or ( \Delta E )) FW50</td>
<td>00</td>
<td>0.6</td>
<td>0.6</td>
</tr>
<tr>
<td>11</td>
<td>0.88</td>
<td>0.88</td>
<td></td>
</tr>
<tr>
<td>( \Delta V ) (or ( \Delta E )) FWHM</td>
<td>00</td>
<td>0.34</td>
<td>0.34</td>
</tr>
<tr>
<td>11</td>
<td>0.5</td>
<td>0.5</td>
<td></td>
</tr>
<tr>
<td>( K_{f} )</td>
<td>00</td>
<td>0.54</td>
<td>0.54</td>
</tr>
</tbody>
</table>

Tab.5.1 Prefactors of the evaluation of the different spot discs with different measurements.
\[ C_{so} \left( \infty f_j \right) = C_{so}(0,f_j) \sqrt{\frac{V_a}{V_b}} \quad C_{so} \left( \infty f_j \right) = C_{so}(0,f_j) \frac{V_a}{V_b} \]  

\[ C_{sl}(0,f_j) = C_{sl}(M,f_j) \left[ 1 + M \left( \frac{V_b}{V_a} \right)^{1/4} \right]^{-4} \]  

\[ C_{cl}(0,f_j) = C_{cl}(M,f_j) \left[ 1 + M \left( \frac{V_b}{V_a} \right)^{1/4} \right]^{-2} \]  

For the imaging mode of figure 5.1(3), \( d_{Gau}, d_{sph}, d_{ch} \) and \( d_{\text{eff}} \) in the image plane \( b \) are determined by

\[ d_{Gau} = 2K_{G_{G_{s_b}}} r_{a} = 2K_{G_{a_b}} r_{a} M \quad M = \frac{\alpha_{11}}{\alpha_{22}} \sqrt{\frac{V_{11}}{V_{22}}} = \frac{f_{22}}{f_{11}} \sqrt{\frac{V_{11}}{V_{22}}} \]  

\[ d_{sph} = K_{sG} C_{so} \left( \infty f_{11} \right) \alpha_{11}^3 M + K_{sG} C_{so2} \left( \infty f_{21} \right) \alpha_{22}^3 \sqrt{\frac{V_{22}}{V_{21}}} \]  

\[ d_{ch} = K_{sG} C_{co} \left( \infty f_{11} \right) \alpha_{11} \frac{\Delta V}{V_{11}} M + K_{sG} C_{co2} \left( \infty f_{21} \right) \alpha_{22} \frac{\Delta V}{V_{21}} \]  

\[ d_{\text{eff}} = \frac{K_{sG} \lambda_{22}}{\alpha_{22}} \quad \lambda_{22} = \frac{h}{\sqrt{2m e V_{22}}} \]  

However, \( d_{Gau}, d_{sph}, d_{ch} \) and \( d_{\text{eff}} \) in figure 5.1(2) and figure 5.1(4) are respectively evaluated by

\[ d_{Gau} = 2K_{G_{G_{s_b}}} r_{a} = 2K_{G_{a_b}} r_{a} M \quad M = \frac{\alpha_{11}}{\alpha_{22}} \sqrt{\frac{V_{11}}{V_{22}}} \]  

\[ d_{sph} = K_{sG} C_{so} \left( \infty f_{11} \right) \left[ 1 + \frac{1}{M_1} \left( \frac{V_{11}}{V_{12}} \right)^{1/4} \right]^4 \alpha_{11}^3 M + K_{sG} C_{so2} \left( \infty f_{21} \right) \left( \frac{V_{22}}{V_{21}} \right)^{3/2} \left[ M_2 + \left( \frac{V_{21}}{V_{22}} \right)^{1/4} \right] \alpha_{22}^2 \]  

56
where

\[ M_1 = \frac{\alpha_{11}}{\alpha_{12}} \sqrt{\frac{V_{11}}{V_{12}}} \]
\[ M_2 = \frac{\alpha_{12}}{\alpha_{22}} \sqrt{\frac{V_{12}}{V_{22}}} \]
\[ M = M_1 \ast M_2 \]  \hspace{1cm} (5.15)

and

\[ d_{chr} = K_{cg} C_{cos 1} \left( \infty f_{11} \right) \left[ 1 + \frac{1}{M} \left( \frac{V_{11}}{V_{12}} \right)^{1/4} \right]^2 \frac{\Delta V}{V_{11}} \alpha_{11} M \]
\[ + K_{cg} C_{cos 2} \left( \infty f_{21} \right) \left( \frac{V_{22}}{V_{21}} \right)^{3/2} \left( M_2 + \frac{V_{21}}{V_{22}} \right)^{1/4} \left( \frac{\Delta V}{V_{22}} \right)^2 \alpha_{22} \]  \hspace{1cm} (5.16)

\[ d_{eg} = \frac{K_{pe}}{\alpha_{22}} \lambda_{22} = \frac{h}{\sqrt{2m} \nu_{22}} \]  \hspace{1cm} (5.17)

in which \( M_1 \) and \( M_2 \) are the magnifications of the first lens and the second lens in the imaging modes of figure 5.1(2) and (4). It should be noted that, for the imaging modes of figure 5.1(2) and figure 5.1(4), the magnification \( M_1 \) and \( M_2 \) (or the total magnification \( M = M_1 \ast M_2 \)) in Eq.(5.14) and Eq.(5.16) are different although the expressions of \( d_{sp} \) and \( d_{chr} \) of these imaging relations are the same. The magnification in these modes are limited in a determined range, as seen from table 2.1.

5.4 Statistical Coulomb interaction aberrations

Statistical Coulomb interaction aberrations can be described and measured with a Boersch effect disc and a trajectory displacement effect disc. In this section we shall again consider the four elementary imaging modes in figure 5.1 for evaluating the statistical Coulomb interaction aberrations. The evaluation will be focused on the image plane \( b \) of the four imaging modes in figure 5.1.

5.4.1 Boersch effect disc in a complete particle optical column

Because of the energy spread caused by the Boersch effect in the beam segments of an imaging system, a new spot disc, the Boersch effect disc, appears in the image plane \( b \). This new spot is found through the chromatic aberration effect in a lens.

The total energy spread in the two trapezoidal beam segments in figure 5.1(1) is

\[ \Delta E_{Boe_{1}} = \Delta E_{Boe_{a}} + \Delta E_{Boe_{b}} = \Delta E_{Boe_{a}}(m, I, V_{a}, r_{a}, \alpha_{0}, P) + \Delta E_{Boe_{b}}(m, I, V_{b}, r_{b}, \beta_{0}, Q) \]  \hspace{1cm} (5.18)

in which \( \Delta E_{Boe_{a}} \) and \( \Delta E_{Boe_{b}} \) are the energy spread in the object-side and in the image-side of the lens, and they are determined by Eq.(3.15) and Eq.(3.21), respectively. However, in Eq.(5.18) only the energy spread \( \Delta E_{Boe_{a}} \) can produce the Boersch effect disc in the image plane \( b \) in figure 5.1(1) through the chromatic aberration effect, i.e.
\[
d_{\text{Boe}_i} = K_{\text{c}_a} C_{\text{co}(\infty f_{a})} \left[ 1 + \frac{1}{M} \left( \frac{V_a}{V_b} \right)^{1/4} \right]^2 \frac{\alpha_c M}{V_a} \Delta E_{\text{Boe}_a}(m, I, V_a, r_a, \alpha_0, P) \tag{5.19}
\]

If a particle optical column consists of a number of lenses and imaging relations, for the example of figure 2.6, all energy spreads produced by the Boersch effect in all beam segments from the source (see figures 2.1 and 2.2) to the considered lens should be included when using Eq. (5.19) to perform the calculation of the spot disc \( d_{\text{Boe}_i} \). For the example of the imaging system with \( n \) lenses, if one calculates the Boersch effect disc in the image plane \( b \) of the \( k \)th lens \((1 < k \leq n)\), the energy spread in Eq. (5.19) should be replaced by

\[
\Delta E_{\text{Boe}_a} = \sum_{i=1}^{k-1} (\Delta E_{\text{Boe}_a} + \Delta E_{\text{Boe}_b}) + \Delta E_{\text{Boe}_a} \tag{5.20}
\]

It is obvious that the corresponding experimental parameters in Eq. (5.20) are different in the different beam segments in this case.

In the case of figure 5.1(2), the total energy spread \( \Delta E_{\text{Boe}_l} \) is the summation of the energy spreads in three trapezoidal beam segments

\[
\Delta E_{\text{Boe}_l} = \Delta E_{\text{Boe}_a}(m, I, V_{11}, r_a, \alpha_{11}, P_1) + \Delta E_{\text{Boe}_a}(m, I, V_{12}, r_a, \alpha_{11} + \alpha_{12}, P_1, |\alpha_{12}|, L)
+ \Delta E_{\text{Boe}_a}(m, I, V_{22}, r_a, \alpha_{22}, Q_2) \tag{5.21}
\]

Based on Eq. (5.16), the Boersch effect disc \( d_{\text{Boe}_l} \) in the image plane \( b \) of figure 5.1(2) is evaluated by

\[
d_{\text{Boe}_l} = K_{\text{c}_a} C_{\text{co}(\infty f_{11})} \left[ 1 + \frac{1}{M_1} \left( \frac{V_{11}}{V_{12}} \right)^{1/4} \right]^2 \frac{\alpha_{11} M}{V_{11}} \Delta E_{\text{Boe}_a}(l, m, V_{11}, r_a, \alpha_{11}, P_1)
+ K_{\text{c}_a} C_{\text{co}(\infty f_{21})} \left( \frac{V_{22}}{V_{21}} \right)^{3/2} \left[ M_2 + \left( \frac{V_{21}}{V_{22}} \right)^{1/4} \right]^2 \frac{\alpha_{22} M}{V_{22}} \Delta E_{\text{Boe}_a}(m, I, V_{22}, r_a, \alpha_{11}, P_1)
+ \Delta E_{\text{Boe}_a}(m, I, V_{22}, r_a, \alpha_{11} + \alpha_{12}, P_1, |\alpha_{12}|, L) \tag{5.22}
\]

For the imaging mode with a cylindrical beam segment shown in figure 5.1(3), the total energy spread is calculated by

\[
\Delta E_{\text{Boe}_l} = \Delta E_{\text{Boe}_a}(m, I, V_{11}, r_a, \alpha_{11} f_{11}) + \Delta E_{\text{Boe}_c}(m, I, V, r_0, L) + \Delta E_{\text{Boe}_a}(m, I, V_{22}, r_a, \alpha_{22} f_{22}) \tag{5.23}
\]

in which the energy spread in the cylindrical beam segment \( \Delta E_{\text{Boe}_c} \) is determined by Eq. (3.23). Based on Eq. (5.11), the total spot disc \( d_{\text{Boe}_l} \) in the image plane \( b \) of figure 5.1(3) is given by

58
\[ d_{\text{Boe},t} = K_{\text{Boe}} \cos (\infty f_{11}) \alpha_{11} M \Delta E_{\text{Boe},t}(m, I, V_{11}, r_0, \alpha_{11}, f_{11}) / V_{11} \]

\[ + K_{\text{Boe}} \cos (\infty f_{21}) \alpha_{21} [\Delta E_{\text{Boe},t}(m, I, V_{11}, r_0, \alpha_{11}, f_{11}) + \Delta E_{\text{Boe},t}(m, I, V, r_0, L)] / V_{21} \]

(5.24)

In the case of figure 5.1(4), the total energy spread \( \Delta E_{\text{Boe}} \) and the total spot disc \( d_{\text{Boe},t} \) induced by the energy spreads in different beam segments are respectively evaluated by

\[ \Delta E_{\text{Boe},t} = \Delta E_{\text{Boe},a}(m, I, V_{11}, r_0, \alpha_{11}, P_1) \]

\[ + \Delta E_{\text{Boe},a}(m, I, V, r_0, + \alpha_{22}Q_2, |\alpha_{21}|, L) + \Delta E_{\text{Boe},a}(m, I, V_{22}, r_0, \alpha_{22}, Q_2) \ (eV) \]

(5.25)

and

\[ d_{\text{Boe},t} = K_{\text{Boe}} \cos (\infty f_{11}) \left[ 1 + \frac{M_1}{M} \left( \frac{V_{11}}{V_{12}} \right)^{1/4} \right] \]

\[ \times \frac{\alpha_{11} M \Delta E_{\text{Boe},a}(m, I, V_{11}, r_0, \alpha_{11}, P_1)}{V_{11}} \]

\[ + K_{\text{Boe}} \cos (\infty f_{21}) \left[ \frac{V_{22}}{V_{21}} \right]^{3/2} \left[ M_2 + \left( \frac{V_{21}}{V_{22}} \right)^{1/4} \right] \]

\[ \times \frac{\alpha_{22} \Delta E_{\text{Boe},a}(m, I, V_{11}, r_0, \alpha_{11}, P_1)}{V_{21}} \]

(5.26)

5.4.2 Trajectory displacement effect disc in a complete particle optical column

Because of the trajectory displacement effect described in chapter 3, another new spot disc, the trajectory displacement effect disc, can be found in the image plane \( b \) of figure 5.1. In figure 5.1(1), the total spot disc \( d_{\text{tra},t} \), produced by the trajectory displacement effect is linearly added, in the image plane \( b \), by

\[ d_{\text{tra},t} = M d_{\text{tra},a} + d_{\text{tra},b} = M d_{\text{tra},a}(m, I, V_b, r_0, \alpha_0, K_0) + d_{\text{tra},b}(m, I, V_b, r_0, \beta_0, Q, K_0) \]

(5.27)

in which \( d_{\text{tra},a} \) and \( d_{\text{tra},b} \) are respectively calculated by Eq.(3.37) and Eq.(3.42).

In the case of figure 5.1(2), the total trajectory displacement effect disc is evaluated by

\[ d_{\text{tra},t} = M(d_{\text{tra},a}(m, I, V_{11}, r_0, \alpha_1, P_1, K_0) + \frac{P}{I} d_{\text{tra},a}(m, I, V, r_0, + \alpha_{11}P_1, |\alpha_{12}|, L, K_0)) \]

\[ + d_{\text{tra},b}(m, I, V_{22}, r_0, \alpha_{22}, Q_2, K_0) \]

(5.28)

in which the value \( d_{\text{tra}}/L \) is the total statistical angular deflection of the beam segment in between two lenses referred to the plane of the lens 1. The angular deflection produces a trajectory displacement distribution in the object plane \( a \), which has a full width (FWHM or FW50) given by \( (P/L)d_{\text{tra},a} \). This is an evaluation approach following Ref.[10]. For the same reason the total trajectory displacement
effect discs in the image planes $b$ of figure 5.1(3) and figure 5.1(4) are respectively given by

$$d_{i.\alpha} = M d_{i.\alpha}(m, I, V_{11}, r_a, \alpha_{11}, r_{11}, K_0) + (f_{22}/L)d_{i.\alpha}(m, I, V_{10}, r_b, \alpha_{11}, r_{11}, K_0)$$

(5.29)

and

$$d_{i.\alpha} = M d_{i.\alpha}(m, I, V_{11}, r_a, \alpha_{11}, P_i, K_0) + (Q_2/L)d_{i.\alpha}(m, I, V_{10}, r_b, \alpha_{11}, P_i, K_0)$$

(5.30)

$$+ d_{i.\alpha}(m, I, V_{11}, r_b, \alpha_{11}, r_{12}, Q_2, K_0)$$

where $d_{i.\alpha}(m, I, V_{11}, r_a, \alpha_{11}, r_{11}, K_0)$ is determined by Eq.(3.43). In Eq.(5.29) and Eq.(5.30), $d_{i.\alpha}(m, I, V_{11}, r_a, \alpha_{11}, r_{11}, K_0)$ and $d_{i.\alpha}(m, I, V_{11}, r_a, \alpha_{11}, r_{11}, K_0)$ are also the angular deflection values referred to the plane of lens 2, which cause the trajectory displacement distributions in the image plane $b$ (f22/L)d_{i.\alpha} and (Q2/L)d_{i.\alpha}, respectively.10

5.5 Space charge effect discs in a complete particle optical column

As described in chapter 4, we mainly consider the first order space charge aberration and the third order space charge aberration. In the following, we do not take into account the laminar flow (but the ANALIC program14 does) for the reason of simplifying the presentation.

Chapter 4 has proven that, for the imaging relation with two trapezoidal beam segments in figure 5.1(1), the space charge defocussing (one of the first order space charge aberrations) and the space charge spherical aberration (one of the third order space charge aberrations) play a major role in the computation of the space charge effect. Accordingly, we shall restrict ourselves to only look into the influence of the space charge defocussing and the space charge spherical aberration in the trapezoidal beam segments on the imaging systems of figure 5.1.

5.5.1 Defocussing distance and defocussing aberration

Because of the space charge effect in the trapezoidal beam segments in the object-side and in the image-side of the lens in figure 5.1(1), the total defocussing distance departing from the image plane $b$ $\Delta z_{i.\alpha}$ is determined by

$$\Delta z_{i.\alpha} = M^2 \left[ \frac{V_b}{V_a} \Delta z_{i.\alpha}(m, I, V_a, r_a, r_p, \alpha_0) + \Delta z_{i.\alpha}(m, I, V_b, r_b, r_p, \beta_0) \right]$$

(5.31)

in which the defocussing distance $\Delta z_{i.\alpha}$ is presented in Eq.(4.52). The total space charge defocussing disc $d_{i.\alpha}$ in the image plane $b$, in terms of the definition of Eq.(4.51), is given by

$$d_{i.\alpha} = 2\beta_0 \Delta z_{i.\alpha} \ast \text{defoc}\%$$

(5.32)

In the case of figure 5.1(2), the total defocussing distance departing from the image plane $b$ $\Delta z_{i.\alpha}$ can be described as

$$\Delta z_{i.\alpha} = M^2 \left[ \frac{V_{22}}{V_{11}} \Delta z_{i.\alpha}(m, I, V_{11}, r_a, r_{11}, P_i, \alpha_{11}) + \Delta z_{i.\alpha}(m, I, V_{22}, r_b, r_{12}, Q_2, \alpha_{22}) \right]$$
\[ \frac{P_1 M_1^2}{L M_1} \sqrt{\frac{V_{22}}{V_{12}}} \Delta z_{\text{foc}_a}(m, I, V, r_a + P_1 \alpha_{11}, r_b + \alpha_{22} Q_2, |\alpha_{12}|) \] (5.33)

In this case the total space charge defocussing disc \( d_{\text{foc}_t} \) in the image plane \( b \) of figure 5.1(2) is defined as

\[ d_{\text{foc}_t} = 2\alpha_{22} \Delta z_{\text{foc}_t} \ast \text{defoc\%} \] (5.34)

The last term of Eq.(5.33) is obtained by the following approach. The defocussing distance departing from the plane \( a \) is first calculated by \( (P_1 \Delta z_{\text{foc}_a} / L)(\alpha_{12}/\alpha_{11}) = (P_1 \Delta z_{\text{foc}_a} / L)[M_1^{-1}(V_{11}/V_{12})^{1/2}] \), here, \( \Delta z_{\text{foc}_a} \) is the defocussing distance departing from the plane of lens 1, which is produced by the space charge effect in the beam segment in between the two lenses. This defocussing distance is then transformed into the defocussing distance departing from the imaging plane \( b \) by multiplying \( M_2^2(V_{22}/V_{11})^{1/2} \). In Eq.(5.33), \( M_1 \) is the magnification of the first lens, and \( M \) the total magnification of the two lens system.

For the imaging relation of figure 5.1(3), the total defocussing distance departing from the image plane \( b \) \( \Delta z_{\text{foc}_t} \) is derived into

\[ \Delta z_{\text{foc}_t} = M_2^2 \sqrt{\frac{V_{22}}{V_{11}}} \Delta z_{\text{foc}_a}(m, I, V_{11}, r_a, r_b + f_{11} \alpha_{11}, \alpha_{11}) + (r_0/L) \Delta r_{\text{sch}1}(m, I, V, r_{0L}) \]

\[ + \Delta z_{\text{foc}_a}(m, I, V_{22}, r_b, r_a + f_{22} \alpha_{22}, \alpha_{22}) \] (5.35)

in which \( \Delta r_{\text{sch}1} \) is presented in Eq.(4.58), and \( r_0 \) is the radius of the cylindrical beam segment in figure 5.1(3). In this circumstance, the total first order spot disc \( d_{\text{foc}_t} \), caused by the space charge effect in the image plane \( b \) of figure 5.1(3) is also calculated by Eq.(5.34). For the same reason, the total defocussing distance departing from the image plane \( b \) \( \Delta z_{\text{foc}_t} \) in figure 5.1(4) can be derived into

\[ \Delta z_{\text{foc}_t} = M_2^2 \sqrt{\frac{V_{22}}{V_{11}}} \Delta z_{\text{foc}_a}(m, I, V_{11}, r_a, r_b + \alpha_{11}, P_1, \alpha_{11}) + \Delta z_{\text{foc}_a}(m, I, V_{22}, r_b, r_a + Q_2 \alpha_{22}, \alpha_{22}) \]

\[ + \frac{M_2 Q_2}{L} \sqrt{\frac{V_{22}}{V_{21}}} \Delta z_{\text{foc}_a}(m, I, V, r_b + Q_2 \alpha_{22}, r_a + P_1 \alpha_{11}, |\alpha_{12}|) \] (5.36)

in which the last term is the defocussing distance departing from the plane \( b \) due to the space charge effect in the convergent beam segment in between the lenses. In this case the total first order defocussing disc \( d_{\text{foc}_t} \), in the image plane \( b \) of figure 5.1(4) is again evaluated by Eq.(5.34).

5.5.2 Space charge spherical aberration

Because of the space charge spherical aberrations in two trapezoidal beam segments of figure 5.1(1), a total third order spot disc \( d_{\text{sch}t} \) can be measured in the plane \( b \)

61
\[ d_{sch} = Md_{sch} (m, I, V_a, r_a, r', P, \alpha) = d_{sch} (m, I, V_b, r_b, r', P, \beta) \]  

in which \( d_{sch} \) is given by Eq. (4.54).

For the imaging mode of figure 5.1(2), the total third order spherical aberration disc \( d_{sch} \) in the image plane \( b \) is calculated by

\[ d_{sch} = Md_{sch} (m, I, V_{11}, r_a, r_a + \alpha_{11}, P, \alpha_{11}) + (P/L)d_{sch} (m, I, V_{b+1}, r_b, P, \alpha_{11}, \alpha_{11}, r_b + Q_2 \alpha_{22}, [\alpha_{11}]) \]

\[ + d_{sch} (m, I, V_{22}, r_b, r_b + Q_2 \alpha_{22}, \alpha_{22}) \]  

in which the term \((P/L)d_{sch}\) is defined by following the definition in Eq. (5.28).

For the same reason of the space charge spherical aberrations in three rotationally symmetric beam segments in figure 5.1(3) and figure 5.1(4), the third order spot discs in the image planes \( b \) of figure 5.1(3) and figure 5.1(4) can be respectively measured with

\[ d_{sch} = Md_{sch} (m, I, V_{11}, r_a, r_a + f_{11} \alpha_{11}, \alpha_{11}) + 2(f_2/L)d_{sch} (m, I, V_{b+1}, r_b) \]

\[ + d_{sch} (m, I, V_{22}, r_b, r_b + f_{22} \alpha_{22}, \alpha_{22}) \]  

and

\[ d_{sch} = Md_{sch} (m, I, V_{11}, r_a, r_a + \alpha_{11}, P, \alpha_{11}) + (Q_2/L)d_{sch} (m, I, V_{b+1}, r_b, P, \alpha_{22}, r_b + P, \alpha_{22}) \]

\[ + d_{sch} (m, I, V_{22}, r_b, r_b + Q_2 \alpha_{22}, \alpha_{22}) \]  

in Eq. (5.39) \( \Delta r_{sch} \) is given by Eq. (4.59).

5.6 Total probe size and I-d relations

In the previous sections, we calculated eight spot discs, \( d_{sph}, d_{spb}, d_{chr}, d_{dfr}, d_{boc}, d_{trc}, d_{foc} \) and \( d_{sch} \), in the image plane \( b \) of the four elementary imaging modes shown in figure 5.1, which are usually met in a charged particle optical column. Based on these evaluations, we are able to further calculate these spot discs for a complete particle optical column that consists of a number of independent imaging units described in figure 5.1. For the example of the optical column in figure 2.6, which consists of two independent imaging units, we can practically evaluate eight spot discs in any image plane. In general, for an optical column with \( l \) independent imaging units, every spot disc in the \( j \)th \((j \leq l)\) image plane \( b \) can be expressed as

\[ d = M_j d_{j-1} + d_j \quad 1 \leq j \leq l \quad d_0 = 0 \]  

where \( d \) represents one of the eight spot discs, and \( M_j \) the magnification of the \( j \)th independent imaging unit. It should be particularly noted that, when one evaluates the different kinds of spot discs \( d \) in different image planes, one is forced to consider the experimental parameters such as the half opening angle, the beam current, the beam potential and so on carefully. As described in chapter 2, for the examples of figure 2.5 and figure 2.6, the experimental parameters, particularly the half opening angle, the beam current and the beam potential, in every beam segment of an independent imaging unit may be very different because of the apertures cutting the beam.
After having defined the individual spot disc in an image plane \( b \) of a complete particle optical column, we can define three total spot sizes in the image plane \( b \) of the column. In all later chapters, these total spot sizes will be repeatedly used for different studies.

The addition of the different lens aberrations has been carefully investigated in Ref.[11], and this addition method was immediately used in Ref.[9,15,16]. In accordance with Ref.[11] we define the total geometrical aberration disc \( d_{\text{tg}} \) in the image plane \( b \) as

\[
d_{\text{tg}} = \left\{ \left[ (d_{\text{sph}}^4 + d_{\text{df}}^4)^{1/3} + d_{\text{Gau}}^{1/3} \right]^{2/1} + d_{\text{chr}}^2 \right\}^{1/2}
\]

(5.42)

in which \( d_{\text{Gau}} \), \( d_{\text{sph}} \), \( d_{\text{df}} \) and \( d_{\text{chr}} \) should be understood as the total spot disc of an optical column, which are respectively added in terms of Eq.(5.41). The total geometrical aberration disc \( d_{\text{tg}} \) is regarded as a measurement of the lens aberrations without taking into account the Coulomb interactions. If the Coulomb interaction effects are considered, another four spot discs constitutes the total Coulomb interaction disc \( d_{\text{ci}} \). Based on the idea of Ref.[11], we define the total Coulomb interaction disc as

\[
d_{\text{ci}} = \left\{ \left[ (d_{\text{sch}}^{1/3} + d_{\text{pce}}^{1/3})^{2/1} + d_{\text{bee}}^{2/1} \right] \right\}^{1/2}
\]

(5.43)

It is clear that \( d_{\text{ci}} \) is a measurement of the impact of total Coulomb effect on an imaging system. The combined measurement for all lens effects and Coulomb effects in a imaging system is the total probe size \( d_{\text{tot}} \). We extend the addition method in Ref.[11], and define the total probe size \( d_{\text{tot}} \) as

\[
d_{\text{tot}} = \left\{ \left[ (d_{\text{sph}} + d_{\text{df}})^{1/3} + (d_{\text{Gau}} + d_{\text{pce}} + d_{\text{bee}})^{1/3} \right]^{2/1} + (d_{\text{bee}} + d_{\text{chr}})^2 \right\}^{1/2}
\]

(5.44)

For a determined particle optical column, if substituting all concerned equations presented previously into Eq.(5.42), (5.43) and (5.44), we find that \( d_{\text{tg}} \), \( d_{\text{ci}} \) and \( d_{\text{tot}} \) are all continuous functions of the basic experiment parameters \((I,m,V,M,r_a,\alpha_0)\). If we go a step further to connect the column parameters with the source parameters by means of Eq.(5.1), we find that these total spot discs are all functions of parameters \((I,m,V,M,r_a,B)\), i.e.

\[
d_{\text{tg}} = f_{\text{tg}}(I,m,V,M,r_a,B)
\]

(5.45)

\[
d_{\text{ci}} = f_{\text{ci}}(I,m,V,M,r_a,B)
\]

(5.46)

\[
d_{\text{tot}} = f_{\text{tot}}(I,m,V,M,r_a,B)
\]

(5.47)

where \( M \) is the total magnification of a particle optical column, \( B \) the reduced source brightness, \( r_a \) the source virtual radius, and \( m \) the particle mass. The current \( I \) and the potential \( V \) can be different in different beam segments. In principle, from Eq.(5.45), Eq.(5.46) and Eq.(5.47) the inverse functions can also be found. The relation between the beam current \( I \) and the spot size \( d \), which is usually referred to as I-d relation, best characterizes a complete particle optical column. In the two-dimensional I-d plane, if one of the experimental parameters \((m,V,M,r_a,B)\) changes, this will result in a determination of a group of I-d curves. These I-d curves can be used to exactly evaluate the design quality of a probe forming instrument.

References

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6 Combined calculation of lens aberrations, space charge aberrations and statistical Coulomb effects in charged particle optical columns

Abstract Optimizing a charged particle optical system utilizing a high brightness source requires the inclusion of the effect of Coulomb interactions in the evaluations. A new computer program package, named ANALIC, has been developed to perform the combined calculation of lens aberrations, space charge aberrations and statistical Coulomb effects in a complete instrument. By making use of an analytical slice method, valid for weak/incomplete collisions, to calculate the Coulomb interactions the program combines reasonable accuracy with high speed. Using ANALIC, an optical system with an arbitrary number of lenses and apertures, an arbitrary mode of imaging and arbitrary distribution of the beam energy can be analyzed directly. The functions, features, organization and calculation approach of the program are reported. As an example of the use of the program a four lens electron probe instrument is analyzed for the demonstration of the combined calculation and optimization process of a particle optical system.

6.1 Introduction

Charged particle optical instruments utilizing high brightness sources are limited not only by lens aberrations but also by Coulomb interactions. Optimization of an optical system requires consideration of these simultaneously. The usual approach of investigating the impact of the Coulomb interactions on a particle optical system is focussed on Monte Carlo simulation\cite{11}. However, using Monte Carlo simulation for a system optimization is very time-consuming since the considered optimization process is a problem with many variables. Analytical equations derived by Jansen\cite{12} and the INTERAC program\cite{13} based on these equations can be used to calculate the Coulomb interactions in beam segments, but it is still difficult to optimize a complete system with an arbitrary number of lenses and apertures, an arbitrary mode of imaging relations and an arbitrary distribution of the beam energy.

The optical system optimization including the evaluation of the Coulomb interactions by using an analytical approach was first reported in Ref.[14]. Examples of full system optimization and design with this new approach are found in Ref.[15, 16], in which the impact of the Coulomb interactions on a focussed ion beam instrument built in our laboratory was carefully investigated. In this paper we try to present the background of the computer program ("ANALIC") which is used for these calculations.

** This chapter is a complete article presented at the 40th Int. Conf. on Electron, Ion and Photon Beam Technology and Nanofabrication, Atlanta, May 28-31, 1996, to be published in J. Vac. Sci. Technol., B14(6), 1996. The authors of the article are Xinrong Jiang, Jim Barth and Pieter Kruit. For reading convenience, the equations, figures and pages in this article are renumbered in line with the order of this thesis. In addition to the presentation in the article, this chapter includes the ANALIC program fortran source code report (250 pages) and the ANALIC program reference manual, which are independently reported.
6.2 Approach of the combined calculation

Figure 6.1 shows a general particle optical system with an arbitrary number of lenses ($L_k$, $k=1..n$) and apertures (position $D_j$ and diameter $D_j$, $j=1..m$), an arbitrary mode of imaging relations with crossovers or without crossovers\textsuperscript{16} and an arbitrary distribution of the beam energy along the optical axis $V(z)$. In every image plane of the lenses, eleven spot sizes ($l=1..11$) are defined:

$$d_{kl} = \{d_{Gau}^{k}, d_{chr}^{k}, d_{sph}^{k}, d_{gy}^{k}, d_{Boe}^{k}, d_{tra}^{k}, d_{foc}^{k}, d_{sch}^{k}, d_{gap}^{k}, d_{tof}^{k}, d_{tot}^{k}\} \quad (6.1)$$

Eq.(6.1) represents a spot size set consisting of the source image disc $d_{Gau}$, the chromatic aberration disc $d_{chr}$, the spherical aberration disc $d_{sph}$, the diffraction aberration disc $d_{gy}$, the Boersch effect disc $d_{Boe}$, the trajectory displacement effect disc $d_{tra}$, the space charge defocussing aberration disc $d_{foc}$, the space charge spherical aberration disc $d_{sch}$, the total geometrical aberration disc $d_{gap}$, the total Coulomb interaction disc $d_{tof}$ and the total probe size $d_{tot}$ in the $k$th image plane of a universal optical system. The three total spot sizes are

$$d_{gap} = \frac{1}{2} \left[ \left( d_{sph}^{4} + d_{gy}^{4} \right)^{\frac{1}{4}} + d_{Gau}^{3} \right]^{\frac{1}{2}}$$ \quad (6.2)

$$d_{tof} = \frac{1}{2} \left[ \left( d_{sch}^{4} + d_{foc}^{4} \right)^{\frac{1}{4}} + d_{Boe}^{3} \right]^{\frac{1}{2}}$$ \quad (6.3)

and

$$d_{tot} = \frac{1}{2} \left[ \left( d_{sph}^{3} + d_{sch} \right)^{\frac{1}{4}} + \left( d_{g}^{2} + d_{foc}^{2} + d_{tra}^{2} \right)^{\frac{1}{4}} + d_{Boe}^{3} \right]^{\frac{1}{2}}$$ \quad (6.4)

d_{gap} is without including the Coulomb effects, $d_{tof}$ is calculated to estimate the relative importance of the Coulomb interaction effects, and $d_{tot}$ is a total combined measurement of the lens effects and Coulomb effects of a particle optical system. The additions in Eqs.(6.2), (6.3) and (6.4) are according to the method presented in Ref.[15,17]. The dependencies on system parameters are expressed as

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66
\[ d_{il} = W_i \left[ \Delta E, d_{ij}, Rm, B, Dz_j, D_j, C_{z}, C_{z}, f_{k1}, f_{k2}, r(z), V(z), I(z) \right] \]

\[(k=1..n; j=1..m; l=1..11) \quad (6.5)\]

All spot discs \( d_{il} \) are the functions of the gun, column and beam parameters. The gun parameters are the source energy spread \( \Delta E \), the source virtual diameter \( d_0 \), the relative particle mass to electron \( Rm \) and the source reduced brightness \( B \). The column is characterized by the aperture positions \( Dz_j \) and diameters \( D_j \), the lens positions \( L_k \), the spherical and chromatic aberration coefficients \( C_{z} \) and \( C_{z} \), the lens focal distances in object-side and image-side \( f_{ik} \) and \( f_{ik} \), and the beam by the beam shape \( r(z) \), the beam energy \( V(z) \) and the beam current \( I(z) \) \((k=1..n; j=1..m)\).

The functions \( W_i \) for the calculation of the lens aberrations are known, the problem is how to determine these functions for the evaluation of the Coulomb interactions. In this paper we outline the approach used to solve this problem, and the reader is referred to Ref. [12,18,19] for a detailed exposition.

Figure 6.2 shows an imaging section around the \( k \)th lens in the general system of figure 6.1. Suppose that there are five apertures in the object-side and image-side and some of them cutting the beam. With the distribution of the beam energy \( V(z) \), the initial condition of the emission of particles and the boundary condition given by aperture positions and diameters, the beam shape \( r(z) \) in the whole system is determined by solving the ray equation:

\[ r'' + \frac{V'(z)}{2V(z)} r' + \frac{V''(z)}{4V(z)} r = 0 \quad (6.6) \]

Eq.(6.6) is well known for the paraxial ray, and can be replaced by a general ray equation. However, in the ANALIC program, we suppose that the lenses are all thin lenses, accordingly, Eq.(6.6) here is only used to determine the beam shape in between lenses. In the program, Eq.(6.6) is solved twice. One is for the dotted line in figure 6.2, which, used to calculate the lens aberrations, is the ray with maximum radial size and going through every aperture. The other is for the outer solid line \( r(z) \), utilized to evaluate the Coulomb effects. The outer ray \( r(z) \) determines the real beam shape of a particle optical column separated by a number of apertures and lenses from the source to the target. The beam current \( I(z) \) is determined based on the brightness \( B \), the aperture position \( Dz \) and diameter \( D \).
The total energy broadening due to the Boersch effect in the whole column of figure 6.1, which is now considered as consisting of several beam sections as figure 6.2, is calculated by

$$\Delta E_{\text{Boe tot}} = \sum_{k=1}^{n} \left[ \int_{z_{\text{Object}}}^{z_{\text{Image}}} F_{\text{Boe}}[r(z), V(z), I(z)] \, dz \right]$$

(6.7)

where \( z_{\text{Object}} \) and \( z_{\text{Image}} \) are the coordinates of the object-plane and image-plane of the kth lens, and \( F_{\text{Boe}}[r(z), V(z), I(z)] \, dz \) is an element value of the energy broadening in a slice (the shadowed area) shown in figure 6.2. \( F_{\text{Boe}} \) is defined as an energy spread function due to the Boersch effect and given by

$$F_{\text{Boe}}[r(z), V(z), I(z)] = \left[ \frac{B_1 D^3 r^4 I(z)^3 V(z)^{-3/2}}{1 + B_2^{-1/4} D^5 r^6 I(z)^5 V(z)^{-1}} \right]^{2/3} (eV.m^{-1})$$

(6.8)

where

$$D_\lambda = \frac{m^{1/2}}{\pi^{2/3} \epsilon_0^{1/2} e^{1/2}}, \quad D_r = \left( \frac{2 \pi \epsilon_0}{e} \right)^{1/3}$$

(6.9)

In Eq.(6.8), the coefficients \( B_1 \) and \( B_2 \) are different for different measurements (FWHM or FW50) of the energy spread\(^{18} \). Eq.(6.8) includes the pencil beam regime and Holtmark regime (characterized by the coefficient \( B_2 \))\(^{12,19} \), however, the Gaussian regime is not included since it is in fact absent in the case of a slice beam segment. To evaluate the Boersch effect disc \( d_{\text{Boe}} \) in the kth image plane, which is found through the chromatic aberration effect\(^{15} \), one has to calculate all energy broadening in front of the kth lens.

The evaluation of the trajectory displacement effect disc \( d_{\text{tra}} \) referred to the image plane of the kth lens (\( k=1\ldots n \)) is expressed as

$$d_{\text{tra}} = M_k \int_{z_{\text{Object}}}^{z_{\text{Image}}} (z-z_{\text{Object}}) F_{\text{tra}}[r(z), V(z), I(z)] \, dz + \int_{z_{\text{Object}}}^{z_{\text{Image}}} (z_{\text{Image}}-z) F_{\text{tra}}[r(z), V(z), I(z)] \, dz$$

(6.10)

where \( M_k \) is the magnification of the kth lens, and \( F_{\text{tra}}[r(z), V(z), I(z)] \, dz \) the statistical angular deflection value in a slice element. \( F_{\text{tra}} \) is defined as an angular deflection function and evaluated by

$$F_{\text{tra}}[r(z), V(z), I(z)] = \left[ \frac{T_1 D^8 r^6 I(z)^8 V(z)^{-1/5}}{T_2 + T_2^{-1/2} D^5 r^6 I(z)^2 V(z)^{-1}} \right]^{7/6} (m^{-1})$$

(6.11)

The coefficients \( T_1 \) and \( T_2 \) distinguish the FWHM from FW50 measurement of the spot size \( d_{\text{tra}} \), and the coefficient \( T_4 \) distinguishes the Gaussian from uniform spatial distribution of the particle beam\(^{18} \). Eq.(6.11) also includes only the pencil beam regime (\( T_4 \) term) and Holtmark regime (\( T_2 \) term) without the Gaussian regime\(^{12,19} \).

Eq.(6.10) is also suited to the evaluation of the space charge defocussing and the space charge
spherical aberration if the function $F_{ra}$ is replaced by $F_{loc}$ and $F_{sch}$ respectively. However, the evaluation is very complicated since the angular deflection functions due to the space charge effect $F_{loc}$ and $F_{sch}$ can not be expressed analytically\textsuperscript{18}. Accordingly, we solve this problem here by following another simpler approach.

Suppose that the beam section determined by the outer ray $r(z)$ in the object-side of the $k$th lens consists of $q$ trapezoidal beam slices, and that the positions of the slices are $z=(z_{kog1}+z_{kog2})/2$ ($g=1..q$), as the a-b-c-d-a area shown in figure 6.2, in which $I_{kog}$, $V_{kog}$ and $\alpha_{kog}$ indicate the beam current, beam energy of the $g$th trapezoidal slice and half opening angle of the slice referred to the object plane $z_{kog}$. In this case, the defocussing\textsuperscript{12,18} from the object plane $z_{kog}$ due to the space charge effect in the $g$th slice ($g=1..q$) is

$$\Delta z_{kog} = \frac{c_0 I_{kog} r_{kog}}{\alpha_{kog}^3} \left[ \frac{\alpha_{kog} (z_{kog2} - z_{kog1})}{r_{kog}} + \frac{r_{kog}}{r(z_{kog2})} - \frac{r_{kog}}{r(z_{kog1})} + 2 \ln \frac{r(z_{kog2})}{r(z_{kog1})} \right]$$  \hspace{1cm} (6.12)

where $r_{kog}=r(z_{kog})$, $c_0$ is taken as unity when the uniform or Gaussian spatial distribution of the particle beam is considered\textsuperscript{12,18}, and

$$\mu_{kog} = \frac{I_{kog}}{4 \pi \varepsilon_0 \sqrt{2e/m V_{kog}}} \quad (g=1..q)$$  \hspace{1cm} (6.13)

For the same reason, the spherical aberration coefficient due to the space charge effect in the $g$th slice can be derived as

$$C_{s,kog} = \frac{c_2 I_{kog} r_{kog}}{2 \alpha_{kog}^5} \left[ \frac{\alpha_{kog} (z_{kog2} - z_{kog1})}{r_{kog}} + 4 \ln \frac{r(z_{kog2})}{r(z_{kog1})} + \frac{6r_{kog}}{r(z_{kog2})} - \frac{6r_{kog}}{r(z_{kog1})} \right]$$

$$- \frac{2r_{kog}^2}{r(z_{kog2})^2} + \frac{2r_{kog}^2}{r(z_{kog1})^2} + \frac{r_{kog}^3}{3r(z_{kog2})^3} - \frac{r_{kog}^3}{3r(z_{kog1})^3} \right] \quad (g=1..q)$$  \hspace{1cm} (6.14)

in which $c_2=0.5$ and $c_2=0$ are taken for the Gaussian and uniform angular distributions of the particle beam respectively.

The total space charge defocussing disc $d_{k,loc}$ and total space charge spherical aberration disc $d_{k,sch}$ in the image plane of the $k$th lens in figure 6.2 should include the contributions from the beam sections in the object-side and image-side of the lens. Accordingly, they are determined by

$$d_{k,loc} = M \sum_{g=1}^{q} \Delta z_{kog} + \sum_{g=1}^{q} \Delta z_{kog} \quad (k=1..n)$$  \hspace{1cm} (6.15)

and

$$d_{k,sch} = \frac{M \sum_{g=1}^{q} C_{s,kog} \alpha_{kog}^3 + \sum_{g=1}^{q} C_{s,kog} \alpha_{kog}^3}{(k=1..n)}$$  \hspace{1cm} (6.16)

Here, the parameters with "i" subscript mean that they are defined in the image-side of the lens in figure 6.2. In Eq.(6.15) the factor defoc% is the fraction of the defocussing, say, 0.05 ~ 0.15 from
our experience point of view, to be considered in the addition of the total spot sizes defined in Eqs.(6.3) and (6.4). The reason for introducing this parameter is because most but not all the space charge defocussing can be corrected\(^2\),\(^18\).

The previous equations are applicable to the beam section with a non-crossover imaging mode\(^16\) by adjusting the integral limits as well as the imaging relation of the lens\(^18\).

### 6.3 Features and organization of ANALIC

In the ANALIC program all parameters defined in Eq.(6.5) for a particle optical instrument are system variables. Changing one or two of them results in a variation of the whole system. The program rapidly performs the combined calculation of the lens aberrations, the statistical Coulomb effects and the space charge aberrations according to the change of the variables, and produces different outputs for system analysis and design. These output functions are divided into tables form, curves form and surfaces plus curves form. The main characteristic of these output functions is that all calculated spot discs \(d_{kl}\) can be recorded with a number of tables, curves and surfaces simultaneously, and the dependencies of the spot discs \(d_{kl}\) on the system variables \(\{\Delta E, d_0, R_m, B, L_4, D_1, D_2, C_5, C_6, f_{k1}, f_{k2}, V(z), I(z)\}\) can be displayed on screen respectively by presenting a group of curves and surfaces. Another important property of the output functions is for system optimization. When two of the system variables vary in determined ranges simultaneously, the program presents the relations between the minimum spot sizes and the optimum variable values. For instance, a probe forming instrument is best characterized by a relation between the probe current \(I\) and minimum probe size \(d_{opt}\) at optimum system magnification \(M_{opt}\)\(^15\),\(^16\),\(^20\). In this case, the program will output an optimized system setting \(\{I, d_{opt}, M_{opt}\}\), in which the optimum magnification \(M_{opt}\) is determined by the system variables \(\{L_4, f_{k1}, f_{k2}, V(z)\}\). This makes it possible to optimize the design procedure of an instrument effectively when taking into account simultaneously the influence of the lens positions \(L_4\), lens imaging relations \((f_{k1} \text{ and } f_{k2})\) and system energies \((V(z))\) on both the lens effects and Coulomb effects.

The ANALIC program is written in Fortran 77 and runs on an IBM compatible PC. The source code consists of eight programs and one input file: ANALIC, READIN, GEOPITICS, INACTION, CURVES, OUTPUT, OPTIMIZE, OPTICS AND INPUT.DAT. ANALIC is a main program. READIN, GEOPITICS, INACTION, CURVES, OUTPUT and OPTIMIZE are the subroutines of ANALIC. OPTICS is an independent program. The source code consists of fifteen thousand lines. Figure 6.3 shows the relationships between the programs.

In figure 6.3, ANALIC controls all subroutines, and outputs the messages to prompt the user to operate the program correctly. READIN imports all parameters and data from the input file.
(INPUT.DAT) for preparing all follow-up calculations and outputs. It also performs the pre-processing for the input data and checks whether the defined parameters and data are reasonable or not. GEOPHTICS calculates the lens aberrations before the Coulomb interactions are considered, including evaluating the imaging relations of a particle optical system and the beam shape defined in Eq. (6.6) and figure 6.2. INACTION is in charge of computing all Coulomb interaction effects presented in section 6.2. CURVES realizes the output function of the curves form, with which the dependencies of the eleven spot discs defined in the target of an optical column d_m on every system variable defined in Eq. (6.5) can be displayed on screen. OUTPUT creates a group of tables which record all calculated dependencies. OPTIMIZE is responsible for a full system optimization. It first creates the surfaces output form and then finds out the optimized setting of an optical system. Finally, the OPTICS program is used to draw a defined particle optical instrument on screen including displaying the geometrical results of the system such as the lens aberrations, the beam shape and imaging relation, etc. It is particularly useful for examining whether a defined optical system is reasonable or not before the Coulomb interactions are taken into account. INPUT, DAT is used as an input file to define a complete particle optical system and the calculation purposes with the ANALIC and OPTICS programs. SGPLOT and GRAFTOOL in figure 6.3 are two commercial software packages which are used to support the display and editing of the curves and surfaces evaluated by the ANALIC program.

6.4 Calculation example using ANALIC

We take a four lens electron beam instrument shown in figure 6.4 to demonstrate the ANALIC program.

The beam energy distribution from the gun to the target V(z) is a step function for simplifying the demonstration. The source parameters are d_s=30 nm, ΔE=0.2 eV and B=10^8 A.m^2.sr^-1, V^-1, and the spherical and chromatic aberration coefficients in the object- side of the lenses are C_s1=30 mm, C_c1 =20 mm, C_s2=C_s3=C_c2=C_c3=0, C_s4 =380 mm and C_c4=57 mm. The beam has Gaussian angular and spatial distributions, and its spot sizes are evaluated with the FW50 measurement.

We first demonstrate the function described as the curves form. D_3 is considered as a system variable, figure 6.5 presents the dependencies of the eleven spot discs on the probe current I when D_3 changes. The calculation condition of figure 6.5 is a) the focal distances f_s1=22 mm, f_s2=44 mm, f_s3=f_s4=30.3 mm, f_s1=f_s2=20.8 mm and f_s1=f_s2=60 mm (the total magnification of the system M=0.825), and b) the aperture diameters D_1=1.2 mm and D_2=0.3 mm. It is found from figure 6.5 that the Coulomb interactions (d_u, d_v, d_w and d_u) are heavily impacting the electron beam instrument because of the high current in front of the third aperture (the current in the section between D_1 and D_3 is I_{D3}=2665 nA, and between D_2 and D_3 I_{D3}=1411 nA) and the low energy sections following
the third lens. It can be easily understood that any change of the system variables defined in Eq.(6.5) will result in a group of curves similar to figure 6.5.

Next we demonstrate the full system optimization. Suppose that the first and third crossovers of the system in figure 6.4 are fixed at the positions of z=195 mm and 510 mm (f11=22 mm, f12=44 mm, f41=f42=60 mm), and that the second crossover position is moved (f21, f22, f31 and f32 changing simultaneously to adjust the system magnification M). The apertures D1 and D2 remain fixed at 1.2 mm and 0.3 mm, and the third aperture D3 is changed over a definite range, thereby resulting in a variation of the probe current I. Figure 6.6 shows the dependencies of the three total spot sizes (d_tgs, d_tcl and d_tot) on the magnification M and probe current I. For every probe current I one can find a minimum probe size d_tgs_opt or d_tcl_opt. Accordingly, a best balance between the chosen probe current I and the minimum probe size d is found, as shown in figure 6.7 (see the curve with marker (d_tgs_opt) and the right curve (d_tot_opt)). The minimum total probe size with the influence of the Coulomb interactions is much larger than that without the Coulomb interactions since the probe size component produced by the Coulomb interactions d_tcs can not be ignored especially in the case of larger magnification, as shown in figure 6.6(2). Comparing figure 6.6(1) with figure 6.6(2) one can find a combination of the current and magnification (I,M) inside which d_tcs is larger than d_tgs. Figure 6.7 also presents two other system optimization processes for comparison. One is the case of changing the first aperture diameter D1 and removing the second and third apertures D2 and D3, and the other changing D2 and removing D3 (D1 is still fixed at 1.2 mm). The magnification M in the two cases varies with the crossover position in between D2 and D3. The minimum probe size d_tgs_opt in the three cases are the same, but the smaller the minimum probe size d_tot_opt, the closer to the source the changing aperture has been placed. This aperture position effect has been further studied in Ref.[20].

We finally look at the optimal setting of the magnification of the electron beam instrument as shown in figure 6.8. The optimal magnifications with the impact of the Coulomb interactions are smaller than that without the Coulomb interactions at the same probe current. The optimal magnification (crossover position), with which the probe size is a minimum, depends on which aperture changes. The optimal settings similar to figure 6.8 can be found in other optimization approaches, for instance, if the first or the third crossover position or one of the lens positions changes.

### 6.5 Discussion

![Image](Fig.6.5 The spot size set (equation (6.1)) varies with one of the system variables (the probe current I).)

72
The ANALIC program can be used to perform a combined calculation of lens aberrations and Coulomb aberrations and to directly optimize a multi-variable particle optical system with an arbitrary number of lenses and apertures, an arbitrary mode of imaging relations and an arbitrary distribution of the beam energy. The accuracy of the program has been checked by using the MONT-EC\textsuperscript{1} and INTERAC\textsuperscript{13} programs and by the experiments\textsuperscript{18} carried out in our laboratory. After having been greatly modified several times and having run more than two years, it is being more and more used in practice for evaluating the Coulomb interactions in charged particle optical instruments. It offers comprehensive results through its strong output functions. In addition, it is also developed to investigate the impact of the Coulomb interactions on a single beam segment, for instance, the segment in front of the first lens, the segment behind the last lens or the segment in between two lenses in figure 6.1. The first segment model is particularly useful to be utilized to study the Coulomb interactions in the source region, the second to investigate the landing properties of a particle beam to target when the last lens plays a major role\textsuperscript{14}, the third to evaluate the influence of an intermediate beam section on a complete system.

The optimization of a probe forming instrument can greatly improve the performance of the system. This can be obviously understood from figure 6.6. The question now is how to find the best optimized system setting? Since many of the system parameters can be variables of the optimization process, solving this problem needs an enormous computation and an effective computer program. This is the basis of developing the ANALIC program.

Fig. 6.6 Illustration of three typical combined calculations.
The linear addition method is used in the evaluations of the Coulomb interactions in a complete column. This is different from the gamma-rule summation method proposed by Jansen. However, the use of the linear addition is based on our studies on this problem, in which we calculated a two lens focussed ion beam system with a Monte Carlo simulation and found that the linear rule is better than the gamma-rule. We also measured the spot sizes in the two lens system at different conditions and found that the measured spot sizes fit the calculated ones with the linear rule summation reasonably. Jansen's equations in fact also use the linear summation within a segment. It is only for adding segments that he suggested the gamma-rule.

The limitations of the approach for the combined calculation of lens effects and Coulomb effects are: a) the lenses in a particle optical column are considered as thin lenses, thereby the influence of the lens field on the Coulomb effects being ignored, b) the fields in the object-side and image-side of an imaging lens are considered only impacting the Coulomb effects but not changing lens effects, thereby the influence of the fields on the geometrical aberrations and imaging relation of the lens being ignored, and c) the derived equations (6.8) and (6.11) are only for weak, incomplete collisions between particles.

The limitations of the ANALIC program are: a) it is only suited for probe forming systems, like FIB, SEM and Gaussian EBPG etc., b) it is only used in the investigations of an axis-symmetric optical column or single beam segment, and c) it can only be used to calculate a particle optical system with a medium or low current density since the program is essentially based on the theory of
the first order perturbation approximation. However, in the analysis of many focussed ion beams and low-voltage electron microscopes we have seen that these regions are most important.

References

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13. G.H. Jansen, INTERAC Program Package (1989), distributed by Delft Particle Optics Foundation, Delft University of Technology, the Netherlands.
7 Influence of Coulomb interactions on choice of magnification, aperture size and source brightness in a two lens focussed ion beam column

Abstract  Focussed ion beam columns with liquid metal ion sources should be optimized to give the highest possible current in a probe of given dimension. A procedure for this optimization is presented, which includes the influence of Coulomb interactions between the particles in the beam. The column is first optimized without including the Coulomb effects and it is found that the optimized magnification and aperture size are independent of the gun brightness. The magnification approaches a constant value in the high current domain, where the gun lens aberrations seriously influence the probe size. The Coulomb effects can be characterized by pointing out a domain in the probe current-probe size plane which is inaccessible, no matter how high the brightness of the gun may be. The approximate position of this inaccessible area can be found with a relatively small numbers of calculations. It is then demonstrated how the beam current as a new function of probe size can be reoptimized by the choice of magnification and aperture size. Coulomb effects turn out to be dominating the probe size except for very small probes and for very large probes.

7.1 Introduction

A focussed ion beam column with a liquid metal ion source is best characterized by the relation between the beam current I and the probe size d. It is rather difficult to determine this relation exactly in the case that geometrical aberrations and Coulomb interaction effects are taken into account simultaneously.

Normally, in the cases of larger demagnification and no Coulomb interaction effects, the final lens dominates the properties of the column. In an optimized situation, the contributions from either chromatic or spherical aberration in this column are made to be of the same order as the geometrical size of the gun image by choosing the appropriate magnification and aperture size. If gun lens aberrations have to be considered, the situation is more complicated, because now the aberration contributions are the combined effect of two lenses, with the relative contribution determined by the magnification. However, if Coulomb effects play a role it is even more difficult to find the I-d relation. These Coulomb effects can be characterized by four contributions to the total spot size: the Boersch effect disc, the trajectory displacement effect disc, the space charge defocussing disc and the space charge spherical aberration disc$^{12}$.

Our approach in this paper is to first optimize the I-d curve without Coulomb effects, in which we find that the choice of magnification and aperture size does not depend on the source brightness. We then check, by changing the source brightness, how much current we can really afford into a certain spot size in the previously optimized column before the Coulomb effects start to dominate. Thus we find a maximum current at each spot size, together mapping out a domain in I-d space that

** This chapter is a complete article published in J. Vac. Sci. Technol., B14(3), (1996). The authors of the article are Pieter Kruit and Xinrong Jiang. For reading convenience, the equations, figures and pages in this article are renumbered in line with the order of this thesis.
seems inaccessible. Finally, by "fine tuning" the column, we try if any other combination of magnification, aperture size and source brightness can get the system to operate at a higher current or smaller probe size. From what we find, we deduce recommendations for the choice of operating conditions. For calculations we use the program ANALIC\(^3\), based on the equations of Jansen\(^1\) and Jiang et al\(^2\).

This is different from the usual approach that can be found in the literature, for instance in Ref.\([4,5,6,7,8,9]\): the influence of the Coulomb effects on a charged particle optical column is generally investigated by means of a Monte Carlo simulation. The latter usually offers a relation between the energy spread or the trajectory displacement and the beam current, but not an optimization of a column. To develop a comprehensive way to search how the Coulomb effects impact a microfocussed beam when the geometrical aberrations and the Coulomb effects are taken into account simultaneously, the authors recently considered the impact of the Coulomb effects on an optimized setting of a probe forming instrument, and introduced the concept of "danger area" in the I-d space\(^10\). In this paper, we further extend this approach by examining how sensitive the "danger area", which we now more appropriately call "inaccessible area", is to fine tuning of the column. The optimized I-d curves that we obtain resemble those presented by Venables et al\(^11\).

Although this paper is not meant as the thorough analysis of one particular column, but rather as a description of what we think is a good procedure to analyze and optimize any column, we can only do this by using an example column built in our laboratory.

### 7.2 Example column

Figure 7.1 shows this column consisting of two uni-potential lenses. A column with two lenses is in fact a very standard configuration, and many calculations have been performed for this kind of column by the Monte-Carlo approach\(^8\) or by the analysis of the lens aberrations\(^12\), \(^13\), \(^14\).

The fixed sizes of the column in figure 7.1 are the distance between the source tip and the first lens \(P_1\) (60 mm, also the object distance of the first lens), the distance between the first lens and the second lens \(L_{12}\) (160 mm) and the distance between the second lens and the target \(Q_2\) (40 mm, the image distance of the second lens). A gallium liquid metal ion source (GaLMIS) is used in this column and its reduced brightness \(B_1\) is typically \(2.10^6\) A.m\(^2\).sr\(^-1\).V\(^-1\). The fixed beam parameters are supposed to be the energy spread of the source \(\Delta E\) (5 eV, FWHM), the virtual source diameter \(d_0\) (50 nm) and the beam potential \(V\) (30 kV). The adjustable parameters of this column are chosen as the diameter of the first lens aperture \(D_1\), the total magnification of the column \(M\) (or the crossover position between the lenses) and the source brightness \(B_1\). We only consider a system with the beam limiting aperture in the first lens, or actually in the gun since we only calculate the interactions for a current in the column which is equal to the

![Fig. 7.1 A two uni-potential lens focussed ion beam column in Delft.](image)
probe current. This is usually not a practical reality. Typically, a fixed aperture is placed on the emitter side of lens 1 and a second aperture between the lenses. In that configuration, the Coulomb interactions can have a far more serious effect, especially at small probe sizes\textsuperscript{10,15}. Taking these apertures into account, however, would not change the analysis procedure, which is the subject of this paper.

The geometrical source image disc $d_{\text{Gau}}$, the spherical aberration disc $d_{\text{sph}}$ and the chromatic aberration disc $d_{\text{chr}}$ in the target plane in figure 7.1 are calculated respectively by

\begin{equation}
 d_{\text{Gau}} = M d_0 = M_1 M_2
\end{equation}

\begin{equation}
 d_{\text{sph}} = 0.177 \alpha_0^3 C_{\text{so1}} (1 + M_1^{-1})^4 M + C_{\text{so2}} (1 + M_2)^4 M^{-3}
\end{equation}

\begin{equation}
 d_{\text{chr}} = 0.34 \alpha_0 \Delta E [C_{\text{co1}} (1 + M_1^{-1})^2 M + C_{\text{co2}} (1 + M_2)^2 M^{-1}] / V
\end{equation}

\begin{equation}
 M_1 = M L_{12} (M P_1 + Q_2), \quad M_2 = (P_1 M + Q_2) / L_{12}
\end{equation}

where $\alpha_0$ is the half aperture angle at the object side of the first lens ($\alpha_0 = 0.5D_i / P_i$). $M_1$ and $M_2$ are the magnifications of the first lens and second lens respectively. For disc sizes, we use the FWHM value, that is the width of the spot containing 50% of the current. For a derivation of the numerical prefactors see Ref.[16]. In our calculation of the lens properties, the spherical and chromatic aberration coefficients are determined at the object side and in the infinite magnification case, i.e. $C_{\text{so1}} = C_{\text{so1}} (\infty, f_i)$, $C_{\text{so2}} = C_{\text{so2}} (\infty, f_i)$, $C_{\text{co1}} = C_{\text{co1}} (\infty, f_i)$ and $C_{\text{co2}} = C_{\text{co2}} (\infty, f_i)$. It is clear that, when the total magnification $M$ changes in figure 7.1, the focal distances $f_1$ and $f_2$ change as well, and because the aberration coefficients $C_{\text{so1}}$, $C_{\text{so2}}$, $C_{\text{co1}}$ and $C_{\text{co2}}$ change with $f_1$ and $f_2$, they also change with $M$. Our calculations show that the properties of the uni-potential lenses in figure 7.1 can be characterized by figure 7.2. Figure 7.2 is based on the original data of the spherical and chromatic aberration coefficients versus the focal distance of a uni-potential lens in Ref.[17].

### 7.3 Optimization without Coulomb interactions

In the optimization of the column in figure 7.1, the addition of different contributions to the total geometrical aberration disc $d_{\text{Gau}}$ is based on the method of Barth et al\textsuperscript{16}, i.e.
\[ d_{\text{g}a} = \left( (d_{\text{sp}}^3 + d_{\text{Gas}}^3)^{1/3} + d_{\text{chr}}^2 \right)^{1/2} = f_{\text{g}a}(M, D_1) \] (7.5)

After substituting equations (7.1), (7.2), (7.3) and (7.4) into equation (7.5), we can easily find that the total geometrical disc \( d_{\text{g}a} \) is a function of the aperture \( D_1 \) and the total magnification \( M \). This relation is shown in equation (7.5) and figure 7.3. The optimized setting of the column \( (M_{\text{opt}}, d_{\text{g}a_{\text{opt}}}) \) can be found from figure 7.3 for every aperture \( D_1 \). The beam current to the target I is determined by

\[ I = \frac{\pi^2}{16} B_r \left( \frac{d_1 D_1}{P_1} \right)^2 \] (7.6)

For the typical brightness of the usual GaLMIS \( B_r = 2.10^6 \) A.m\(^2\).sr\(^{-1}\).V\(^{-1}\), the relation between the current I and the minimum total geometrical disc \( d_{\text{g}a_{\text{opt}}} \) in figure 7.3 is indicated by the middle solid curve in figure 7.4. The detailed values at every optimized setting are listed in table 7.1 (see middle column).

When we look at the magnification \( M_{\text{opt}} \), for which we get the smallest total geometrical disc \( d_{\text{g}a_{\text{opt}}} \) at a given current I we find that it approximately becomes constant in the range of larger apertures \( D_1 \). The cause of this effect can be found in the contribution of the gun lens aberration: the geometrical image of the source becomes negligible compared to the gun lens aberration at large \( D_1 \) values. The optimized relation between the aberrations of the first and second lens does not change with \( D_1 \). The middle dashed curve in figure 7.4 is the I-\( d_{\text{g}a} \) relation at the constant magnification \( M = 0.8 \). Two other calculations are performed in the cases of low brightness \( B_r = 4.10^5 \) A.m\(^2\).sr\(^{-1}\).V\(^{-1}\) and high brightness \( B_r = 10^7 \) A.m\(^2\).sr\(^{-1}\).V\(^{-1}\), thereby acquiring the corresponding I-d relations shown in figure 7.4.

**Fig.7.3** Total geometrical aberration disc \( d_{\text{g}a} \) versus the total magnification of the column \( M \) at different apertures \( D_1 \).

**Fig.7.4** Relation between the beam current I and the total geometrical disc \( d_{\text{g}a} \), \( B_r = B_r \).
7.4. We realize that the liquid metal ion source can generally only be operated in a narrow range of source brightness. The low brightness value is under the usual operation threshold of the GaLMIS. The high brightness value, if obtainable at all, is accompanied by a large energy spread. We introduce these different brightness values for the sake of the argument. The optimized settings of $M$ and $D_1$ for the high and low brightness cases are also listed in table 7.1 (the middle column). We assume that $B_t$ is increased at constant virtual source size and at constant $\Delta E$.

It should be noted that figure 7.3 does not depend on the source brightness $B_t$. This means that the optimization of a column without including the Coulomb effects is independent of the brightness, and that the optimal l-d curves in figure 7.4 with different brightness are parallel. We also want to remind the reader that the advantage of a higher brightness source is so obvious that any possible increase of the brightness is worth fighting for. Unfortunately, when Coulomb effects occur in the column, matters are not so simple.

7.4 Influence of Coulomb effects

Usually, the spot discs due to the Coulomb effects include $d_{Boe}$, $d_{trm}$, $d_{loc}$ and $d_{sch}$, which, respectively, characterize the spot produced by the Boersch effect, the trajectory displacement effect, the space charge defocusing effect, and the space charge spherical aberration effect. $d_{Boe}$ is found through the chromatic aberration effect, for the column of figure 7.1, it is evaluated as

$$d_{Boe} = 0.34 \alpha_0 (\Delta E_{Li} C_{co1} (1 + M_1^{-1}) M + (\Delta E_{L1} + \Delta E_{L12}) C_{co2} (1 + M_2^{-1} M^{-1})) / V$$ (7.7)

where $\Delta E_{L1}$ is the energy broadening produced by the Boersch effect in the first section, and $\Delta E_{L12}$ the energy broadening in the section between the two lenses.

All those spot discs induced by the Coulomb effects are functions of the particle mass, the beam potential, the beam current and the shape of a beam segment (the opening angle, the length etc.). The addition of these spot discs, which are all supposed to be a measurement of FW50, results in the total Coulomb interaction effect disc $d_{tei}$. We define $d_{tei}$ in close similarity to $d_{iga}$ as

$$d_{tei} = \left[ \left( d_{sch}^4 + (d_{loc}^2 + d_{trm}^2)^{1.3/2} \right)^{2/1.3} + d_{Boe}^2 \right]^{1/2}$$ (7.8)

Therefore, $d_{tei}$ is a measurement of the influence of the total Coulomb interaction effect. The combined total FW50 size of the probe can be characterized by the total probe size $d_{tot}$. It is defined as

$$d_{tot} = \left[ \left( d_{sch}^4 + (d_{sch}^2 + d_{sch}^2)^{1.3/2} \right)^{2/1.3} + (d_{Boe} + d_{sch})^2 \right]^{1/2}$$ (7.9)

To give an indication of the dependency of $d_{Boe}$, $d_{trm}$, $d_{loc}$, $d_{sch}$, $d_{iga}$, $d_{tei}$ and $d_{tot}$ on the aperture $D_1$, and implicitly on the beam current $I$, we calculated these spot discs with the program Analytic for $M=0.8$ and the usual brightness of $B_t = 2.10^8$ A.m$^2$.sr$^{-1}$.V$^{-1}$ when the aperture $D_1$ changes from 0.05 mm to 0.9 mm. For every spot disc in equation (7.9), this program linearly adds all contributions from the four individual trapezoidal beam segments in figure 7.1, it then calculates the total spot sizes in terms of equations (7.5), (7.8) and (7.9) in the target plane of figure 7.1. Figure 7.5 shows the dependencies of seven spot discs on the aperture $D_1$. In the calculation of figure 7.5, we supposed that the beam current has a Gaussian spatial and angular distribution. The latter is of course not realistic if the beam is apertured, but if the current angular distribution is uniform, the space charge spherical aberration effect $d_{sch}$ is zero. In practice, most of the space charge defocusing effect can be corrected. For this reason, we only use an arbitrary fifteen percent of the defocusing for the
calculation of figure 7.5.

From figure 7.5 we learn that the Boersch effect disc $d_{\text{Boes}}$, the 15% of space charge defocusing disc $d_{\text{defo}}$, and the space charge spherical aberration disc $d_{\text{sph}}$, are much smaller than the trajectory displacement effect disc $d_{\text{tra}}$ and the total geometrical disc $d_{\text{g}}$. This means that the trajectory displacement effect dominates the Coulomb effects. We also learn that the trajectory displacement effect disc $d_{\text{tra}}$ is larger than the total geometrical disc $d_{\text{g}}$ in the intermediate aperture range.

The central question in our optimization is now: can we find an other combination of magnification, aperture size and source brightness, for which the Coulomb effects are less decremental to the performance of the column? One possible approach is to calculate the performance for all possible combinations of these three parameters and find the largest current at each particular probe size $d_{\text{sc}}$. However, we shall first try a simpler approach, following the reasoning that we recently presented. The argument is based on the consideration that for one required spot size, the optimized values of $M$ and $D_1$ do not depend on the source brightness as long as Coulomb effects are negligible. In that case we ask for each spot size and the related optimized configuration, how much beam current $I$, or how much source brightness $B_s$, is allowed before the Coulomb effects start to dominate the performance of the column. More precisely, we calculate the current $I$ for which $d_{\text{sc}} = d_{\text{gopt}}$ for the $(M_{\text{opt}}, D_1)$-combinations of figure 7.4 or table

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**Fig. 7.5** Seven spot discs in the target plane of figure 7.1 versus aperture $D_1$.

**Fig. 7.6** The inaccessible area of the column in figure 7.1, in which the Coulomb effects dominate, $B=B_s$.
7.1 The result is given in figure 7.6. The figure can be interpreted as indicating which current-spot size combinations can be obtained without worrying about Coulomb effects, and which (I-d) combinations can not be obtained without taking Coulomb effects into account. In fact, it seems that we cannot make the later (I-d) combinations at all, in other words: the shaded area seems inaccessible. At this point we must be cautious with too definite a conclusion: the area is only inaccessible when we stick to the (M, D₁) combinations that were found from an optimization that did not take the Coulomb effects into account.

7.5 Full optimization of the column

Our question now is: can we gain by choosing different magnification M, different aperture size D₁ and different source brightness Bₜ, than followed from the optimization without taking the Coulomb effects into account?

We calculated the total probe size dₜ (equation (7.9)) as a function of magnification M in three brightness value cases (high brightness Bₜ=10⁷, medium 2.10⁶ and low 4.10⁵ A.m².s⁻¹.V⁻¹) when the aperture D₁ changes from 0.05 mm to 0.9 mm. We determined the optimal magnification and spot size (Mₜₐₚ, dₜ opt) in a similar way as (Mₜₐₚ, dₜₐ opt) were found from figure 7.3 when no Coulomb effects were taken into account. With these optimal points, figure 7.7 was made, which represents the distribution map of the optimal working points of the column. Table 7.1 lists all values of the optimal working points of figure 7.7.

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Fig. 7.7 Distribution map of the optimal points of the column in figure 7.1. The dotted lines are identical with figure 7.4, figure 7.6 and table 7.1. The thick line is the inaccessible area border line.
For comparison the I-d relations (the dotted lines) of figure 7.4 and the inaccessible area border line in figure 7.6 are also indicated.

For the brightness values $B_r = 2 \times 10^6$ and $B = 10^7$ A.m$^2$.sr$^{-1}$.V$^{-1}$, we further calculated the total probe size $d_{ox}$ at the magnification with which the total geometrical disc $d_{gs}$ takes the minimum value $d_{gs\ opt}$. These calculations are shown in figure 7.8. The curves $m_1$ and $h_1$ give the I-d relation if no Coulomb effects are taken into account. The curves $m_2$ and $h_2$ give the I-d relation if $M$ and $D_1$ are fully optimized (last column in table 7.1) including Coulomb effects. The curves $m_3$ and $h_3$ give the I-d relation if $M$ and $D_1$ are taken from the optimization of figures 7.3 and 7.4, so as if Coulomb effects do not exist, but the probe size is calculated including the Coulomb effects. From figure 7.7, figure 7.8 and table 7.1, we find that:

a). when the Coulomb effects occur, the minimum probe size point moves to smaller magnifications (table 7.1).

b). in the intermediate apertures, the total probe size $d_{ox}$ ($m_3$ and $h_3$ curves in figure 7.8) at the magnification with which the total geometrical disc $d_{gs}$ takes the minimum value $d_{gs\ opt}$ is larger than the minimum total probe size $d_{ox\ opt}$. This shows that the full optimization including the Coulomb effects is particularly important in this area. The minimum total probe size $d_{ox\ opt}$ is much larger than the minimum total geometrical disc $d_{gs\ opt}$ at the same current level. This means that the parallel I-d relationships shown in figure 4 in different brightness cases do not exist any more when Coulomb effects occur, and that the probe size at the target expands sharply when the aperture $D_1$ runs into the intermediate sizes.

7.6 Discussion

We are now in a position to discuss the practical optimization of the operating parameters of ion beam columns in which Coulomb interaction effects influence the probe size. Of course, if a full theoretical analysis of the column is available, one can choose the theoretical parameters from a table

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Fig. 7.8 Comparison between different probe sizes in (1) medium brightness $B_r = 2 \times 10^6$ and (2) high brightness $B_r = 10^7$ A.m$^2$.sr$^{-1}$.V$^{-1}$.
like our table 7.1. However, this will not often be the case, and more over, one needs to know the brightness of the source for the choice of magnification and aperture size, but that brightness value is not an experimentally given parameter. So in a practical situation we recommend to first set the source to stable, high brightness operating conditions, then choose a beam current to work at (by inserting the appropriate aperture) and then minimize the spot size by varying the magnification. This procedure does not differ much from what is the established procedure in the absence of Coulomb interactions, however, the resulting magnification will now depend on the brightness of the source. Note that this procedure depends on the fact that the current does not change with magnification, which is only the case if the aperture is at the source side of the column. We have not analyzed what should be done if the aperture is in the final lens, because this is the wrong position if Coulomb effects occur. However, in a previous study on electron columns, we concluded that the sloping part at the right side of the inaccessible area border is not affected by a larger semi-angle, while the horizontal part drops to smaller I-values.

It is very difficult to first choose a spot size at which one wants to work and then tune the system for a maximum current, although for many applications this is the way one would want to work. However, from figures 7.7 and 7.8 it is clear that for bright sources, the gain in obtainable probe current is very limited when changing the probe size from 0.03 to 0.3 µm. This indicates that for the small probe sizes one can use the same aperture. This is very different from what has to be done for low brightness sources, in the absence of Coulomb interaction effects: changing the probe size by a factor of 10 can then lead to a gain in probe current by a factor of 50 to 500, the exact factor depending on which aberration, Cc or C*, dominates.

The inaccessible area shows clearly what the limitations of a column are. In order to get to I,d values inside that area the column design has to be changed. For small probe sizes it is advantageous to aperture the beam as closely to the source as possible. The effect of having a crossover in between lenses 1 and 2 is mainly caused by a different contribution of the aberrations, although the Coulomb interactions are also influenced. The design changes that have most effect are a shortening of the column and an increase of acceleration voltage. Figure 7.9 and figure 7.10 present these design considerations, which are all the full optimization results before (dmin) and after (dopt) the Coulomb interactions are taken into account. Figure 7.9 shows how the optimized probe sizes in the configuration of figure 7.1 change with the beam potential, assuming Cc and C* values independent of beam potential. Figure 7.10 presents three column designs. The column length in design 1 is P1=40 mm, L12=100 mm and Q2=25 mm, in design 2 P1=60 mm, L12=160 mm and Q2=40 mm (the same as figure 7.1), and in design 3 P1=90 mm, L12=240 mm and Q2=60 mm, using the same lenses characterized by figure 7.2. We see that shortening the column length or accelerating the beam
can decrease the Coulomb interactions, although these effects are obscured in figures 7.9 and 7.10 because the geometrical aberrations are also decreased. The latter is a result of using the same lenses in all calculations, while in practice one would have to adapt the lens design. A 0.1 μm probe size with about 1.0 nA current can be obtained by using both the 60 kV beam potential and the design 1 configuration.

The analysis in this paper is based on analytical equations for the interaction effects. The accuracy of the results is expected to be within 10 or 20%1, especially when the interaction effects are not yet very strong, that is in the low current regime. We did not calculate the interaction effects in the regime just in front of the ion source, before the first aperture. In fact, we assumed that the beam was apertured even there, and already accelerated to the final value. The motivation for neglecting this region is that the effects very close to the emitter are usually incorporated in the properties of the virtual source.

Our calculations are concerned with the full width-50% values of the current density distributions. For most application, this is the value of interest. However, Coulomb interaction effects can yield distributions with very long tails1, the precise distribution depending on the details of the beam properties. As a general rule, for the lower currents, these tails will be longer than for the higher currents, although even there we expect a Lorentzian distribution rather than a Gaussian distribution.

For our calculation at different brightness values, we assumed that the energy spread ΔE is always 5 eV. In a more realistic comparison of the effect of brightness increase, we would have to take into account that ΔE rises sharply with Bμ. In a chromatically limited probe one would maximize Bμ/ΔE2.

7.7 Conclusions

Without Coulomb effects, the optimum setting for aperture and magnification of a focussed ion beam column does not depend on the brightness of the source. For high currents, when the source lens aberrations have to be taken into account, the optimum value of the magnification approaches a constant, simplifying the operation considerably.

The influence of Coulomb effects on the performance of a column can be presented in a comprehensive way by indicating an inaccessible area in the probe current - probe size plane. The awareness alone of such an inaccessible area can save the operator of the instrument a considerable amount of time in trying to tune the system. In the presence of the Coulomb interactions it is advisable to position the beam limiting aperture as closely to the source as possible. Not only does this minimize the effects, it also simplifies the tuning of the column. Particularly for high brightness sources, it is important to tune the column with the aim to minimize the Coulomb effects. In general
one shall choose a smaller magnification of the source than in the absence of interactions.

If the aperture is in the gun, Coulomb effects do not limit the ultimate resolution of an ion beam column: at low currents, in our example column < 0.2 nA, they do not play a role. At probe sizes larger than a certain value, in our column > 1 \mu m, the effects are not a limiting factor either, mainly because the combined aberrations of the source lens and the probe lens have increased the probe size to a level where other effects are invisible.

Acknowledgement

The authors thank Dr. J.E. Barth, Ir. E. Koets and Dr. Ir. C.W. Hagen for their beneficial discussions.

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8 Comparison between different imaging modes in focussed ion beam instruments

Abstract  In a two-lens focussed ion beam instrument, one can choose to either have a crossover in between the lenses or not. For a representative instrument, it is shown that the optimized probe size of the non-crossover mode is smaller than that of the crossover mode. Both the lens aberrations and the statistical Coulomb effects are responsible for this effect. We analyzed the differences for a large range of beam currents and found that in the absence of statistical Coulomb interactions, the difference can be as much as a factor 1.6. In the presence of Coulomb interactions, the difference increases to a factor 1.8.

8.1. Introduction

Lens aberrations and statistical Coulomb interactions play an important role in focussed ion beam instruments used for mask repair or subsurface structure analysis. A focussed ion beam instrument contains an optical column consisting of lenses and apertures. In our previous investigations of the Coulomb interactions in particle optical columns\textsuperscript{1,2}, we concluded that Coulomb interactions can seriously limit the performance of focussed ion beam systems, more so if they are equipped with high brightness sources. The specific problem we want to address in this paper is the following: which mode in figure 8.1 is best from the smallest probe size point of view? In other words: is the presence of an intermediate crossover deteriorating the performance, or perhaps even solely responsible for the statistical Coulomb effects?

Ref.\textsuperscript{[3]} reported the use of the divergent imaging mode of figure 8.1.(b) in a low voltage scanning electron microscope, but no evaluations were presented. Ref.\textsuperscript{[4,5,6]} investigated different imaging modes with the calculation of the geometrical aberrations in focussed ion beam columns, but the Coulomb interactions in these imaging modes were not included. Ref.\textsuperscript{[7]} and Ref.\textsuperscript{[8]} respectively computed the Coulomb effects in the cylindrical mode of figure 8.1(c) and the divergent mode of figure 8.1(b) with a Monte Carlo simulation, but magnification and aperture size were not varied in order to compare optimized results.

The approach in this paper is to compare the optimized beam current-probe size (I-d) relations in different imaging modes, where we include the probe broadening caused by statistical Coulomb interactions.

The investigation is based on a practical focussed ion beam column built in our laboratory, as shown in figure 8.1. For practical calculations, we assume that 1) the column is a two uni-potential lens column with the aperture D\textsubscript{1} in the first lens. In fact we assume the current to be limited right from the source, in order to find the "best case" values for the Coulomb effects. The beam potential is 15 kV, and the column fixed sizes are P\textsubscript{1}=60 mm, L=160 mm and Q\textsubscript{2}=40 mm, 2) a gallium liquid metal ion source is used and its reduced brightness is assumed to be B=2.10\textsuperscript{6} A.m\textsuperscript{2}.sr\textsuperscript{-1}.V\textsuperscript{-1},

** This chapter is a complete article published in Microelectronic Engineering 30, 249-252(1996). The authors of the article are Xinrong Jiang and Pieter Kruit. For reading convenience, the figures and pages in this article are renumbered in line with the order of this thesis.
the energy spread of the source \( \Delta E = 5 \) eV (FWHM), and the virtual source diameter \( d_0 = 50 \) nm, and 3) the chromatic and spherical aberrations of the lenses depend on the strength of the lenses and thus change with the chosen mode and the magnification. When the imaging mode and the magnification \( M \) are determined, we can obtain the focal distances \( f_1 \) and \( f_2 \). With \( f_1 \) and \( f_2 \), the geometric aberration coefficients at the object-side and in the infinite magnification case \( C_{\text{sol}}(f_1, M = \infty) = C_{\text{cos}}(f_1, \infty), C_{\text{sol}}(f_2, \infty) \) and \( C_{\text{cos}}(f_2, \infty) \) can be evaluated following the approach described in Ref.[2].

All evaluations including both the lens aberrations and the Coulomb effect aberrations are performed with the full width 50% values of the current density distributions (FW50) in this paper. We only take the statistical Coulomb effects (the trajectory displacement effect disc \( d_{\text{ta}} \) and the Boersch effect disc \( d_{\text{bo}} \)) into account, ignoring the space charge aberrations (the space charge defocussing disc \( d_{\text{sc}} \) and the space charge spherical aberration disc \( d_{\text{sca}} \))\(^2\). We consider the case in which the angular distribution of the current density is uniform, such that the space charge spherical aberration disc \( d_{\text{sca}} \) is zero\(^3\). We further assume that the space charge defocussing is totally corrected, causing the defocussing disc \( d_{\text{sc}} \) to be zero.

The program ANALIC\(^1\) is used to calculate the total geometric aberration disc \( d_{\text{tg}} \) without including the Coulomb effects and the total probe size \( d_{\text{tot}} \) with inclusion of the Coulomb effects at the targets of the different modes in figure 8.1 when the aperture size \( D_1 \) and the magnification \( M \) change simultaneously. The equations used in the calculation of the probe sizes \( d_{\text{tg}} \) and \( d_{\text{tot}} \) are presented in Ref.[2,9].

8.2. I-d relations in different modes

For the crossover mode of figure 8.1(a), it is shown in figure 8.2(a) and figure 8.2(b) how the total geometric disc \( d_{\text{tg}} \) and the total probe size \( d_{\text{tot}} \) vary with the aperture size \( D_1 \) and magnification \( M \) respectively. For all magnifications \( M \) (from 0.1 to 10), \( d_{\text{tg}} \) and \( d_{\text{tot}} \) increase with the aperture size \( D_1 \) (from 0.01 to 1.0 mm), or with the beam current \( I \). For each aperture size \( D_1 \), the dependencies of \( d_{\text{tg}} \) and \( d_{\text{tot}} \) on the magnification \( M \) display a minimum. The minimum probe size \( d_{\text{tg}} \) or \( d_{\text{tot}} \) opt.
is found at the optimal magnification $M_{opt}$. It is noted that the surface of $d_{tot}$ lies above that of $d_{ga}$ because of the statistical Coulomb interactions, especially in the intermediate aperture ranges.

For the non-crossover modes in figures 8.1(b), (c) and (d), the beam imaging relations depend on the magnification $M$. Figure 8.1(b) and figure 8.1(d) show that a divergent beam and a convergent beam appears between the lenses when the magnification $M$ changes from $Q_2/(L+P_1)$ to $Q_2/P_1$ and from $Q_2/P_1$ to $(L+Q_2)/P_1$, respectively. When $M=Q_2/P_1=f_2/f_1$, the beam between the lenses is a cylindrical beam. For the same reasons as for the crossover imaging mode, the total geometric disc $d_{ga}$ and the total probe size $d_{tot}$ of the non-crossover modes are functions of the aperture size $D_1$ and the magnification $M$, as shown in figure 8.3.

In figure 8.3, the change of the aperture size $D_1$ (or the beam current $I$) is identical to that of figure 8.2, but the magnification $M$ is taken in the range from $M=0.2$ to 2.0 according to the fixed distances $P_1$, $L$ and $Q_2$. When $0.2 < M < 2/3$, $M=2/3$ and $2/3 < M < 2$, figure 8.3 corresponds to the imaging modes in figures 8.1(b), (c) and (d), respectively. From figure 8.3, one can also find a minimum probe size $d_{ga_{opt}}$ or $d_{tot_{opt}}$ at an optimal magnification $M_{opt}$ for every aperture size $D_1$ (or every beam current $I$). Accordingly, from figure 8.2 and figure 8.3, we can determine the dependence of the beam current $I$ on the minimum probe size $d$ (I-d relation) for different imaging modes. Figure 8.4 shows four I-d relations: $I-d_{ga_{opt}}$ and $I-d_{tot_{opt}}$ relations in the crossover and non-crossover modes, respectively. From figure 8.4 it is concluded that 1) no matter whether the statistical Coulomb effects are included or not, the minimum probe size in the non-crossover modes is less than that of the crossover mode over the full current range, and 2) the impact of the statistical Coulomb effects on the non-crossover modes is less than that on the crossover mode. Since the deflection error of a ray in a lens is proportional to the deflection and the lens deflections in the crossover mode are always greater than in the non-crossover mode for the same total magnification, the shift of the I-d curves to larger $d$ values is to be expected. For a discussion of the difference in the trajectory displacement for the two modes see Ref. [10]. For instance, the minimum total geometric disc $d_{ga}$ in the crossover mode is 1.6 times greater than in the non-crossover mode at a current of 3.0 nA. Including Coulomb effects, the minimum total probe size $d_{tot}$ in the crossover mode is 1.8 times greater than in the non-crossover mode at the same current.

The shape of the I-d curve follows from the differing dependencies of the individual contributions
to d on D$_1$ (or I) and M. The source image size d$_{gam}$ is decreased by decreasing M. The trajectory displacement effect disc d$_{tr}$ increases with current and decreases with M. The chromatic aberration contribution increases with current via the Boersch effect. Because decreasing M requires increasing the lens deflections, d$_{chr}$ and d$_{sph}$ will increase with decreasing M. The minimum probe size is obtained when the magnification balances the contributions decreasing or increasing with decreasing M. The I-d dependencies of the individual contributions at optimum magnification for minimum total probe size are shown in figure 8.5. We see that d$_{tr}$ becomes more important than d$_{gam}$ when the current I > 0.2 nA. When I > 2 nA d$_{sph}$, which increases as D$_1^3$, becomes more important than d$_{chr}$ which increases linearly with D$_1$. The spherical aberration dominates the probe size for the largest D$_1$ (I > 5 nA). Here the magnification balance is between the spherical aberration contributions of the first and second lens.

8.3. Conclusions

The optimized probe size of the non-crossover modes is smaller than that of the crossover mode of a focussed ion beam instrument over the full current range. The optimal results show that the minimum probe sizes of the crossover mode are 1.6 and 1.8 times greater at the current 3.0 nA than those of the non-crossover modes of a practical focussed ion beam instrument before and after the statistical Coulomb effects are considered respectively. Our further investigations show that this conclusion is valid for different beam energies and source brightness values and that it is also applicable to the case of electron beam instruments.

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References

Intermediate aperture effect in charged particle optical instruments

Abstract A new particle optical phenomenon, the intermediate aperture effect, which influences the performance of charged particle optical instruments, is described in this chapter. The intermediate aperture effect is considered as a fact that in a particle optical column the Coulomb interaction aberrations dominate over lens aberrations in a special region. For a general particle optical column, the intermediate aperture effect is best characterized by pointing out a danger area, which is a combination set of the aperture size and magnification. However, in the case of an optimized particle optical column, the intermediate aperture effect is found in an intermediate aperture range. These relationships are analyzed in this chapter both for the general particle optical column and for practical electron and ion beam instruments. Finally, the essential grounds how the intermediate aperture effect occurs in a particle optical column are investigated for pointing out the approaches of people getting away from this effect in order to enhance the resolution of charged particle optical instruments.

9.1 Introduction

When performing a full evaluation for a charged particle optical column, which includes the calculation of lens aberrations and Coulomb interaction aberrations, one can find a new particle optical phenomenon: only in a special region, do the Coulomb interactions between particles dominate the column. Out of this region, however, the lens aberrations absolutely dominate over the Coulomb interactions, thereby the impact of the Coulomb interactions on an optical column can practically being ignored.

The fact that occurs in this special region is referred to as an intermediate aperture effect. We have already met the intermediate aperture effect many times, for instance in figures 7.5, 7.6, 7.9, 7.10, 8.4 and so on of this thesis. This implies that the intermediate aperture effect is in fact a general particle optical phenomenon. The purpose that we investigate the intermediate aperture effect is that we can clearly understand its characteristics and stay away from this effect when we design or operate at a particle optical system.

Only few reports deal with the intermediate aperture effect. Ref.[1,2] noted the calculation of an inaccessible area, but that is a part of expressions of the intermediate aperture effect, not the essence of this effect. The intermediate aperture effect can be described by different manners. Ref.[3] evaluated the probe current I - probe size d relations for different imaging modes of a practical optical system and found that the intermediate aperture range is important. However, this range is also one of expressions of the intermediate aperture effect.

We describe the intermediate aperture effect in this chapter by means of the concepts of a danger area and an intermediate aperture range. For a general particle optical column, the danger area clearly points out where the intermediate aperture effect occurs. However, for an optimized particle optical column, the intermediate aperture range indicates how the intermediate aperture effect plays a role. The former description will be found simpler than the latter.

We try to research into the intermediate aperture effect for general particle optical columns. But for quantitative calculations we can only take practical columns for examples. Accordingly, three different particle optical columns will be investigated. In the last section of this chapter, we shall
look into the essence why the intermediate aperture effect occurs in a particle optical instrument.

We shall again use ANALIC program\(^{4,5}\) to perform all quantitative calculations for different example optical columns in order to further check the capabilities of the program in the use of solving different problems.

9.2 General column and example columns

We restrict ourselves to observe the intermediate aperture effect of a focussed particle optical column in the target plane.

A charged particle optical system model is already described in figure 2.5 and calculated in chapter 6. No matter how complicated or simple a focussed particle optical column may be, what one is most interested in is the properties of the probe. The total magnification of a column M, the probe size at the target d and the beam current to the target I are normally used to best characterize the probe properties. Accordingly, in this chapter we shall evaluate the intermediate aperture effect by means of the important parameters M, d and I. One example column of the general optical system in figure 2.5 is shown in figure 9.1, which is a four lens column found in an electron beam pattern generator. The source is a cold field emitter with a reduced brightness \(B=10^8\) A.m\(^2\).sr\(^{-1}\).V\(^{-1}\), a source virtual diameter \(d_0=30\) nm and an energy spread \(\Delta E=0.2\) eV (FWHM). The beam potential \(V\) is 7.5 kV in the object-side of the first lens, and 30 kV in others. The first and the third crossover positions of the column are always fixed at 270 mm and 470 mm, while the second crossover position is moved in between the second lens and the third lens for adjusting the total magnification of the column M. The magnifications of the first lens and the fourth lens are \(M_1=4\) and \(M_4=0.25\). The aberration coefficients (\(C_4\) and \(C_5\), i=1,2,3,4) are defined at the object-side and in the case of the infinite magnification, where \(C_{4i}=16.5\) mm, \(C_{5i}=12.8\) mm, \(C_{6i}=380\) mm and \(C_{7i}=57\) mm. \(C_2\), \(C_3\), \(C_5\) and \(C_6\) are supposed to be zero for simplifying the calculation of the geometrical aberrations. This does not influence the conclusion of this chapter. Besides, we shall further investigate the intermediate aperture effect in a two lens focussed ion beam column and a three lens focussed electron beam column. These practical optical columns can all be included in the model of the general optical system in figure 2.5.

If we consider the general optical column in figure 2.5 as the system of a black box, the input signals of this system are \(d_0\) and \(I_{in}\), and the output signals \(d\) and \(I_{out}\). Here, \(d\) represents one of the eleven spot sizes shown in figure 2.5. The input current \(I_{in}\) is determined by

\[
I_{in}=(\pi d_0 \alpha_0/2)^2 B V_{1i}
\]

(9.1)

where \(d_0\) is the virtual source diameter, B the source reduced brightness and \(\alpha_0\) the half opening angle at the virtual source (see Eq.(2.4)). The output current \(I_{out}\) is limited by system apertures, and the spot sizes at the target \(d\) by lens aberrations and Coulomb effects. Our investigation is concentrated on the output of the system, i.e. the relation between the output current \(I_{out}\) and the spot sizes \(d\). We shall simply write \(I_{out}\)

\[
\text{Fig.9.1 An electron beam pattern generator column with four lenses and three crossovers.}
\]

93
as I in the rest of the chapter without declaring it any more.

9.3 Intermediate aperture effect

9.3.1 Danger area of an optical column

It was pointed out in chapter 5 that all spot discs at the target are the functions of the current I and magnification M when a particle optical system operates at a stable state, i.e. the source parameters \(d_0, \Delta E, B, m\) as well as the column configuration and its geometrical parameters are all determined. In a coordinate system, variables \((d, I, M)\) constitute a curved surface, and the surface function is determined by

\[
d = q(I, M)
\]  

(9.2)

Among the eleven spot discs in figure 2.5, we choose the total geometrical aberration disc \(d_{ga}\) and the total Coulomb interaction disc \(d_{ci}\) to look into the dependencies of them on the magnification M and current I. The surface functions of variables \((d_{ga}, I, M)\) and variables \((d_{ci}, I, M)\) are respectively defined as

\[
d_{ga} = f(I, M)
\]  

(9.3)

and

\[
d_{ci} = F(I, M)
\]  

(9.4)

where \(f\) and \(F\) express the surface functions of the total geometrical aberration disc \(d_{ga}\) and the total Coulomb interaction disc \(d_{ci}\). These functions are determined by Eq.(5.42) and Eq.(5.43) (or Eq.(5.45) and Eq.(5.46)). For the example column of figure 9.1, the dependencies of the \(d_{ga}\) and \(d_{ci}\) on the magnification M and current I were calculated with ANALIC program, as shown in figure 9.2(1) and figure 9.2(2). In the calculation of figure 9.2, the aperture sizes \(D_2, D_3\) and \(D_4\) in figure 9.1 are supposed to be so large that the apertures do not cut the current when the aperture size \(D_1\) (or the current I) changes from 0.03 mm (0.4164 nA) to 3 mm (4164 nA). The total magnification M varies from 0.1 to 10 with the moving of the crossover position in between the second lens and third lens. All spot discs which constitute \(d_{ga}\) and \(d_{ci}\) in

Fig.9.2 The dependencies of the total geometrical aberration disc \(d_{ga}\) (1) and the total Coulomb interaction disc \(d_{ci}\) (2) on the current I and magnification M.
terms of Eq.(5.42) and Eq.(5.43) were evaluated with the FW50 measurement method\textsuperscript{1,6}. 15\% of the space charge defocussing aberration is considered in the addition of $d_{\text{ui}}$ (see Eq.(5.43)). The current density is assumed as Gaussian spatial distribution and uniform angular distribution (i.e. KK=10).

We learn from figure 9.2(2) that the Coulomb interactions really play a role in the optical column of the electron beam instrument. In the region of larger magnifications and aperture sizes, the total Coulomb interaction disc $d_{\text{ui}}$ can be larger than the total geometrical aberration disc $d_{\text{qa}}$. Accordingly, we meet here a question: In which combinations of the aperture size $D_{i}$ (the current $I$) and the magnification $M$ of the electron beam column, is the total Coulomb interaction disc $d_{\text{ui}}$ larger than the total geometrical aberration disc $d_{\text{qa}}$?

To find these combinations we are forced to solve the spatial crossing curve between the surface $d_{\text{qa}}$ and surface $d_{\text{ui}}$. In terms of Eqs.(9.3) and (9.4) this crossing curve is determined by

$$f(I,M)-F(I,M)=0 \quad \text{and} \quad d_{\text{qa}}=f(I,M) \quad (9.5)$$

For the example column of figure 9.1, the crossing curve given by Eq.(9.5) was solved, as the thick line shown in figure 9.2.(1). The identical curve to Eq.(9.5) can also be given by

$$f(I,M)-F(I,M)=0 \quad \text{and} \quad d_{\text{ui}}=F(I,M) \quad (9.6)$$

This crossing curve is indicated by the thick line of figure 9.2(2). Looking at the area surrounded by the crossing curves in figure 9.2(1) and figure 9.2(2), we find that inside the area the total Coulomb interaction disc $d_{\text{ui}}$ is much larger than the total geometrical aberration disc $d_{\text{qa}}$. This means that in this region the Coulomb interactions in fact dominate the resolution of the electron beam instrument.

Figure 9.3 shows the spatial crossing curve in figure 9.2 and its projections in M-I plane, d-M plane and d-I plane. These projection curves in three planes are respectively determined by

$$f(I,M)-F(I,M)=0 \quad \text{(in M-I plane)} \quad (9.7)$$

$$f [f_{i}^{-1}(d_{\text{qa}},M),M]-F [f_{i}^{-1}(d_{\text{qa}},M),M]=0 \quad \text{(in d-M plane)} \quad (9.8)$$

$$f [I f_{M}^{-1}(d_{\text{qa}},I)]=F [I f_{M}^{-1}(d_{\text{qa}},I)]=0 \quad \text{(in d-I plane)} \quad (9.9)$$

where $f_{i}^{-1}$ and $f_{M}^{-1}$ express the inverse functions of the function $f$ defined by Eq.(9.3) with respect to
I and M respectively.

The projection curve in (I,M) plane indicates the combinations of the current I and magnification M with which the Coulomb interaction aberrations dominate over the lens aberrations. Accordingly, the area surrounded by the curve determined by Eq.(9.7) is defined as a danger area. Inside the area the total Coulomb interaction disc $d_{\text{Coul}}$ is much larger than the total geometrical aberration disc $d_{\text{GA}}$, out of which, however, the lens aberrations dominate the column and the influence of the Coulomb interactions on the column is relatively slight.

Another important fact is that the total geometrical aberration disc $d_{\text{GA}}$ is independent of the source reduced brightness B, however, the total Coulomb interaction disc $d_{\text{Coul}}$ increases with the brightness B rapidly. Accordingly, it can be easily imagined from figure 9.2 that the higher the source brightness, the larger the danger area of an optical column will be. To quantitatively investigate this problem, two new spatial crossing curves were calculated based on the column of figure 9.1. Figure 9.4 shows the projections of these spatial crossing curves in M-I plane and d-I plane.

These curves were calculated in the cases of the high brightness $B=5 \times 10^8 \text{ A.m}^2\text{sr}^{-1}\text{V}^{-1}$, the medium brightness $B=10^8 \text{ A.m}^2\text{sr}^{-1}\text{V}^{-1}$ and the low brightness $B=4 \times 10^7 \text{ A.m}^2\text{sr}^{-1}\text{V}^{-1}$. The danger area calculated with the medium brightness in figure 9.4 is identical to that in figure 9.3. It can be seen that the danger area is small when the brightness only decreases 2.5 times compared to the case of the medium brightness, however, the danger area becomes very large when the brightness increases 5 times. It can also be found that the sharp change of the danger area in different brightness values occurs in the regions of the smaller magnification and higher current. In the regions of the lower currents or larger magnifications, the danger area changes slightly with the different source brightness values.

The danger area can also be found in the optical column of a focussed ion beam instrument. Taking the gallium ion beam column in figure 7.1 for example, we calculated the danger areas in different beam potentials and different source brightness values, as shown in figure 9.5. The calculation conditions of figure 9.5 are the same as those in chapter 7. Figure 9.5 shows that the danger area moves to the lower current region when the beam potential decreases, however, the danger area extends to the smaller magnification and the higher current range when the source brightness increases. This means that the best approach of staying away from the danger area is to increase the

Fig.9.4 Influence of the source brightness on the danger area of a particle optical column.
beam energy, instead, to increase the brightness of the source.

### 9.3.2 Intermediate aperture range

The danger area of an optical column shows the combination of the aperture size and magnification with which the Coulomb interactions dominate the aberrations of the column. However, a particle optical column is usually optimized in practice. From figure 9.2(1) and figure 7.3, we learn that, no matter whether in an electron beam column or ion beam column, we can find a minimum total geometrical aberration disc at the optimum magnification in the case of different aperture sizes (or different beam currents). This fact leads us to find a special aperture range to evaluate the impact of the Coulomb interactions on an optimized particle optical column. We shall call this special range the intermediate aperture range.

In the curved surface of the total geometrical aberration disc $d_{ga}$, which is defined as Eq.(9.3), all optimum points $(d_{ga\text{ opt}}, l_{opt}, M_{opt})$ constitute an optimum spatial curve determined by

$$d_{ga\text{ opt}}=f(l_{opt}, M_{opt}) \quad (9.10)$$

where $(l_{opt}, M_{opt})$ indicates the optimum combination of the aperture size and magnification with which the total geometrical aberration disc $d_{ga}$ is a minimum value $d_{ga\text{ opt}}$. From the optical point of view, Eq.(9.10) only denotes a curve, not a surface, because for every beam current $l_{opt}$ there are only one optimum magnification $M_{opt}$ and one minimum total geometrical aberration disc $d_{ga\text{ opt}}$. For the example of figure 9.2(1), the optimum curve defined by Eq.(9.10) really exists, as shown in figure 9.6 (see curve 1-1). The projection curve 1'-1' of the spatial curve 1-1 in I-d plane is just the I-d relation curve, which was many times discussed in chapters 6, 7 and 8.

For the impact of the Coulomb interactions on a particle optical column, we consider such a ques-
tion: What is the obtainable beam current \( I \) when the total Coulomb interaction disc \( d_{ci} \) reaches at the minimum total geometrical aberration disc \( d_{ga_{opt}} \) for every optimum magnification \( M_{opt} \)? This question can be expressed as

\[
I = F_1^{-1}(d_{ga_{opt}}, M_{opt}) \tag{9.11}
\]

The solution of Eq.(9.11) is also a spatial curve because for every optimum magnification \( M_{opt} \), there is only one minimum total geometrical aberration disc \( d_{ga_{opt}} \) (see figure 9.2(1)). Taking the column of figure 9.1 for example again, Eq.(9.11) was calculated, and is indicated in figure 9.6 (see curve 2-2). The projection of the curve 2-2 in the I-d plane is the curve 2'-2'. It can be found that the curve 1-1 and curve 2-2 have two spatial crossing points A and B. The projection of points A and B in the I-d plane is points A' and B', and the projection of points A' and B' on the I-axis is points A'' and B''. The shaded area in figure 9.6 is the inaccessible area, and the curve 2'-2' the border line of the inaccessible area.

2'-2' curve can now be understood as the I-d relation between the beam current I and the total Coulomb interaction disc \( d_{ci} \) in the case of the optimum magnification \( M_{opt} \). It can be seen that only when the current is higher than \( I_A \) (40 nA), but lower than \( I_B \) (1200 nA), is the total Coulomb interaction disc \( d_{ci} \) larger than the minimum total geometrical aberration disc \( d_{ga_{opt}} \). On basis of Eq.(9.1), the aperture sizes \( D_{1A} \) and \( D_{1B} \) of the first lens can be calculated when the currents I are equal to \( I_A \) and \( I_B \), respectively, i.e. \( D_{1A} = 0.294 \) mm and \( D_{1B} = 1.611 \) mm.

For a general particle optical column defined in figure 2.5, the similar curves and crossing points to those in figure 9.6 can be found in principle. Accordingly, for a general optimized particle optical column we define the aperture size range from \( D_{1A} \) to \( D_{1B} \) as the intermediate aperture range, and the current range from \( I_A \) to \( I_B \) as the intermediate current range.

Note that for an optimized particle optical column the intermediate aperture range is a minimum aperture range in which the Coulomb interactions dominate the optimized optical column, but out of which the impact of the Coulomb interactions on the column can be ignored. There is only one intermediate aperture range for a particle optical column.

When a particle optical column operates at different source brightness values or different beam potentials, the intermediate aperture ranges are different. Moving the curves 1'-1' and 2'-2' in figure 9.6 to figure 9.7, we can look into this problem in detail.

All curves in figure 9.7, including the curves 1'-1' and 2'-2', were calculated with the same conditions as figure 9.2 based on the electron beam column of figure 9.1. Figure 9.7 shows four I-\( d_{ga_{opt}} \) relations (between the current I and minimum total geometrical aberration disc \( d_{ga_{opt}} \)) in four brightness cases (\( B = 5 \times 10^8, 10^9, 4 \times 10^7 \) and \( 2 \times 10^7 \) A.m².sr⁻¹.V⁻¹). For an optimized particle optical column there is only one inaccessible area border line even though this column operates at different brightness values. This also means that for every source brightness the inaccessible area of the opti-
mized optical column is the same. The reason is that the minimum total geometrical aberration disc \( d_{gs, \text{opt}} \) and the optimal magnification \( M_{\text{opt}} \) in Eq. (9.11) are independent of the source brightness \( B \). Figure 9.7 clearly indicates that the higher the source brightness the larger the intermediate aperture range will be. When the brightness \( B = 2.5 \times 10^7 \text{ A.m}^{-2}.\text{sr}^{-1}.\text{V}^{-1} \), the \( I-d_{gs, \text{opt}} \) curve is tangential to the inaccessible area border line and the intermediate aperture range is equal to zero. Accordingly, there is no intermediate aperture range in the case of brightness \( B = 2 \times 10^7 \text{ A.m}^{-2}.\text{sr}^{-1}.\text{V}^{-1} \).

9.3.3 Definition of the intermediate aperture effect

We are now able to define the intermediate aperture effect. The intermediate aperture effect is considered as a particle optical phenomenon, in which the impact of the Coulomb interactions between particles is stronger than that of the lens aberrations on a particle optical column when the column operates at a danger area or an intermediate aperture range.

For a general particle optical column, the danger area best characterizes the aperture and magnification combinations, in which the intermediate aperture effect occurs. However, for an optimized particle optical column, the intermediate aperture range clearly shows where the intermediate aperture effect occurs. Accordingly, the intermediate aperture effect is directly related to the concept of the danger area or the intermediate aperture range. If the danger area or the intermediate aperture range is found to be zero, we can conclude that there is no intermediate aperture effect in a particle optical column.

9.4 Influence of aperture position on intermediate aperture effect

We now consider a different situation for a further investigation on the intermediate aperture effect. In the general particle optical column of figure 2.5, suppose that the changing aperture is the last one \( D_m \) instead of the first \( D_1 \). The first aperture size is fixed in this case. Figure 9.8 presents an example column of this kind of particle optical instruments.

Figure 9.8 shows a focussed electron beam optical column with three lenses and two apertures. The first aperture size \( D_1 \) is fixed, and the third (last) aperture size \( D_3 \) adjustable, thereby the current to the target \( I \) being a variable. The second crossover position is fixed at 280 mm, but the first crossover position can be moved along the axis, thereby the total magnification of the column \( M \) being another variable. Therefore, the total geometrical aberration disc \( d_{gs} \) and the total Coulomb interaction disc \( d_{ci} \) at the target can be again expressed as Eq. (9.3) and Eq. (9.4).

The beam potential at the object-side of the first lens is 7.5 kV, the others are all 50 kV. The geometrical aberration coefficients \( C_i \) and \( C_c \) are defined at the object-side and in the case of the infinite magnification, here, \( C_{i1} = 70 \text{ mm}, C_{i2} = 66 \text{ mm}, C_{c1} = C_{c2} = 0, C_{c3} = 79 \text{ mm} \) and \( C_{c3} = 32 \text{ mm} \). The column of figure 9.8 is different from the columns in figure 9.1 and figure 7.1 because only the first aperture plays a role in the latter columns. The focussed electron beam is cut by both the first aperture and the last aperture in the column of figure 9.8. Accordingly, the calculations for the lens aberrations and for the Coulomb interactions in this column are different. The narrow (the shaded) focussed beam is used to evaluate the lens aberrations, and the wide (real) beam is for the calculation of the Coulomb interactions. When the magnification \( M \) and aperture size \( D_3 \) change simultaneously, the two beam shapes may be very different.

The ANALIC program\(^5\) is again used to calculate the total geometrical aberration disc surface \( d_{gs} = f(I, M) \) and the total Coulomb interaction disc surface \( d_{ci} = F(I, M) \) for the column of figure 9.8. The results are presented in figure 9.9. Note that the current \( I \) in figure 9.9 is the current to the tar-
get. For every magnification M, the maximum third aperture size is determined by

$$D_{3\text{max}} = \frac{Q_0 D_1}{P_1 M} \sqrt{\frac{V_{11}}{V_{32}}} \quad (9.12)$$

This means that for every magnification M the maximum current to the target I_{out,max} is equal to the input current of the column I_{in}. It is meaningless that the aperture size D_3 is larger than D_{3\text{max}} in this investigation. Accordingly, the changing range of the variable D_3 is supposed to be less than D_{3\text{max}}. Figure 9.9 was calculated at D_3=1 mm. Figure 9.9(1) is similar to figure 9.2 (1), however, figure 9.9(2) is very different from figure 9.2(2). In the case of larger magnifications the total Coulomb interaction disc d_{cli} increases with the magnification M, almost being independent of the aperture size D_3. The reason of this effect is that, compared to the contribution of the beam segments from the tip to the third lens, the contribution to the total Coulomb interaction disc d_{cli} from the last beam segment is so small that it can be ignored. In the larger demagnification case, d_{cli} increases with the beam current I, because the total Coulomb interaction disc in the beam segments of front of the last lens is demagnified, and the contribution to d_{cli} from the last beam segment plays a role. For every beam current I, there is a minimum total geometrical aberration disc d_{ga opt} and a minimum total Coulomb interaction disc d_{cli opt}, but their optimum magnifications are different.

There is a spatial crossing curve between the surfaces d_{ga}=f(I,M) in figure 9.9(1) and d_{cli}=F(I,M) in figure 9.9(2). This crossing curve has been calculated, as shown in figure 9.9(1) and figure 9.9(2) (see the thick curves). This crossing curve is also very different from that in figure 9.2. Accordingly, the characteristics of a particle optical column with an adjustable last aperture are different from those with an adjustable first aperture. In order to look into these differences in detail the crossing curve in figure 9.9 is moved to figure 9.10 (see the thick and unenclosed spatial curve) for the comparisons.

For the three lens electron beam column of figure 9.8, we also calculated the total geometrical aberration disc surface d_{ga} and the total Coulomb interaction disc surface d_{cli} when the first aperture size D_1 is considered as one of the variables and the last aperture size D_3 is assumed to be large enough without cutting any current. In this case, the spatial crossing curve between the d_{ga} surface and d_{cli} surface is obtained, as shown in figure 9.10 (see the thick and closed spatial curve).

Figure 9.10 also indicates the projections of the two different spatial crossing curves in three planes. In the I-M plane we find the danger areas for the two different working modes of the electron beam column in figure 9.8: One is that the first aperture D_1 changes, but the last aperture D_3 opens, and the other is that the last aperture D_3 changes, but the first aperture is fixed at D_1=1 mm. In the former case, the danger area is very small. This means that the Coulomb interactions dominate the column only for very limited combination of the current and magnification, instead, the lens aberrations in fact dominate the column for most of combination of the current and magnification. Another important characteristic in the former case is that the danger area appears in the higher current range. This implies that we can practically stay away from the danger area without losing much of the wanted current. By contrast to the former case, the situation in the latter is opposite: the danger area is not only very large but also in the lower current range. The danger area in the latter case almost covers
the range from the beginning current of this calculation to a very high current and from a very small magnification to a very large magnification (M = 0.03 to 10). Accordingly, for most of the combination of the current and magnification, the Coulomb interactions absolutely dominate the column in this case.

Let us further look into the differences between the two operating modes in the column of figure 9.8 by investigating their inaccessible areas and intermediate aperture ranges. Figure 9.11 gives the comparison of these differences. The curves without markers in figure 9.11 are the I-d_{gas opt} relations of the column in figure 9.8 in three source brightness values: B = 5 \times 10^7, B = 10^8 and B = 2 \times 10^8 A.m^{-2}.sr^{-1}.V^{-1}. Note that the I-d_{gas opt} relation obtained with the D_1 changing mode is identical to that with the D_3 changing mode because we use Eq. (9.12) relation and the shaded beam segments in figure 9.8 to calculate the total geometrical aberration disc d_{gas}. However, the inaccessible area border line is very different in these operating modes, as shown in figure 9.11. We see that the obtainable current before the total Coulomb interaction disc d_{el} reaches the minimum total geometrical aberration disc d_{gas opt} in the D_1 changing mode is much higher than that in the D_3 changing mode.

If we look at the intermediate aperture ranges, from figure 9.11 we can also easily find the big difference between the two different operating modes. Taking the brightness B = 10^8 A.m^{-1}.sr^{-1}.V^{-1} for example, the intermediate aperture range in the D_1 changing mode is from D_1 = 0.453 mm (or I = 95 nA) to D_1 = 0.476 mm (or I = 165 nA), however, the intermediate aperture range in the D_1 changing mode is from D_3 = 0.252 mm (or I = 0.12 nA) to D_3 = 0.614 mm (or I = 205 nA). The latter range is much larger than the former. In the case of low brightness B = 5 \times 10^7 A.m^{-2}.sr^{-1}.V^{-1}, the intermediate aperture range is zero in the D_1 changing mode, but the intermediate aperture range is still large in the D_3 changing mode. Finally, we go a step further to compare the total minimum probe size d_{tot opt} for the two different operating modes in the column of figure 9.8. We calculated four I-d_{tot opt} relations with a source brightness B = 10^8 A.m^{-2}.sr^{-1}.V^{-1}. The results are presented in figure 9.12. The solid and broken curves without a marker in figure 9.12 are the I-d_{gas opt} relation and I-d_{tot opt} relation in the D_1 changing mode, respectively. The solid curves with three different markers are the I-d_{tot opt} relations in the D_3 changing.

Fig. 9.9 The total geometrical aberration disc d_{gas} = f(I, M) (1) and the total Coulomb interaction disc d_{el} = F(I, M) (2) in a three lens electron beam instrument.
mode when the first aperture size \( D_1 \) is respectively taken as 0.25 mm, 0.5 mm and 1 mm. From the results of figure 9.12 we find that for the \( D_1 \) changing mode the minimum total probe size \( d_{tot \text{ opt}} \) is very close to the minimum total geometrical aberration disc \( d_{sg \text{ opt}} \). When the current is lower than 20 nA, there is almost no difference between \( d_{sg \text{ opt}} \) and \( d_{tot \text{ opt}} \). However, for the \( D_3 \) changing mode, the minimum total probe size \( d_{tot \text{ opt}} \) is much larger than the minimum total geometrical aberration disc \( d_{sg \text{ opt}} \) for every beam current. The larger the aperture size \( D_1 \), the larger the difference between \( d_{tot \text{ opt}} \) and \( d_{sg \text{ opt}} \) will be.

**Fig. 9.10** Two different spatial crossing curves and their projections in three planes for an identical three lens electron beam column.

### 9.5 Essence of the intermediate aperture effect

We are now at a position to answer such a question: What is the essence of the intermediate aperture effect? To investigate this problem, we take the four lens electron beam column of figure 9.1 for example again, and calculate the distributions of all eleven spot sizes indicated in figure 2.5. Figure 9.13 shows the relations between the beam current \( I \) and the different spot sizes when the total magnification of the column \( M \) equals unity. The calculation conditions of figure 9.13 are the same as those in figure 9.2. Accordingly, the total geometrical aberration disc \( d_{sg} \) and the total Coulomb interaction disc \( d_{ci} \) in figure 9.13 are exactly equal to those in figure 9.2 when \( M=1 \). In figure 9.13 the space charge spherical aberration disc \( d_{sc} \) is zero because in the calculation of figure 9.2 we supposed that the current angular distribution is uniform.²

Looking at the distributions of the different spot sizes with the beam current (or with the first aperture size \( D_1 \) in the column of figure 9.1), we can divide the aperture size \( D_1 \) into three ranges. (1) In the smaller range of the aperture sizes, the source image \( d_{ga} \), the chromatic aberration \( d_{ch} \) and the diffraction aberration \( d_{df} \) dominate the column. (2) In the range of the intermediate aperture sizes, the trajectory displacement effect plays a major role, all other aberrations become less important. In this range the total Coulomb interaction disc \( d_{ci} \) is approximately equal to the trajectory displacement effect disc \( d_{tr} \), and the total Coulomb interaction disc \( d_{ci} \) is larger (or much larger) than the total geometrical aberration disc \( d_{sg} \). Another important characteristic in this range is that the slope of \( d_{ci} \) is opposite to that of \( d_{sg} \). In other magnification cases, we can also find these characteristics from figure 9.2. These characteristics are the basis that we are able to obtain the spatial crossing curve and to define the danger area or the intermediate aperture range of an optical column. (3) In the range of the larger aperture sizes, the geometrical spherical aberration absolutely dominates the column, all other aberrations become marginal. Accordingly, the total probe size \( d_{tot} \) in figure 9.13 mainly comes...
from three contributions: the source image disc \( d_{\text{sur}} \), the trajectory displacement effect disc \( d_{\text{tr}} \), and the spherical aberration disc \( d_{\text{sp}} \).

Although the previous analysis is based on a given magnification (\( M = 1 \)), the explanation for the essence of the intermediate aperture effect is in fact applicable to an optimized optical column, in which there is always a balance between the size of source image and the size of lens aberrations, and there are different optimum magnifications for the balance. Looking at figure 9.7, we find that the I-d line below the point A' is dominated by the chromatic aberration, and up the point B' by the spherical aberration. In between the points A' and B' there is also an opposite varying slope between the curve 1'-1' and curve 2'-2', and the Coulomb effects (the curve 2'-2') dominate over this range.

In summary, the intermediate aperture effect is based on the fact that, in the range of the intermediate aperture sizes, the trajectory displacement aberration dominates over all other aberrations, and the changing slope of the total Coulomb interaction disc \( d_{\text{tr}} \) is opposite to that of the total geometrical aberration disc \( d_{\text{gs}} \). The intermediate aperture range is just located in the position where the lens aberrations transit from the source image and chromatic aberration to the spherical aberration. In this transition the Coulomb interaction effects are stronger than the lens aberration effects, as a result the intermediate aperture effect occurs in this transition.

### Fig. 9.11 The different inaccessible areas and intermediate aperture ranges in different operating modes of an electron beam column.

### 9.6 Conclusions

There is a determined combination set of the aperture size (the current) and magnification of a particle optical column, in which the Coulomb interaction aberrations dominate over the lens aberrations. This special particle optical fact has been described as the intermediate aperture effect.

Two concepts have been developed to investigate the intermediate aperture effect. For a general particle optical

### Fig. 9.12 Influence of different column apertures on the I-d relation of a full optimized electron beam instrument.
column, the danger area is used to indicate where the intermediate aperture effect occurs. The projection of the spatial crossing curve between the total geometrical aberration surface and the total Coulomb interaction surface in the I-M plane determines the danger area. For an optimized particle optical column, the intermediate aperture range is utilized to point out the place where the intermediate aperture effect plays a role. The intermediate aperture range is found from the crossing points between the I-d_{tg} \_opt\ relational curve and the inaccessible area border line. There is only one intermediate aperture range in an optimized particle optical column.

The intermediate aperture effect is highly sensitive to the source brightness and beam energy. The higher the source brightness or the lower the beam energy, the larger the danger area and the intermediate aperture range will be.

The intermediate aperture effect is also sensitive the aperture position. The optical properties of the three lens electron beam instrument in the D_i changing mode are much better than those in the D_j changing mode. This conclusion is drawn from both the investigation of the intermediate aperture effect and the analysis of the full column optimization. As a general rule, there is an always advantage if the apertures of a particle optical column are placed as close to the source as possible.

The essence of the intermediate aperture effect in a particle optical column is due to the fact that the trajectory displacement effect dominates the column when the lens aberrations transit from the source image and the chromatic aberration to the spherical aberration of the column, and in this transition the total lens aberration and the total Coulomb interaction aberration present an opposite changing slope.

References

7. P. Kruit and X.R. Jiang, Influence of aperture position in focussed ion beam systems on statistical Coulomb interaction effects, presented at SPIE'96 Int. Symp. on Charged-Particle Optics II, 4-9 August, 1996, Denver.

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**Fig. 9.13** The distributions of the different spot sizes at the target of a four lens electron beam optical column when the total magnification of the column M equals unity.
10 Influence of aperture position in focussed ion beam systems on statistical Coulomb interaction effects

Abstract In a series of recent studies, we evaluated the effects of statistical Coulomb interactions on the obtainable probe sizes and probe currents in Focussed Ion Beam (FIB) systems. In order to find the fundamental limits, we assumed that the final probe current was selected by an aperture very close to the source. However, in practical FIB’s, the aperture is somewhere halfway the column, so the current is much higher in the first part of the column, with associated stronger Coulomb interactions. We have now analyzed the influence of the aperture position on the FIB performance and found that the position is very important, but only in the range of small probe sizes or low probe currents. Many FIB’s have a fixed first aperture close to the source to limit the beam current early on and then a second aperture to select the final probe current. We have also analyzed the effect of the fixed aperture and found that it controls the statistical Coulomb interactions only if the current is limited very substantially, which then makes it impossible to operate in high current mode.

Keywords: Charged Particle Optics, Coulomb Interactions, Focussed Ion Beam, Lens Aberrations

10.1 Introduction

The Coulomb interaction effects in focussed ion beam (FIB) systems can deteriorate the resolution or, alternatively, seriously limit the beam current at a given resolution. Using a Monte Carlo simulation, Hirohata et al 1 searched for the aberration properties induced by the space charge effect for a two lens focussed ion beam column, Vijgen et al 2 calculated the statistical Coulomb interactions in a shaped ion beam pattern generator, and Vijgen 3 later evaluated the Coulomb effects in a two lens ion beam system. From the analytical approach, Kruij et al 4 looked into an optimized ion beam system using Jansen’s equations 5 for Boersch effect and trajectory displacement effect. Kruij et al 6 and Jiang et al 7 then fully optimized a two lens focussed ion beam column and analyzed the different imaging modes in the system including a combined evaluation of the lens aberrations and the Coulomb interaction aberrations by using the ANALIC program 8, which is a new computer software package used to perform this kind of combined calculation for charged particle optical instruments. With an experiment, de Jager et al 9 demonstrated the influence of Coulomb interactions on the current density for a one-lens focussed ion beam column: the current density on the target even decreases with increasing beam current. Bi et al 10 measured the probe size of a two-lens focussed ion beam system at different magnifications and different imaging modes and found that the Coulomb effects dominate the system especially at larger magnifications.

Focussed ion beam instruments are equipped with apertures. In our previous studies 4,6,7, we analyzed the impact of Coulomb effects on focussed ion beam systems through changing the diameter

** This chapter is a complete article published at SPIE '96 Int. Symp. on Charged-Particle Optics II, Denver, August 4-9, 1996. The authors of the article are Pieter Kruij and Xinrong Jiang. For reading convenience, the equations, figures and pages in this article are renumbered in line with the order of this thesis.
of an aperture, i.e. the probe current of a system, thereby having found that in an intermediate aperture range the Coulomb interaction aberrations dominate a focussed ion beam system. We described this effect by using the concept of a "danger area"\(^6\) or an "inaccessible area"\(^6\). In order to find the fundamental limits, our previous studies were limited to the situation in which it is assumed that the aperture is placed at a position very close to the source. However, many practical FIB instruments have a fixed first aperture close to the source to limit the beam current early on and then a second aperture to select the final probe current. It is the aim of this paper to study how the second aperture position influences the statistical Coulomb interactions in a FIB system.

We shall fully optimize the FIB system for different aperture positions including taking the Coulomb effects in the whole column into account. The simulations in this paper include two imaging modes: with a crossover and without crossover in between lenses. For calculations we use the ANALIC program\(^9\).

10.2 Influence of aperture position on column optimization

The optimization procedure is based on a two lens and two aperture focussed ion beam (FIB) system built in our laboratory, as illustrated in figure 10.1. The source parameters in the system are described as \(d_0\) (the virtual diameter of a liquid metal ion source, 50 nm), \(\Delta E\) (the source energy spread, 5 eV for FWHM) and \(B\) (the source reduced brightness, \(2.10^6\) A.m\(^2\).sr\(^{-1}\).V\(^{-1}\)). This system can work in both the crossover mode and the non-crossover mode. The comparison between these imaging modes was analyzed in Ref.[7]. In our experience the operation of the non-crossover mode is as easy as that of the crossover mode. The first aperture, which is used to limit the beam current, is fixed at position \(dz1 = 3\) mm. The second aperture \(D_2\) is movable along the z-axis. We shall consider eight typical \(D_2\) positions: \(dz2 = 3\) mm (\(dz1\)), 30 mm (0.5P), 60 mm (P), 100 mm (P+0.25 L), 140 mm (P+0.5L), 180 mm (P+0.75L), 220 mm (P+L) and 240 mm (P+L+0.5Q). Here, \(P\) is the object distance of the first lens, \(Q\) the image distance of the second lens and \(L\) the distance between the lenses. The variation of the magnification \(M\) results from the changes of the focal distances \(f_{11}, f_{12}, f_{21}\) and \(f_{22}\), thereby resulting in the changes of the lens aberration coefficient\(^6\). The column length is fixed at \(P = 60\) mm, \(L = 160\) mm and \(Q = 40\) mm, and the beam potential at \(V_0 = V = V_1 = 15\) kV.

To perform the system optimization, a combined measurement of the total probe size at the target \(d_{tot}\) is defined as\(^6,8,11\):

\[
d_{tot} = \left\{ \left[ d_{wh} + \left( d_{Gau} + d_{tro} \right)^2 \right]^{\frac{1}{2}} + \left( d_{Roo} + d_{cho} \right)^2 \right\}^{\frac{1}{2}}
\]

(10.1)
The different contributions from the source image $d_{\text{int}}$, the chromatic aberration blur $d_{\text{chr}}$, the spherical aberration blur $d_{\text{sph}}$, the Boersch effect blur $d_{\text{boe}}$ and the trajectory displacement effect blur $d_{\text{tra}}$ are calculated independently. The calculation of the lens aberrations ($d_{\text{chr}}$ and $d_{\text{sph}}$) in our FIB system follows the approach reported in Ref. [6], the evaluation approach of the statistical Coulomb effects ($d_{\text{boe}}$ and $d_{\text{tra}}$) are presented in Ref. [8]. We always use the FWHM value of the diameter, which for a Gaussian distribution is almost equal to the FWHM value, but for other distribution might be very different, usually larger than the FWHM value.

It is most useful and realistic to compare the influence of aperture position on column performance at the same probe current. To demonstrate this kind of optimization in a large range, we suppose that the first aperture $D_1$ has a diameter 62.4 $\mu$m so that the maximum current behind $D_1$ is then 20 nA.

For one aperture position $dz2$, the total probe size $d_{\text{tot}}$ is a function of the probe current $I$ and the column magnification $M$ when the probe current limiting aperture $D_1$ changes its diameter. For instance, the solid lines in figure 10.2 show the relation of $d_{\text{tot}}$=f(I,M) when $dz2$=0.5P. In order to compare the aperture position effect at the same probe current level for different aperture positions, we suppose that the $D_2$ aperture size changes to create the same probe current no matter what position the aperture is. For this, it is necessary to assume different $D_2$ values for each magnification, which is not a practical situation, but an important modeling exercise. Accordingly, the relation of $d_{\text{tot}}$=f(I,M) can be calculated for the $D_2$ position $dz2$=P+0.75L with the same current level as $dz2$=0.5P, yielding the broken lines of figure 10.2. It is found from figure 10.2 that a) there is a minimum total probe size $d_{\text{tot, min}}$ for every probe current $I$ and every $D_2$ aperture position $dz2$, and b) the farther the $D_2$ aperture

**Figure 10.2** The total probe size $d_{\text{tot}}$ varies with the magnification $M$ and the probe current $I$. The results given are for crossover mode.

**Figure 10.3** A best balance between the probe current $I$ and the minimum probe size $d$ is found in the crossover mode of figure 10.1 for eight aperture positions $dz2$. 

107
is away from the source, the larger the probe size will be.

Based on the observation of figure 10.2, we calculate the relation of \( d_{wa} = f(I, M) \) for a large range of the probe current \( I \) (from 2 pA to 20 nA) and magnification \( M \) (from 0.01 to 10) when the aperture \( D_2 \) is located in the eight typical positions. We then find the relations between the probe current \( I \) and the minimum probe size \( d \) for every \( D_2 \) position. These relations are presented in figure 10.3. The corresponding probe current and minimum probe size symbolized as 1, 2, 3, 4, 5, and 6 in figure 10.2 can be found in figure 10.3. We also present the minimum total geometrical aberration disc \( d_{ga} \) in figure 10.3, which does not include the Coulomb interactions (let \( d_{ra} = d_{oa} = 0 \) in equation (10.1)). Note that \( d_{ga} \) is independent of the \( D_2 \) aperture position \( dz_2 \). Accordingly, the \( I-d_{ga} \) curve in figure 10.3 is valid for all \( D_2 \) positions.

We can now clearly understand from figure 10.3 that it is always advantageous to aperture the beam with \( D_2 \) as close to the source as possible. Figure 10.3 presents a best balance between the obtainable probe current \( I \) and the minimum probe size \( d \) for the crossover mode of the FIB system in figure 10.1. Performing the same simulation as we did in the crossover mode for the non-crossover mode of figure 10.1, figure 10.4 is obtained.

To design a focussed ion beam column, one has to choose the aperture size \( D_2 \) under the best I-d relations of figures 10.3 and 10.4. For instance, when the second aperture is positioned in the range of \( P \leq dz_2 \leq (P + L) \), the relation between the aperture size \( D_2 \) and the probe current \( I \) is determined by

\[
D_2 = \frac{PD_1}{dz_2} \left[ \frac{I}{I_c} \right]^{1/2} \left| 1 - (dz_2 - P) \frac{PM_{opt}(I) \pm Q}{LPM_{opt}(I)} \right| \quad (10.2)
\]
where $M_{\text{opt}}$, which is a function of the probe current $I$, is the optimum magnification with which the total probe size $d_{\text{opt}}$ takes a minimum, as shown in figure 10.2. $I$ is the total current behind the aperture $D_1$, and calculated by

$$I = \frac{\pi^2}{4} d_0^2 \left( \frac{D_1}{2d_0} \right)^2 V_0 B$$ (10.3)

Equation (10.2) is applicable to both the crossover mode and the non-crossover mode. The former requires to use the symbol of "+", and the latter "-".

Figure 10.5 and figure 10.6 show the dependencies of the aperture size $D_2$ on the probe current $I$ at different aperture positions for the crossover mode and the non-crossover mode respectively. It is seen that most of aperture sizes $D_2$ are between 10 $\mu$m to 1000 $\mu$m, which are normal aperture sizes. Figures 10.3 and 10.5 (or figures 10.4 and 10.6) constitute the design basis under the optimization of a focussed ion beam column, they indicate where one should place the aperture, what size to choose and which probe size $d$ and probe current $I$ one can expect.

The first aperture $D_1$, the size of which was fixed at 62.4 $\mu$m, in the previous investigations, can also strongly influence the statistical Coulomb interactions in the focussed ion beam column of figure 10.1. We now repeat the evaluations of figures 10.3 and 10.4 by considering four $D_1$ sizes: 15 $\mu$m, 62.4 $\mu$m, 125 $\mu$m and 300 $\mu$m. Figures 10.7 and 10.8 show a part of the results of the computations, which represent how the first aperture size plays a major

Fig.10.6 The same dependencies as figure 10.5 for the non-crossover mode of figure 10.1.

Fig.10.7 Influence of the first aperture on the minimum probe size under the optimization of the column of figure 10.1. The second aperture is placed at $d_{z2}=0.5P$ and the crossover mode is used.
role in the column optimization. Figures 10.7 and 10.8 are the situations in which the crossover mode is considered and the second aperture $D_2$ are placed at 0.5$P$ and $P+0.5L$ respectively. For comparison the c0 and c1 curves in figure 10.3 are also given in figures 10.7 and 10.8.

We see from figure 10.7 that the minimum probe size varies with the $D_1$ size at the same probe current level even though the second aperture $D_2$ is placed close to the source ($dz2=0.5P$). The farther the aperture $D_2$ is away from the source, the stronger the influence of the first aperture size $D_1$ on the minimum probe size will be. This effect can be found from figure 10.8, in which the probe size with a larger $D_1$ size can be several times greater than that with a smaller $D_1$ size in the lower current range.

### 10.3 Discussions

#### 10.3.1 About the column optimization

In most practical focused ion beam systems, a fixed first aperture $D_1$ is positioned close to the source to limit the beam current early on and then a halfway second aperture $D_2$ is used to select the final probe current $I$. In the previous optimization, we supposed that only the current passing through the first aperture $D_1$ produces the Coulomb interactions in the source region. This is not so in reality. In the considered system, the $D_1$ aperture with size 62.4 $\mu$m allows 20 nA current to the column. The current in front of the $D_1$ aperture is in fact much higher than this value. The higher current in this region will contribute to a large energy spread due to the Boersch effect, but the probe size broadening due to the trajectory displacement effect is so small that it can be ignored compared to the virtual source size of 50 nm$^{12}$.

All calculations are performed for a brightness $B=2.10^6$ A.m$^2$.sr$^{-1}$.V$^{-1}$. One could reason that the interactions will change when the gun is operated at a different brightness. However, in our calculations presented in Ref.[6] we have shown that this can not improve the situation.

We see from figure 10.2 that for every probe current $I$ the total probe sizes at different aperture positions are going to be close to each other in the range of larger demagnification (smaller values of $M$). This effect is because the lens geometrical aberrations dominate the system due to the larger beam angle induced by the larger demagnification. However, for the larger magnifications, the Coulomb interactions become dominant and the farther the second aperture is away from the source, the stronger the Coulomb interactions will impact the system. As a result of the balance between the
geometrical aberrations and the Coulomb aberrations, a minimum probe size is found for every probe current, which is in fact an indication of the transfer from the domination of the geometrical aberrations to that of the Coulomb interactions.

The column optimization of figures 10.3 and 10.4 shows that it is always advantageous in principle to position the aperture as close to the source tip as possible. However, it is normally very crowded around the tip region in a practical system and it is difficult to have an adjustable device for the change of the aperture. In this case we can use an additional aperture to partly compensate the influence of the aperture position effect on the column performance. Figure 10.9 shows this simulation experiment for the crossover mode. In the simulation the first aperture $D_1$ is still at $dz1=3$ mm with diameter 62.4 $\mu$m (the maximum current behind $D_1$ is 20 nA). An additional aperture $D_2'$ is inserted at the position $dz2'=0.5P$. We demonstrate three $D_2'$ sizes: $D_2'=44$, 88 and 140 $\mu$m, corresponding to the maximum current behind $D_2'$ 0.1 nA, 0.4 nA and 1 nA. The adjustable aperture $D_1$ is positioned at $dz2=P+L$. We calculated the new configuration with three apertures. The results of this simulation are presented in figure 10.9. For comparison, figure 10.9 also presents the previous I-d relations c0, c1 and c7 in figure 10.3. We learn from figure 10.9 that the additional aperture $D_2'$ can partly limit the Coulomb interactions in the lower probe current range. For the higher probe currents, it seems difficult to obtain much benefit from the additional aperture.

We find from figures 10.3 and 10.4 that the non-crossover mode is better than the crossover mode no matter what position the $D_2$ aperture is. The operation of the non-crossover mode is not a problem, but its limitation is the magnification range. For the non-crossover mode shown in figure 10.1, the magnification $M$ is limited in

$$M_{\text{min}} = \frac{Q}{L+P} < M < \frac{L+Q}{P} = M_{\text{max}}$$  \hspace{1cm} (10.4)

Accordingly, the magnification $M$ can only change from $M_{\text{min}} \approx 0.2$ to $M_{\text{max}} \approx 3.3$ for the configuration of figure 10.1. In normal case this range is enough.

10.3.2 About the aperture size and position

Many practical focussed ion beam systems use a fixed aperture $D_2$ in between lenses to select the probe current. In this case the question is where the $D_2$ aperture can best be positioned and what size should be chosen. We realize from figures 10.5 and 10.6 that only the $D_2$ aperture size is variable.
can an optimum I-d relation be obtained no matter where the aperture is positioned. Accordingly, for the operation mode with a fixed D₂ aperture what one can choose is to select an appropriate aperture position and size to obtain an I-d relation which can approach the optimum one reasonably. For the crossover mode we find from figure 10.5 that the D₂ size only changes slightly around 70 μm when the aperture is placed at d₂=\(P+0.5L\) and when the probe current I is lower than 800 pA. With this aperture size and position we calculate the I-d relation so that figure 10.10 is obtained. In the evaluation the probe current I is selected by moving the crossover position, thereby resulting in a variation of the column magnification M of 0.05 to 50. The first aperture size D₁ is fixed at 62.4 μm, producing a maximum column current of 20 nA. Three optimum I-d relations shown in figure 10.3 (c0, c1 and c5) are also included in figure 10.10 for comparison.

We see from figure 10.10 that the I-d curve with the fixed D₂ size of 70 μm is in good agreement with that obtained by optimizing the combination of the D₂ size and column magnification (c5) in the probe current range from 10 pA to 1 nA, which covers the normal currents used in focussed ion beam systems. This result for a fixed aperture in between the lenses is consistent with the Monte Carlo calculations of Vijgen⁴ performed for only two current values. In this current range the crossover is located in front of the D₂ aperture. In the high current range of 4 nA to 20 nA the former I-d line can again be fitted, if the crossover is behind the D₂ aperture. Note that reducing the current below 4 nA with this crossover position is a very bad situation. We also calculated the I-d relations with other D₂ sizes, for instance D₂=40, 50, 60, 80, 90 and 100 μm respectively, and found that the obtained I-d lines in these calculations also fit the optimum one (c5) in some current ranges, but the agreement between them is worse than that with the D₂ size of 70 μm especially in the normal current range of 10 pA to 1 nA.

We see that in the lower current range, the Coulomb interactions increase the probe size by a factor of about 3 at a given current, or limit the probe current by a factor about 20 at a given probe size. One might wonder if this effect can be reduced by choosing a smaller D₁ aperture. Figure 10.8 shows, however, that one then has to reduce the D₁ size substantially, to values under 15 μm, which then also limits the maximum current to less than 1 nA.

Figure 10.11, which was produced by performing similar simulations to figure 10.10 for two other D₂ positions, shows that placing the D₂ aperture at d₂=\(P+0.25L\) is a bad choice. We find that only in a very small range of the current does the I-d line with a fixed D₂ size of 70 μm fit the optimum I-d line (c4), instead, in most crossover positions the former line stays far away from the latter.
However, in the case of \(dz2=P+0.75L\) the I-d line with a fixed \(D2\) size of 200 \(\mu\)m is consistent with the optimum line (c6) in the high probe currents of 0.2 nA to 20 nA, but losing the agreement in the low probe currents.

Figure 10.12 shows the situation of the non-crossover mode. We calculated the I-d lines for five sizes of the \(D2\) aperture, which was positioned at \(dz2=P+0.5L\). We find every I-d line corresponding to a fixed \(D2\) size fits the optimum one (nc5 in figure 10.4) only in a very small probe current range, however, the probe sizes in a determined probe current range for every \(D2\) size are smaller than those obtained by optimizing the combination of the \(D2\) size and magnification in the crossover mode (c5 in figure 10.1).

10.4 Conclusions

Only one I-d relation at optimum magnification would be enough to characterize a FIB system if there were no Coulomb interactions. See curve c0 in figure 10.3 for the crossover mode and nc0 in figure 10.4 for the non-crossover mode of imaging in the two lens system considered here. In fact Coulomb interactions can dominate the I-d relation. The fundamental limits are found when the probe current selecting aperture is positioned very close to the source, in our demonstrations \(dz2=dz1=3\) mm. Curves c1 and nc1 show that, for the intermediate current range, there is a substantial irreducible increase in the minimum probe size. Both the lens aberrations and the Coulomb interaction effects are smaller for
the non-crossover mode. In practice only a fixed D₁ aperture, limiting the maximum current, can be placed very close to the source. With the probe current selecting aperture D₂ placed away from the source the probe size at lower currents are also affected by Coulomb interactions. To limit the aperture position effect, the best choice is to place the probe current selecting aperture (D₂) as close to the source as possible and to reduce the source aperture size (D₁) as far as possible.

A problem is that both magnification M and aperture size D₂ must be variable in order to minimize the probe size over the complete current range. However it is possible to select the current by changing the column magnification when a fixed sized (D₂) aperture is positioned between the lenses. The best position is at the middle of the lenses. For the non-crossover mode the current range is limited at each choice of the D₂ aperture size (figure 10.12). Using the crossover mode a fixed D₂ size can be found which allows good performance over the complete usual probe current range.

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References

11 Influence of Coulomb interactions on low-voltage scanning electron microscopes

Abstract Without an optimization procedure, low-voltage scanning electron microscopes (LVSEM) could suffer strongly from Coulomb effects. For a representative LVSEM, it is shown that the Coulomb effect blur can be more than one order of magnitude greater than the source image in full probe current range. After having reset the first aperture and optimized the combination of the magnification and the probe current selecting aperture, the probe size in the instrument reduces 20 times compared to without the optimal procedure when the system runs at 1 nA probe current and 1 keV landing energy. For a diffraction limited LVSEM system, it is found that positioning an aperture in the low energy probe section does more harm than good. However, placing an aperture with suitable size in the Coulomb-tube of the instrument can approach the optimum performance which is obtained by optimizing the aperture size and magnification simultaneously, thereby simplifying the configuration and reducing the cost of the system.

11.1 Introduction

There is increasing interest in low-voltage scanning electron microscopes (LVSEM) in last decades since the advantages are being more and more recognized and used in the areas of the development and manufacture of microelectronic and optoelectronic components\(^1,2\). A large number of low voltage approaches are reported in literature, as summarized by Ref.[3]. Besides, the low voltage probe forming techniques are also being used in the transmission electron microscopes (TEM)\(^4,5,8\) and focussed ion beam (FIB) systems\(^7\).

Generally speaking, a LVSEM system operates at 0.2-20 keV landing energies, 1-100 nA probe currents and 2-200 nm probe sizes. These properties are attractive for wafer inspection and electron beam testing because of the reduced charging, the negligible radiation damage and the higher signal/noise ratio. However, a LVSEM system could also result in two problems. One is the higher chromatic aberration of probe forming lenses at the low voltages, and the other is the beam broadening caused by the mutual Coulomb repulsion including the Boersch effect, the trajectory displacement effect and the space charge effect. The use of a low probe energy is in fact mainly responsible for the deterioration of the LVSEM resolution due to the Coulomb interactions between electrons.

Because of these advantages and disadvantages, the high-resolution low-voltage particle optics becomes the first consideration of a LVSEM system design. Without taking into account the Coulomb interactions, Beck et al\(^1\) looked into low-voltage probe forming columns for electrons, Ximen et al\(^8\) concentrated on the theoretical calculation of probe size of LVSEM systems, and Meisburger et al\(^9\) noted the design of low-voltage electron-optical system for the high-speed inspection of the integrated circuits. With including the impact of the Coulomb effects, Barth et al\(^10\) analyzed the e-e interactions in the intermediate crossover of LVSEM systems for searching the probe size - probe current dependence, and Kruit et al\(^11\) investigated the trajectory displacement limitation of the probe current for a 1 keV LVSEM instrument.

This chapter presents a novel approach which is different from the usual\(^10,11\) for the investigation of the influence of the Coulomb effects on low-voltage scanning electron microscopes. A combined optimization of aperture sizes, magnification as well as the column length in a representative LVSEM system is considered. We shall first discuss the properties of two typical LVSEM instruments, one is a high-current low-voltage electron beam column reported in Ref.[1], and the other a three-lens scanning electron microscope (3L-SEM). We then concentrate ourselves only on the evaluation of Coulomb effects in the latter system. This is because the system has many characteristics similar to commercial LVSEM's and to the FEG-SEM column reported in Ref.[12], and has many important
optical properties: the high brightness Schottky gun, the Coulomb-tube beam transportation, the beam energy jumping, the low energy landing and the multi-aperture selecting current. The full system optimization for the 3L-SEM is finally considered, from which we find that some of LVSEM properties are very different from those of general charged particle optical instruments.

In all calculations of the Coulomb effects in the whole column from the gun to the target, we use the numerical evaluation method, which is described in section 3.4 of this thesis since the considered LVSEM columns can not be modelled as a series of narrow crossover beam segments. This method is included in the ANALIC program\textsuperscript{13}. Accordingly, this program is again used in the study of this chapter. The FWH50 measured spot disc, which is the width of containing 50\% particles in a determined beam distribution\textsuperscript{14}, is considered in all evaluations of the lens aberrations and Coulomb interaction aberrations.

11.2 General column characteristics of LVSEM

We mainly describe here the general properties of two typical low-voltage scanning electron microscopes (LVSEM).

Figure 11.1(1) illustrates a high-current low-voltage electron beam system with unity magnification and telecentric ray path using a single-pole condenser lens (SPCL) and a single-pole immersion objective lens (SPIOL)\textsuperscript{1}. This belongs in fact to our two-lens optical model described as figure 2.3 and table 2.1. The beam potential is $V_j = V = 10$ kV and $V_f = 1$ kV in our symbolization in table 2.1, in which $eV_f = 1$ keV is the final landing energy of the low-voltage system. The optical properties of the SPCL (lens $L_1$), referred to its object-side, are characterized by the focal distance $f_1 = 15$ mm, the spherical aberration coefficient $C_1 = 13.2$ mm and the chromatic aberration coefficient $C_\alpha = 11.5$ mm. However, the properties of the SPIOL (lens $L_2$), referred to its image-side, are described as $f_2 = 5.01$ mm, $C_2 = 1.05$ mm and $C_\alpha = 0.83$ mm. A ZrO/W <100> Schottky-cathode is used in the system of figure 11.1(1) with the angular current density $dI/d\Omega = 1$ mA/sr, the virtual source diameter $d_0 = 20$ mm and the source energy spread $\Delta E = 0.15$ eV (FWHM). The column of figure 11.1(1) is 115 mm long including a working distance of $Q = 8$ mm.

Because of the requirements of the low landing energy and the high probe current, the influence of the Coulomb interactions on the resolution of the system in figure 11.1(1) should be considered. Accordingly, the column performance was investigated by using the ANALIC program\textsuperscript{13} based on the previous conditions, as presented at figure 11.2, in which 15 percent of the space charge defocussing (defoc.\% = 0.15 in Eq.(5.32)) is considered. The eleven spot sizes in figure 11.2 were evaluated in line with the definition of chapter 6, and the probe current was assumed to be selected by an adjustable aperture at the center of the first lens, thereby, the current varying from 4 nA to 4000 nA.
As can be seen from figure 11.2 that the Coulomb interactions are really impacting the low-voltage high-current electron beam system of figure 11.1(1). In the probe current range from 30 nA to 500 nA, the total Coulomb interaction disc \( d_{\text{int}} \) is larger than the total geometrical aberration disc \( d_{\text{tg}} \). Accordingly, if the column configuration is not changed, the system can only operate at the currents less than 30 nA in order to stay away from the influence of the Coulomb effects. This system can of course be optimized to enhance its performance with the same approach as we did in chapters 7 and 8. This identical exercise is omitted here.

Figure 11.1(2) schematically illustrates a three-lens scanning electron microscope (3L-SEM) equipped with three apertures. The maximum current is selected by the first aperture \( D_1 \) in the gun lens \( L_1 \). Equipped with a Schottky emitter, the source has a diameter 20 nm and the angular current density 0.4 mA/sr at a fixed extraction voltage of 5 kV (the source energy spread \( \Delta E = 0.4 \) eV). In the Coulomb-tube (the beam sections from the first lens \( L_1 \) to the second lens \( L_2 \)), the electrons have an energy \( V_2 = V_p \), where \( V_p \) is the probe energy from the second lens to the target (in our definition \( V_{22} = V_{32} = V_p \)). The landing energy of the system \( V_p \) can vary from 0.2, 0.5, 1.0, 2.0, 5.0, 10, 20 to 30 kV. A fraction of the first selected current by \( D_1 \) is removed at the second aperture \( D_2 \), which is located in front of the combined lens \( L_2 \). The gun lens and the combined lens image the source with variable magnification \( M_{12} = M_1 \ast M_2 \) onto the center plane of the electrostatic lens \( L_3 \). Here, \( M_1 \) and \( M_2 \) are the magnifications of the lenses \( L_1 \) and \( L_2 \). The final probe current \( I \) is selected by adjusting \( M_{12} \) and the third aperture \( D_3 \), which is positioned at the center of the third lens. In the system, only the aberrations of the final lens \( L_3 \) are significant and taken into account. The chromatic and spherical aberration coefficients of this lens in object-side are \( C_{33} = 25 \) mm and \( C_{33} = 100 \) mm.

Considered as one of typical charged particle instrument models in chapter 1, the column of figure 11.1(2) includes many important optical characteristics of a probe forming system: the Schottky gun, the multi-aperture selecting current, the beam energy jumping, the low energy landing, the Coulomb-tube electron beam transportation and the different imaging modes, etc.

11.3 Impact of Coulomb effects on 3L-SEM column

The aperture settings of the 3L-SEM column in figure 11.1(2) is the diameter \( D_1 = D_2 = 500 \mu m \), \( D_3 = 100 \mu m \) and the position \( D_{z1} = 5 \) mm, \( D_{z2} = 110 \) mm and \( D_{z3} = 290 \) mm. Thus, the beam current in front of the second aperture \( D_2 \) is 3.1 \( \mu A \). This is a high current, with which the beam sections in front of \( D_2 \) could suffer strongly from the Coulomb interactions. The beam current behind \( D_2 \) depends
on the magnification $M_{1,2}$, and is greatly limited by the third aperture $D_3$. The beam section in between the second lens and the third lens could also suffer from the Coulomb effects because of its low energy. Since the lens $L_3$ is demagnifying the crossover and the aperture $D_3$ cuts most of the beam, the beam angle is so small that the lens aberrations from the first and second lenses can be ignored. Accordingly, the aberration coefficients $C_{cl1}$, $C_{cl2}$, $C_{c2}$ and $C_2$ are assumed to be zero. However, the third lens $L_3$ is important, because not only it suffers from the chromatic and spherical aberrations but also the diffraction aberration.

Based on the previous considerations, the lens aberrations and the Coulomb interactions in the column of figure 11.1(2) was evaluated by using the ANALIC program\textsuperscript{13}. The evaluation is divided into two groups: the lower probe energies (0.5 keV and 1 keV) and the higher probe energies (20 keV and 30 keV), as shown in figure 11.3 and figure 11.4, respectively, in which we present the dependencies of four spot sizes on the probe current. The variation of the current is realized by moving the crossover position in between the first and second lenses. It is seen that, in the lower current range, the total geometrical aberration disc $d_{geo}$ is much larger than the source image $d_{gau}$. The reason of this effect is that the diffraction aberration disc $d_{d}$ and the chromatic aberration disc $d_{chr}$ play a major role in the addition of the lens aberrations. This is a common characteristic of LVSEM systems. However, $d_{gau}$ is approaching $d_{geo}$ with the increase of the probe current. In this case, $d_{d}$ and $d_{chr}$ remain the same as before, instead, the source image increases with the current, i.e. with the magnification.

Looking at the total Coulomb interaction disc $d_{cia}$ in figures 11.3 and 11.4, we find that the Coulomb interactions dominate over the lens aberrations in a very large probe current range. In the full probe current range, $d_{cia}$ is much larger than the source image $d_{gau}$. The lower the probe energy, the larger the deviation between $d_{cia}$ and $d_{gau}$ will be. For instance, in the low probe energy mode ($V_p=0.5$ keV or 1 keV), the total Coulomb interaction disc $d_{cia}$ can be more than one order of magnitude greater than the source image $d_{gau}$.

As can be seen from figure 11.3 and figure 11.4 that the higher probe energy can decrease the Coulomb interactions, but this is not an effective approach to limit the Coulomb effects in the 3L-SEM system. The reason is that the influence of the Coulomb effects on the system performance is mainly produced in the long beam sections behind the second lens, in which the beam current is very high and a large fraction of the currents can not pass through the third aperture to the target. This results in a wrong output: low probe current with large probe size.

It comes to the conclusion that the 3L-SEM system suffers strongly from the Coulomb interactions. The adjustment of the column magnification or the probe energy of the system can not limit the Coulomb effects obviously. The only approach to effectively control the Coulomb effects

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure11.3.png}
\caption{The probe-size probe-current dependencies of the 3L-SEM system with lower landing energies (0.5 keV and 1 keV).}
\end{figure}
is to change the column configuration.

11.4 New aperture and imaging modes of 3L-SEM column

We learn from figure 11.3 and figure 11.4 that, in the original column configuration of the 3L-SEM system of figure 11.1(2), the diffractive and chromatic aberrations dominate the system only in a very low current range, instead, the Coulomb interactions absolutely determine the total probe size $d_{\text{tot}}$ in a very large probe current range. Accordingly, it is clear that the D1 and D2 apertures must be dramatically reduced in size to limit the Coulomb effects.

First of all, we consider the new aperture settings of the system. The first aperture size $D_1$ equals 30 and 50 micron can give maximum currents 11 and 31 nA. This is the desired current range of the 3L-SEM. $D_2$ aperture needs to be less than 60 micron to significantly reduce the Coulomb interactions in the low energy section after L2 lens. We then consider using the non-crossover imaging modes, which was modeled in chapter 2 and discussed in chapter 815, in order to further reduce the Coulomb effects because the crossover in the Coulomb-tube is mainly responsible for the energy spread due to the Boersch effect in this region.

Taking into account $D_1 = D_2 = D_3 = 50 \mu m$, a set of graphs showing the Coulomb interaction blur (the trajectory displacement and additional chromatic aberration due to the Boersch effect19) were evaluated by again using the ANALIC program for two magnification modes. The first is for magnification with the crossover and the second for the non-crossover in the Coulomb-tube. The latter system setting is also modeled as figure 2.6. Figure 11.5 shows the results of the evaluation. For the non-crossover mode, the magnification M is more restricted in range, for instance, the magnification in the Coulomb-tube $M_{12}$ can vary from 1.1 to 11 in the case of 1 keV probe energy.

It is seen from figure 11.5 that the Coulomb effects have been greatly limited in the column with a new aperture setting. For the higher probe energies ($V_p = 20$ keV and 30 keV), the coulomb effects no longer become a significant factor in the whole probe current range, and for the lower probe energies ($V_p = 0.5$ keV and 1 keV), the Coulomb effects start to play a role only after the current reaches nano-amperes. Our another understanding to figure 11.5 is that the non-crossover mode gives a smaller Coulomb effect blur for every probe energy since there is less Boersch effect in the Coulomb-tube. It is also found from figures 11.5(3) and (4) that there is a dramatic increase of the probe size but without any enhancement of the current in the higher current range. The reason of this effect is that all currents behind the aperture $D_1$ pass through the second aperture $D_2$ and the third aperture $D_3$, and the beam half-angle in the probe sections becomes smaller and smaller while the magnification in the Coulomb-tube becomes larger and larger. As a result, the trajectory displacement

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Fig.11.4 As figure 11.3, for higher landing energies (20 keV and 30 keV).
Fig. 11.5 Comparison between the crossover and non-crossover imaging modes of the 3L-SEM system with new aperture settings.

in the Holtsmark regime increases with the decrease of the half-angle$^{14,17}$.

11.5 Optimization of 3L-SEM column

We have realized that the suitable aperture sizes $D_1$ and $D_2$ can greatly improve the performance of the 3L-SEM system at lower probe energies. We are now at a position to answer such a question: Can we gain more by optimizing the combination of the system magnification, aperture size as well as the column length? To investigate this problem in a wider magnification or probe current range, we use the crossover mode of the column.

11.5.1 Aperture size optimization

First of all, we answer such a question: How the probe size depends on the column magnification $M$ and probe current $I$ simultaneously? Assume that the first aperture size $D_1 = 50 \mu m$, this allows 31 nA current into the column. In this case, figure 11.6 shows the dependencies of the total probe size $d_{tot}$ on the probe current $I$ and magnification $M$ for two modes: the $D_2$ size changes but $D_3$ open (figure 11.6(1)) and the $D_2$ is open but $D_3$ size changes (figure 11.6(2)), in which the probe energy $V_p$ is 1 keV. Note that the probe current $I$ varies not only with the aperture sizes ($D_2$ or $D_3$) but also with the magnification ($M$) in the evaluation. We learn from figure 11.6 that 1) it is very necessary to optimize the 3L-SEM column since the probe size $d_{tot}$ varies strongly in the magnification $M$ - current $I$ domain, 2) for every probe current $I$ there is a minimum probe size found at an optimum magnification, 3) the total probe size in figure 11.6(2) is much larger than in figure 11.6(1). This implies that the Coulomb interactions in the 1 keV beam section are very serious, 4) in the larger magnification range, there is an optimum current $I$ or aperture size $D$ in figure 11.6(1), but not in figure 11.6(2), with which the probe size is a minimum. This means that the 3L-SEM is a system
limited by the diffractive and chromatic aberrations (figure 11.6(1)), but the aberrations become less important when the Coulomb effects dominate (figure 11.6(2)), and 5) in the smaller magnification range, the probe size increases with the probe current monotonically.

Based on figure 11.6, we can further evaluate the optimized system setting. This is presented in figure 11.7, in which we also give a similar optimum setting for a case where the first aperture size is smaller ($D_1 = 30 \mu m$). Looking at the three minimum probe sizes in two modes, we find that, in the $D_2$-change mode, the total minimum probe size $d_{tot}$ is very close to the total geometrical aberration disc $d_{ga}$ in the lower currents less than 4 nA, in which the Coulomb interactions in the column become minimal. However, the Coulomb effects play a major role in the higher currents. The probe size in the $D_2$-change mode is much larger than in the $D_2$-change mode because of the aperture position effect described in chapter 10. This effect mainly occurs in the low beam energy segment in between the second and third lenses.

We conclude from figure 11.7 that placing an adjustable aperture at $D_2$ position is much better than that at $D_3$ position. With a $D_2$-change aperture, the Coulomb effects can be greatly limited especially in lower probe current range.

11.5.2 Simplified aperture setting

We are now to try a simpler approach: Is it possible to effectively limit the Coulomb effects in the 3L-SEM system by simply placing an aperture with fixed size at the $D_2$ position and by removing the $D_3$ aperture? If this could be realized, we would simplify the configuration and operation and reduce the cost of the system. This question is answered in figures 11.8 and 11.9.

Figure 11.8 shows four probe current-total probe size dependencies for four fixed $D_2$ aperture sizes: $D_2 = 20, 40, 50$ and $70 \mu m$, in which the first aperture size $D_1 = 50 \mu m$ and the probe energy

**Fig.11.6** Dependencies of the total probe size on the probe current and column magnification in the cases of (1) $D_2$ changes, $D_1$ open and (2) $D_2$ open, $D_3$ changes.

**Fig.11.7** The optimum I-d relations of the two aperture modes in figure 11.6.
$V_s=1$ keV are considered. For comparison, figure 11.8 also includes the optimized I-d dependencies in figure 11.7. We see from figure 11.8 that the I-d curve with the aperture $D_2=40 \mu m$ is close to the optimized I-d curve with $D_2$-change mode. Furthermore, when the $D_2$ aperture size is fixed at 50 $\mu m$, the I-d curve approaches the optimum I-d curve reasonably in the full current range. We also see that the I-d curves with $D_2=20$ and 70 $\mu m$ are in agreement with the optimum I-d curve in the higher currents. Accordingly, the best choice is to place an aperture with size around 50 $\mu m$ at the $D_2$ position, with which the I-d relation is almost equivalent to that with an optimized combination of the aperture size $D_2$ and magnification M. The same conclusion can also be found by changing the first aperture size. For instance, figure 11.9 shows the similar evaluation to figure 11.8, but the aperture size $D_1$ in figure 11.9 is 30 $\mu m$. We see from figure 11.9 that taking a fixed aperture size $D_2$ in the range from 45 to 50 $\mu m$ can obtain an approximate result to that with optimized $D_2$ size and magnification M.

The reason producing the previous important characteristics in the 3L-SEM system is because the lens aberrations in the Coulomb-tube are absent and the Coulomb effects are very weak after using the new aperture setting. Moving the crossover position can only slightly change these effects in the Coulomb-tube. However, the lens aberrations (mainly the diffractive and chromatic aberrations) and the Coulomb effects are all strong in the low energy (1 keV) probe section. Using the third aperture to control the Coulomb effects is very limited since the landing probe is only 25 mm long (see figure 11.1(2)), oppositely, it cuts a large fraction of the probe current. When the third aperture is utilized, the diffraction becomes dominant over the chromatic aberration, thereby causing an increase of the total lens aberration. Accordingly, using the third aperture is more harm than good. Without the third aperture we can make use of a "most suitable" second aperture to balance the different effects in the low energy probe section.

11.5.3 Column length optimization

We have understood that the low energy probe section determines the performance of the 3L-SEM system, in which both the lens effects and Coulomb effects play an important role. This leads us to consider more questions: How does the probe energy influence the 3L-SEM performance? Can we benefit from the adjustment of the probe length? The similar investigations to these problems have been done in chapter 7, in which we optimized a two-lens focussed ion beam column at different
beam energies (figure 7.9) and column lengths (figure 7.10). Are the properties in chapter 7 applicable to the 3L-SEM system?

Figure 11.10 shows that the dependencies of the probe current I on the minimum probe size d at different probe energies ($V_p$ = 0.2, 0.5, 1, 5 and 20 keV). They are obtained by optimizing the $D_2$ aperture size and the magnification $M$ (the crossover position in between the first and second lenses). The first aperture size $D_1$ is fixed at 50 µm, with which the maximum current to the column is 31 nA. The third aperture $D_3$ is removed, thereby creating a large probe current range. It can be seen from figure 11.10 that with the probe currents lower than 1 nA the Coulomb effects have been totally controlled even at a very low probe energy (0.2 keV). In this current range only the diffractive and chromatic aberrations play a role. The higher the probe energy, the smaller the diffractive and chromatic aberrations will be. This results in the sharp variation of the probe size at different energies. In the currents higher than 1 nA the Coulomb effects become dominant especially in the lower probe energy range. When the probe energy is higher than 5 keV, the Coulomb effects can be ignored even in the full current range.

We learnt from figure 7.10 that shortening a column length can obtain a smaller probe size at the same probe current. However, this is not always true. Figure 11.11 presents an evidence. In the evaluation of figure 11.11, the distance between the second and third lenses in the 3L-SEM column of figure 11.1(2) is taken four values $L_{23}$ = 75, 150, 300 and 600 mm, but the image distances of the second lens and the third lens remains unchanged (50 mm and 25 mm respectively, as seen from figure 11.1(2)). The probe energy is $V_p$ = 1 keV, the aperture size $D_1$ 50 µm and the aperture $D_3$ absent. The I-d curves are obtained by optimizing the aperture size $D_2$ and magnification $M$.

Figure 11.11 gives a surprising result. We see that the longer the column length, the smaller the total geometrical aberration disc $d_{tg}$ in the full current range. This implies that in the considered aperture size ($D_3$) and column length ($L_{23}$) changing ranges the diffractive aberration is always dominant over the spherical and chromatic aberrations. The total probe size $d_{tg}$ including the Coulomb effects is very close to the total geometrical aberration disc $d_{tg}$ in the currents lower than 2 nA. The longer the column length, the closer they will be. This is because the Coulomb effects are more demagnified by the smaller magnification due to the longer $L_{23}$. In the currents higher than 2 nA, the Coulomb effects play a major role no matter which column length is considered.

11.6 Conclusions
Low-voltage scanning electron microscopes (LVSEM), which are normally equipped with a high brightness gun for the example of Schottky emitters, suffer from the Coulomb interactions, especially, when they operate at higher currents. This current limitation is about 30 nA in the low-voltage high-current electron beam system of figure 11.1(1).

Before the column is optimized, the Coulomb effects deteriorate the performance of the 3L-SEM system strongly, and the Coulomb effect blur can be one order of magnitude greater than the source image in the full current range.

Without changing the basic configuration, the Coulomb effects in 3L-SEM system have been greatly reduced by resetting the first aperture size and optimizing the combination of the magnification and the probe current selecting aperture. With these actions, the total probe size found in figure 11.9 is only 23 nm when the system runs at 1 nA probe current and 1 keV landing energy, which is close to the source virtual diameter 20 nm and only 5 percent of the total probe size before the optimization of the system at the same conditions (see figure 11.3).

Using the third aperture in the 3L-SEM column is more harm than good. The combined optimization of the aperture size D2 and magnification M can be approached by making use of a fixed aperture at D2 position and by removing the third aperture D3, thereby simplifying the configuration and reducing the cost of the system.

Enhancing the probe energy is always advantageous. Using 20 or 0.2 keV probe energy, a 2.5 or 60 nm probe size is found from figure 11.10 at 100 pA current. For a diffractively limited system, shortening the column length can not increase the resolution in the lower current range, even in the higher current range, the result of this effort is also limited (figure 11.11).

References

18. P. Kruit and X.R. Jiang, Influence of aperture position in focussed ion beam system on statistical Coulomb interaction effects, presented at SPIE'96 Int. Symp. on Charged-Particle Optics II, 4-9 August, Denver, 1996.
12 Verifications of ANALIC program

Abstract  This chapter intends to check the correctness and reliability of the ANALIC program, which is a new computer software package having been developed to perform the full system optimization including the combined calculation of lens aberrations and Coulomb effects in charged particle instruments. Three approaches are utilized for this objective. The analytical approach shows that the accuracy of the ANALIC program is as good as that of the INTERAC program. The deviation between the evaluations of the two programs for Coulomb effects is less than 5%. From the Monte Carlo (MC) simulation approach, the ANALIC program fits the MONTEC program reasonably for the evaluations of the trajectory displacement effect in the whole current range and of the Boersch effect in the lower current range, but it seems overestimating the Boersch effect in the higher current range. The ANALIC program is considered as more accurate than the MC simulation for the evaluation of the space charge effect. Compared to the MC simulation, it is also found that the linear-rule summation used in the ANALIC is better than the gamma-rule summation in the INTERAC, but this is not the final conclusion since this problem is still being investigated. Finally, the measurements of the probe size in two practical ion beam instruments further show that the calculated results with the ANALIC are in agreement with those from the experiments at different operating modes of the systems.

12.1 Introduction

For the combined calculation of the lens aberrations and Coulomb interaction effects in a particle optical column, the program ANALIC\(^1\) has been developed on the basis of 1) the optical models of chapter 2, 2) the beam segment equations of chapters 3 and 4 and the combined evaluation equations of chapter 5. It means that to verify the program ANALIC is to prove the correctness of chapters 2, 3, 4 and 5, which are the theoretical part of this thesis.

The ANALIC program has been successfully used in the design of the focused ion beam system (chapter 7)\(^4\), in the evaluation of different imaging modes of an optical system (chapter 8)\(^3\), in the investigations of the intermediate aperture effect (the inaccessible area and the danger area etc. in chapters 7 and 9) and the aperture position effect (chapter 10)\(^4\) as well as the calculation of the Coulomb interactions in low-voltage scanning electron microscopes (chapter 11) because of its strong abilities of performing the combined calculation and full system optimization. Are these studies reliable? What is the accuracy of the program when it is applied to these studies?

It is the objective of this chapter to answer these questions.

We shall verify the ANALIC program by using three methods: the analytical approach, Monte Carlo simulation approach and experimental approach. No other ways have been reported so far being used to verify the evaluation of the Coulomb effects in charged particle optical instruments.

The INTERAC program\(^5\) is fully based on the analytical equations derived by Jansen\(^6\) for the evaluation of the Coulomb effects in particle beam segments. Accordingly, first of all, we shall compare the ANALIC program with the INTERAC program for looking into how the results obtained by the programs fit each other. We then compare the ANALIC program with the MONTEC program\(^7\), which is one of successful Monte Carlo simulation programs\(^8,9,10\) in the study of the Coulomb effects, in order to obtain a understanding what is the difference between the analytical approach and the Monte Carlo simulation. We believe that this comparison is important because their approaches of evaluating the Coulomb effects are very different\(^6\). We finally compare the ANALIC program with our experiments, with which we can say that the charged particle optical instruments
are really limited by the Coulomb effects because not only can the effects been estimated with computer programs but also can they been measured with instruments. Only very few examples have been reported in the measurement of the Coulomb effects in particle optical systems.

**Tab.12.1 Comparison between the evaluations of the Coulomb interactions in a one-lens focused ion beam system with ANALIC program and INTERAC program.**

<table>
<thead>
<tr>
<th>Aperture D (mm)</th>
<th>0.05</th>
<th>0.08</th>
<th>0.1</th>
<th>0.2</th>
<th>0.5</th>
<th>1.0</th>
<th>2.0</th>
<th>5.0</th>
<th>8.0</th>
</tr>
</thead>
<tbody>
<tr>
<td>Current I (nA)</td>
<td>2.186e-3</td>
<td>5.597e-3</td>
<td>8.746e-3</td>
<td>3.498e-2</td>
<td>2.186e-1</td>
<td>8.746e-1</td>
<td>3.498e+0</td>
<td>2.186e+1</td>
<td>5.597e+1</td>
</tr>
<tr>
<td>$\Delta E_{\text{beam}}$ (eV)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>ANALIC</td>
<td>5.162e-6</td>
<td>3.383e-5</td>
<td>8.250e-5</td>
<td>1.322e-3</td>
<td>5.094e-2</td>
<td>2.133e-1</td>
<td>4.270e-1</td>
<td>1.005e+0</td>
<td>1.692e+0</td>
</tr>
<tr>
<td>INTERAC</td>
<td>2.966e-6</td>
<td>1.944e-4</td>
<td>4.745e-4</td>
<td>7.591e-3</td>
<td>1.063e-1</td>
<td>2.135e-1</td>
<td>4.265e-1</td>
<td>1.055e+0</td>
<td>1.645e+0</td>
</tr>
<tr>
<td>$d_{\text{m}}$ (µm)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>ANALIC</td>
<td>5.149e-6</td>
<td>3.375e-5</td>
<td>8.239e-5</td>
<td>1.318e-3</td>
<td>5.065e-2</td>
<td>2.015e-1</td>
<td>4.032e-1</td>
<td>1.004e+0</td>
<td>1.603e+0</td>
</tr>
<tr>
<td>INTERAC</td>
<td>2.975e-5</td>
<td>1.938e-4</td>
<td>4.732e-4</td>
<td>7.506e-3</td>
<td>1.005e-1</td>
<td>2.016e-1</td>
<td>4.029e-1</td>
<td>9.861e-1</td>
<td>1.556e+0</td>
</tr>
</tbody>
</table>

### 12.2 Comparison between ANALIC and INTERAC

In this section, the Coulomb interactions in a one-lens focused ion beam system is investigated by using both the ANALIC program and the INTERAC program. This example column is the ion beam pattern generator system with two lenses built in our laboratory, as shown in figure 7.1 or figure 8.1. This system can also operate at a simpler mode, only using one lens, when the first lens is turned off. In this case, the sketch of the column is shown in figure 12.1, and its symbolization in figure 5.1(1). The object distance P and image distance Q of the one-lens column are 230 mm and 50 mm, the reduced source brightness $B=2\times10^6$ A.m$^2$.sr$^{-1}$.V$^{-1}$, the virtual source radius $r_v=25$ mm and the energy spread of the source $\Delta E=5$ eV (FWHM). The lens of this column is a unipotential lens, which is designed to withstand 30 kV high voltage. Accordingly, the magnification of the column M is 0.2174, and the focal distance $f=f_s=f_n=41.1$ mm. This results in the spherical and chromatic aberration coefficients $C_{\text{s}}(\infty,f_s)$ and $C_{\text{c}}(\infty,f_s)$ to be 4945 mm and 113.3 mm, according to the same calculation as that for figure 7.2. The beam energy is 15 keV, which is the usual energy of the system.

Suppose that the spatial and angular distributions of the beam current in the example column are all Gaussian, i.e. $\text{KK}=11$. The beam current increases from 2.2 pA to 56 nA when the aperture size D varies from 0.05 mm to 8.0 mm. We first calculated the spherical aberration, the chromatic aberration, the Boersch effect, the trajectory displacement effect and the space charge effect by using
the concerned formulas presented in chapter 5. These formulas are in fact included in the ANALIC program. We then did the same calculation with the INTERAC program. The main results from the two calculations are listed in table 12.1.

In the evaluation with the INTERAC program, we considered the whole column in figure 12.1 as two semi-crossover beam segments. The total Coulomb interaction effects listed in table 12.1 are the linear summation of the contributions from the two segments. In INTERAC program, the summation from different contributions can also be realized based on a gamma-rule. The difference between the linear-rule and gamma-rule summations will be discussed in the next section.

The comparison in table 12.1 is mainly focused on the total energy spread $\Delta E_{\text{foc}},$ (FWHM and FW50) due to the Boersch effect in the two beam segments, the total trajectory displacement effect disc $d_{\text{tra}},$ (FWHM and FW50) in the image plane $b,$ the total space charge defocussing distance $\Delta z_{\text{foc}},$ departing from the image plane $b$ and the total space charge spherical aberration disc $d_{\text{sch}},$ in the image plane $b$ of figure 12.1. It can be seen from table 12.1 that the difference between two calculations is very small and that the relative error in every current case is less than 5%.

Reviewing chapter 5 we know that the evaluations of $\Delta E_{\text{foc}},$ $d_{\text{tra}},$ $\Delta z_{\text{ch}},$ and $d_{\text{sch}},$ in table 12.1 are based on equations (5.18), (5.27), (5.31) and (5.37), however, these equations are further based on the results of chapters 3 and 4. Therefore, the limited departure between the two calculations in table 12.1 is in fact a proof that our models and equations from chapter 2 to chapter 5 are correct and accurate. For this reason it comes to the conclusion that the calculation accuracy with the ANALIC program is as good as that with INTERAC program over the full variable range usually met in a charged particle optical column.

12.3 Comparison between ANALIC and MONTEC

In this comparison calculation, we again use the configuration of the two lens focussed ion beam system shown in figure 7.1, but the calculation approach is a little bit different from chapter 7, in
which the combined calculation of the lens aberrations and Coulomb effects as well as the full system optimization are the main topic. We here only concentrate ourselves on the evaluation of the Coulomb interactions without including the lens aberrations, thereby taking lens aberration coefficients \( C_{a1}=C_{a2}=C_{e1}=C_{e2}=0 \). Besides, the source energy spread \( \Delta E \) is assumed to be zero. The crossover is fixed at \( z=156 \) mm for the total column magnification \( M=1 \). The first aperture size is also fixed at \( D_1=0.2 \) mm, and the variation of the beam current \( I \) is realized by changing the voltage on the extractor. The beam energy in the whole column is 30 keV.

First of all, we use a Monte Carlo (MC) simulation method to evaluate the Coulomb interaction effects in the column of figure 7.1. This technique offers us a direct approach to determine the impact of Coulomb interactions on the properties of a complete particle optical instrument. The essential part of a MC simulation is a ray tracing routine, which computes the particle trajectories by numerical integration of the equations of motion, taking into account the mutual Coulomb repulsion. One of the programs of the Monte Carlo simulation, named MONTEC, was written by Jansen\(^7\), which includes the DRIFT1, DRIFT2 and DRIFT3 simulations. DRIFT1 is based on a numerical ray-tracing algorithm, operating with variable time step. DRIFT2 is a semi-analytical ray-tracing routine, based on a reduction of the full N-body problem to two-particle interactions\(^6\). This algorithm is typically one to two orders of magnitude faster than DRIFT1, thereby being referred to as Fast Monte Carlo (FMC) simulation\(^13\). However, DRIFT3 is for the simulation of the high particle density region found in the vicinity of the source, which is also based on a reduction to two-particle interactions. We only use DRIFT1 and DRIFT2 algorithms in our computations.

Figure 12.2 shows four ion position plots for the two-lens focussed ion beam system of figure 7.1 with the evaluation of DRIFT1, which are found in the target plane of the system (\( z=260 \) mm) with total 1500 gallium ions. Figure 12.2(1) is the unperturbed particle positions, which were computed without taking into account the Coulomb interactions. In this case, all ions are focussed on the target without the radial expansion of the ions. Accordingly, figure 12.2(1) shows the ideal source image. However, with the increase of the beam current from \( I=0.1 \) nA through \( I=1.0 \) nA to \( I=10.0 \) nA, the ion beam rapidly expands in the radial direction due to the mutual Coulomb repulsion, as can been seen from figure 12.2(2) through figure 12.2(3) to figure 12.2(4), respectively.

In addition to the particle position distributions of figure 12.2, the energy spread distribution \( \rho(\Delta E) \) generated in the whole column of figure 7.1 due to the Boersch effect was also evaluated by using the DRIFT1 algorithm, as shown in figure 12.3. This distribution trend was expected and described in figure 3.2. After having completed a simulation, the MONTEC program gives an even polynomial function of six terms for fitting both the particle position distribution and the energy spread distribution, as can be seen from figure 12.3. With this fit function, the Coulomb interaction
effects are evaluated by using the FW50 or FWHM measurement. Figures 12.2 and 12.3 can also be calculated by using the DRIFT2 algorithm of the MONTEC program.

By using the same conditions as the MONTEC program did in figures 12.2 and 12.3, we also calculated the Coulomb interactions in the focused ion beam system of figure 7.1 with the ANALIC program and the INTERAC program. Figures 12.4, 12.5 and 12.6 show the complete comparisons of the results obtained from different algorithms.

We see from figure 12.4 that for the evaluation of the total energy spread $\Delta E$ in the whole column of figure 7.1, the DRIFT1 algorithm closely fits the DRIFT2, and the ANALIC closely fits the INTERAC with a linear-rule summation. In the lower current range, the ANALIC and the INTERAC with a linear-rule fit MONTEC reasonably, however, there is a larger deviation between the former and latter evaluations in the case of a higher current range. The reason is that the former evaluation is based on the first-order perturbation approximation\textsuperscript{6,14}, which assumes that the deviations of the actual positions of the field particles at time $t$ from the unperturbed trajectories at the same time are small, however, this assumption will become unrealistic more and more with the increase of the current higher and higher. Accordingly, the ANALIC and INTERAC algorithms overestimate the Boersch effect in the higher current range. Looking at figure 12.4, we find that the INTERAC with a gamma-rule summation greatly overestimates the Boersch effect in the lower current range. This is unreasonable. What we can explain for this effect is that the gamma-rule summation is not correct or not necessary to be used for the addition of different contributions. This is not the final conclusion, the reason of which is still under investigations\textsuperscript{15,16}.

We see from figure 12.5 that for the evaluation of the trajectory displacement effect $d_{\text{tra}}$ in the column of figure 7.1 by using five algorithms.
greatly overestimates the trajectory displacement effect in a lower current range but also underestimates the effect in a higher current range.

The evaluation of the space charge defocussing distance with four algorithms is presented in figure 12.6. In this calculation, the ANALIC is still in closely agreement with the INTERAC with a linear-rule summation. The DRIFT1 fits the DRIFT2 only in the higher current range, but failing in the lower current range. Compared the MONTEC with the ANALIC or the INTERAC with a linear-rule, they fit well in the higher current range, but failing in the lower current range. We believe that the evaluation of the space charge defocussing distance with the ANALIC is more accurate than that with the MONTEC in the lower current range, the reasons are 1) there are very few approximations in the derivation for the analytical equations of evaluating the space charge defocussing aberration in chapter 4 in the lower current range, and 2) there is a difficult determination of the defocussing distance with a Monte Carlo simulation in the lower current range.

**Fig. 12.6** The evaluation of the space charge defocussing distance $\Delta z_{ foc }$ with four algorithms.

**Fig. 12.7** Comparison between the calculated probe size with the ANALIC program and the measured probe size with the mode one experiment.

12.4 Comparison between ANALIC and experiments

We now discuss the measurements of the Coulomb interactions in two focussed ion beam instruments and the comparison between the calculated Coulomb effects with the ANALIC program and the measured Coulomb effects from our experiments.

12.4.1 Comparison with mode one

Two approaches are used in our measurements of the Coulomb effects in focussed ion beam systems. One is the mode (mode one) in which the beam shape in the whole optical column is fixed but
the emission current of the source is variable, and the other is the mode (mode two) in which the emission current is constant but the beam shape varies either with the column magnification or with the aperture size or with the aperture position. The design of the two experimental modes is based on the fact that the Coulomb effects depend not only on the beam energy (the particle mass, current and potential) but also on the beam geometry (the beam segment length and beam angle). These dependencies were already described in chapter 6, for instance in Eq. (6.5).

The probe size of a charged particle optical instrument can be measured by, for instance, scanning the beam over a knife edge and measuring the beam current variation while the beam scanning\textsuperscript{18}. In the knife edge scanning method, the 12-88% measured width of the beam can be easily proven to be equal to the spot size with the FW50 measurement\textsuperscript{6} if the measured beam is supposed to be in Gaussian distribution. It is obvious that the measured probe size can be regarded as the total probe size $d_{\alpha x}$ defined as Eq. (5.44), which is a combined measurement of the lens aberrations and the Coulomb effects in a practical system.

With the knife edge scanning method, the mode one experiment was carried out in the ion beam pattern generator (IBPG) system shown in figure 1.1, in which the total probe size in the image plane of the second lens $d_{\alpha x}$ was measured at different Ga\textsuperscript{+} probe currents, as shown in figure 1.3. We now evaluate the total probe size $d_{\alpha x}$ in the same system by using ANALIC program and the same conditions as the experiment did. The result of this evaluation is shown in figure 12.7, in which we also indicate the measured $d_{\alpha x}$ shown in figure 1.3 for comparison.

We see from figure 12.7 that 1) both the measured $d_{\alpha x}$ and the calculated $d_{\alpha x}$ increase with the probe current. The higher the current the larger the deviation between the ideal source image and the total probe size including the Coulomb effects will be, and 2) the calculated probe size fits the measured probe size reasonably. Taking into account greater than 20% of space charge defocusing aberration \textup{defoc}\% > 0.2 in Eq. (5.34)) in the addition of the total probe size (Eq. (5.44)) results in an overestimation of the Coulomb effects, however, without including the defocusing (\textup{defoc}\% = 0) gives a underestimation. Based on this observation, accordingly, it seems better to choose the parameter \textup{defoc}\% to be between 0.1 and 0.15 when using the ANALIC program.

**12.4.2 Comparison with mode two**

To demonstrate the mode two experiment, one requires to vary the beam shape. This can be realized by changing either the aperture size or aperture position or crossover position. For the experiment we used the two-lens focussed ion beam system built in our laboratory, as shown in figure 12.8. This system can be considered as being equipped with four apertures. The first aperture,
staying away from the tip DZ₁=1 mm, is in fact the extractor with a diameter D₁=1 mm. The second is the source lens aperture with the distance DZ₂=4 mm and diameter D₂=1 mm. The third is the real aperture used to select the beam current with the distance DZ₃=10 mm and diameter D₃=50 μm. The fourth is also a real aperture which is placed at DZ₄=88 mm with size D₄=50 μm and used to select the probe current.

As seen from figure 12.8, the probe current is greatly limited by the third and fourth apertures. The current passing through D₃ is normally less than 0.1% of the tip emission current.

In the measurement of the total probe size dₜₜ, the beam energy in the whole column is 14589 eV, the current in the beam section between the third and fourth apertures is about 800 pA. The knife edge scanning method was again used for the 12-88 % measurement mentioned previously. The total probe size dₜₜ was measured at different beam shapes and different probe currents by changing the column magnification M. The variation of the magnification results from the adjustment of the voltages on the electrodes of the two lenses. The measured probe size dₜₜ is shown in figure 12.9, in which we see that the probe size varies with the magnification and a minimum probe size is found.

The evaluation of the Coulomb effects is different from that of the lens aberrations in the system of figure 12.8. For the latter calculation, one can only consider the shaded beam sections of figure 12.8, however, for the former, the beam sections (including the beam segments in the source region) surrounded by the outer ray, have to be taken into account. Accordingly, the numerical evaluation method described in chapter 3 was used for the calculation of the statistical Coulomb effects in the practical system of figure 12.8. Figure 12.9 presents three calculated total spot sizes, the total geometrical aberration disc dₕₕ, the total Coulomb interaction disc dₜₜ and the total probe size dₜₜ, which are defined as Eq.(5.42), Eq.(5.43) and Eq.(5.44), respectively. In figure 12.9, the evaluation
of the lens aberrations is followed the approaches described in chapter 7. Because of the large changing range of the beam shape and the probe current with the magnification M, a peak and a minimum probe sizes are observed in figure 12.9. It can be seen that the lens aberrations dominate the system in larger demagnifications, but the Coulomb interactions become a main factor in larger magnifications. The calculated total probe size is in reasonably agreement with the measured probe size especially in around the magnification where the minimum probe size is found.

If the fourth aperture in figure 12.8 is removed, the probe current remains the same for every magnification or crossover position. In this case, the probe size was again measured and calculated respectively in a large range of the magnification, as shown in figure 12.10. It is found from figure 12.10 that the calculated total probe size is still reasonably consistent with the measured probe size.

In order to check the capability and accuracy of the ANALIC program more widely, we now consider another imaging mode of the system in figure 12.8. Since the practical system of figure 12.8 can operate at both the crossover mode and the non-crossover mode based on the optical requirements listed in table 2.1, we now use the non-crossover mode instead of the crossover mode and repeat the previous exercise. Without the fourth aperture D₄, the total probe size dₜot was measured and calculated respectively in the possible magnification range of the non-crossover mode. The results are presented in figure 12.11. We see from figure 12.11 that the calculated probe size with the ANALIC program is close to the measured probe size in the case of the non-crossover mode of the instrument.

In the evaluations of figures 12.9, 12.10 and 12.11, 15% of space charge defocussing (defoc% = 0.15) was assumed in the addition of the total probe size. The beam was supposed with an uniform angular distribution, thereby the space charge spherical aberration disc dₛ is being considered as zero.

12.4.3 Error analysis

We learn from figures 12.7, 12.9, 12.10 and 12.11 that the deviation between the measured probe size and the calculated probe size still remains although the agreement of them is reasonable in a larger variable change range. The main reasons causing the deviation are investigated as follows.

1) The Gaussian beam is an ideal limit beam. There is no Gaussian beam in practice no matter how to change the system variables including the beam current. A practical beam can only stay either in the pencil beam regime or in the Lorentzian regime or in the Holtsmark regime, but the problem is that the practical beam changes from one regime to another when one of system variables varies. When measuring the probe size with the knife edge scanning method, it is very difficult to determine what percentage range of the current should be considered to fit the FW50 measurement because we
in fact do not know what is the real regime of the measured beam. For a large variable changing range, it is an approximation to simply assume that the measured beam is Gaussian and that the 12-88% measurement is equal to the FW50 measurement. However, in the calculation of the total probe size, the FW50 measurement really means the width containing the 50% beam current no matter which regime the calculated beam stays. This implies that in our previous comparisons the definition of the measured probe size is, to a certain extent, different from that of the calculated probe size.

2) For the evaluations of the lens aberrations and the Coulomb effects in a practical optical column with the ANALIC program, the lenses are ideally regarded as thin lenses, but, they are in fact not. Accordingly, the magnification value of the measured probe size could be different from that of the calculated probe size in figures 12.9, 12.10 and 12.11. In other words, there is a shift between the measured probe size and the calculated probe size in the magnification domain.

3) The accumulated error and the summation error are partly responsible for the deviation between the measured and the calculated probe sizes. Because every individual spot size is independently evaluated based on different models, every evaluation has an error to a certain extent. The accumulated error increases when the calculated spot sizes are summarized together by using the method of a power addition (Eq.(5.44)). On the other hand, the addition equation of the total probe size (Eq.(5.44)) is only a simple extension of the equation (Eq.(5.42)) used to summarize the lens aberrations\(^9\). In the case of a large variable range, this extension method is not proven to be accurate enough yet.

12.5 Conclusions

The correctness and reliability of the ANALIC program have been verified through three approaches described in this chapter.

The accuracy of the program is as good as that of the INTERAC program since their relative deviation of the evaluation for Coulomb effects is less than five percent. The reason of the good agreement is that both the ANALIC and the INTERAC are commonly based on the theories of the first order perturbation approximation and the approximate two-particle dynamics. Note that the conclusion is only applicable to the case of the linear-rule summation.

Compared to the results obtained by using the MONTEC program, the INTERAC program with a gamma-rule summation greatly overestimates the Boersch effect and the trajectory displacement effect in the lower current range, however, the ANALIC program with a linear-rule summation is consistent with the MONTEC. For the evaluation of the trajectory displacement effect in the higher current range, the ANALIC still fits the MONTEC reasonably, but the INTERAC underestimates this effect. Both the ANALIC and the INTERAC with a linear-rule overestimate the Boersch effect in the higher current range. The Monte Carlo simulation seems failing in the evaluation of the space charge effect in the lower current range, instead, the ANALIC can present not only simpler but also more accurate studies in this range.

Compared to the results measured practically, which are obtained from two experimental approaches, the calculated probe size with the ANALIC program is also in agreement with the measured probe size in a large changing range of system variables. This further explains that the linear-rule summation is applicable to the addition of the Coulomb effects from the different contributions in different beam segments of a complete particle optical column.
Acknowledgement

The author of this thesis thanks Dr. Jianhua Bi for his work on measuring the probe sizes in figures 12.9, 12.10 and 12.11.

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5. G.H. Jansen, INTERAC Program Package (1989), distributed by Delft Particle Optics Foundation, Delft University of Technology, the Netherlands.
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13 Further investigations on Coulomb interactions in charged particle optical columns

Abstract This chapter deals with four different studies, which belong to our further investigations on Coulomb interactions. First of all, it looks into the space charge aberrations in an accelerating or decelerating field and presents the equations used to evaluate the field aberration, the first order aberration and the third order aberration in charged particle optical columns. It then evaluates the statistical Coulomb effects in the vicinity of a Schottky emitter and in the whole region of a high brightness electron source. As a result, a group of quantitative dependencies of the Coulomb effects on the source parameters are presented, with which we conclude that the Boersch effect plays a major role in the high brightness source, but the trajectory displacement effect is negligible. Next, it investigates the Coulomb effects in ALG-1000 ion beam lithography system, which is considered as a typical ion beam projection column with accelerating and decelerating fields. Based on what we find in the study, it predicts that it is difficult for the considered ALG-1000 system to achieve an expected resolution at or below 0.18 μm. Finally, it estimates the dependence of the relative position between a test particle and a field particle on time. This relation is considered as particularly important in the study of an incomplete collision between two particles.

13.1 Introduction

Following a similar approach of evaluating the laminar flow in a drift space, Hutter¹ used the method presented by Vibrans² to calculate the spreading of an electron beam in an accelerating field. However, this is in fact not a calculation of the space charge aberrations in accelerating or decelerating field. A complete investigation of the space charge aberrations in a crossover beam segment was the work by Jansen³, but which did not take into account the acceleration of the beam. In chapter 4 of this thesis, we derived the general ray equation that includes the acceleration and the space charge effect and calculated the space charge aberration discs in the object or image plane of a lens system, but in which the evaluation of the space charge aberrations was still limited in a drift space. For these reasons, this chapter is first to research into the space charge aberrations in an accelerating or decelerating field.

The evaluation of the Coulomb effects in charged particle sources is considered as a difficult subject. Therefore, only a very small number of reports on the topic can be found in literature. Using a Monte Carlo simulation method, Ward⁴ calculated the virtual source size for a liquid metal ion source including taking the Coulomb interactions into account. A total different approach from Ward’s will be used in this chapter for the investigation of the Coulomb interactions in high brightness electron sources. Based on the optical model of a Schottky emitter described in section 2.2 and Ref.[5] and the numerical evaluation model of the statistical Coulomb effects presented in section 3.4 and Ref.[6], we shall study the dependence of the statistical Coulomb effects on the source parameters. The investigation will be carried out not only in the vicinity of the emitter but also in the whole region of the source.

The resolution of particle beam projection instruments is also limited by the Coulomb interactions. This problem is investigated in this chapter by evaluating the field defocussing size due to the acceleration, the energy spread due to the Boersch effect and the stochastic position blur due to the statistical angular deflection in the well-known ALG-1000 ion beam lithography system⁷.⁸.⁹. The
presented evaluation approach may be applicable to calculate the Coulomb effects in other particle projection systems, for instance SCALPEL\textsuperscript{10} and ALPHA5X\textsuperscript{11}, since these instruments have a similar configuration.

The last part of the chapter is focussed on the study of the relation between the relative position of two particles and time, in which we mainly pursue to find simpler expressions of the relation since the considered problem is so important that it in fact becomes a key of evaluating the statistical Coulomb effects.

13.2 Space charge aberrations in accelerating and decelerating fields

Figure 13.1(1) shows a convergent beam segment in an uniform accelerating (or decelerating) field. The beam potentials in the planes of $z=0$ and $z=Q$ are $V_1$ and $V_2$, and the potential distribution $V(z)$ and electric field distribution $E$ in the beam segment are determined by

$$V(z)=V_1\left[1+\frac{\rho z}{Q}\right] \quad (13.1a)$$

$$E=-V_1\frac{\rho z}{Q}, \quad \rho=\frac{V_2}{V_1} \quad (13.1b)$$

Suppose that $r_p(z)$ and $r_{0p}(z)$ are the arbitrary trajectory and the characteristic trajectory before the accelerating field and the space charge effect are taken into account, and that $r_{0p}(z)_{z=0}=r_f$ as well as $r_{0p}(z)_{z=Q}=r_b$. An arbitrary particle ray $r(z)$ under the impacts of the accelerating field and the space charge effect is determined by the general ray equation Eq.(4.15). The relations between $r(z)$ and $r_b(z)$ as well as $r_{0p}(z)$ are expressed as Eq.(4.25). To be able to analytically solve the ray equation, we assume that the errors $\delta r_f(z)=r(z)-r_f(z)$ and $\delta r_{0p}(z)=r_0(z)-r_{0p}(z)$ in Eq.(4.25) are relatively small. Here, $r_f(z)$ is a characteristic trajectory with the influence of the field and the space charge effect. With this assumption, we can substitute $r(z)$ with $r_f(z)$ and $r_0(z)$ with $r_{0p}(z)$ in the right-side expression of Eq.(4.15). In this case, the solution of the general ray equation can be determined by
\[ r(z) = C_1 \left( \frac{r_f + 2 \frac{r_f - r_b}{\rho - 1}}{} \right) - C_2 \left[ \frac{2 \frac{r_f - r_b}{\rho - 1}}{1 + \frac{\rho - 1}{Q}} \right] \]

\[ - \frac{2Q}{\rho - 1} \int_0^z \left[ 1 + \frac{\rho - 1}{Q} \right] f(\xi) d\xi + \frac{2Q}{\rho - 1} \left[ 1 + \frac{\rho - 1}{Q} \right] \int_0^z \left[ 1 + \frac{\rho - 1}{Q} \right] f(\xi) d\xi \]

where

\[ f(z) = \mu_1 \left[ 1 + \frac{\rho - 1}{Q} \right]^{-3/2} \left[ c_0(z) \frac{r_p(z)}{r_{qp}(z)^2} + c_2(z) \frac{r_p(z)^3}{2r_{qp}(z)^4} + c_4(z) \frac{r_p(z)^5}{3r_{qp}(z)^6} + \cdots \right] \]  

(13.2)

(13.3)

\[ \mu_1 = \frac{l}{4\pi \sqrt{2\eta} \epsilon_0 V_1^{3/2}} \]  

(13.4)

In Eq. (13.3), the coefficient \( c_{2i}(z) \) (\( i = 0, 1, 2, \ldots \)) has the same meanings as those in Eq. (4.10). The solution Eq. (13.2) is applicable to the beam segment with any shape \( r_{qp}(z) \) and \( r_p(z) \). \( C_1 \) and \( C_2 \) are the integral constants determined by the characteristic trajectory \( r_{qp}(z) \). If \( r_{qp}(z) \) is supposed to be a straight line, i.e. \( r_{qp}(z) = r_f(r_f - r_b)/Q \), \( C_1 = C_2 = 1 \). In the following discussion we mainly consider this case. Eq. (13.2) can be expressed as

\[ r(z) = r_{fed}(z) + r_{1st}(z) + r_{3rd}(z) + r_{stb}(z) + \ldots \]  

(13.5)

where \( r_{fed}(z) \) is an aberration caused by the accelerating field and calculated by

\[ r_{fed}(z) = r_f + 2 \frac{r_f - r_b}{\rho - 1} - 2 \frac{r_f - r_b}{\rho - 1}(1 + \gamma z)^{1/2}, \quad \gamma = \frac{\rho - 1}{Q} \]  

(13.6)

\( r_{1st}(z) \) is the first order aberration produced by the space charge effect. It is evaluated by

\[ r_{1st}(z) = -2\mu_1 \frac{c_0(\xi)r_p(\xi)d\xi}{\gamma} + 2\mu_1 \frac{(1 + \gamma z)^{1/2}}{r_{qp}(\xi)^2} \int_0^z \frac{c_0(\xi)r_p(\xi)d\xi}{(1 + \gamma \xi)r_{qp}(\xi)^2} \]  

(13.7)

And, the third order aberration induced by the space charge effect is determined by

\[ r_{3rd}(z) = -\mu_1 \frac{c_2(\xi)r_p(\xi)^3d\xi}{\gamma} + \mu_1 \frac{(1 + \gamma z)^{1/2}}{r_{qp}(\xi)^4} \int_0^z \frac{c_2(\xi)r_p(\xi)^3d\xi}{(1 + \gamma \xi)r_{qp}(\xi)^4} \]  

(13.8)

It is seen from Eq. (13.5) that the particle ray \( r(z) \) with the combined impacts of the accelerating field and the space charge effect consists of a series of components described as the field aberration \( r_{fed}(z) \), the first order space charge aberration \( r_{1st}(z) \), the third order space charge aberration \( r_{3rd}(z) \) and so on. The space charge aberrations are determined by not only the space charge effect but also the accelerating field. This makes the problem more complicated than what we studied in chapter 4.

To calculate the integrals of Eqs. (13.7) and (13.8), we suppose that the characteristic trajectory
\( r_{\text{op}}(z) \) and the arbitrary trajectory \( r(z) \), which are the particle rays before the accelerating field and the space charge effect are considered, are determined by straight lines, i.e.

\[
\begin{align*}
    r_{\text{op}}(z) &= r_{1} - \alpha z \quad (\alpha > 0) \quad \text{and} \quad r_{\text{op}}(z) &= r_{1} - \beta_{0} z \quad (\beta_{0} > 0) \\
\end{align*}
\]  

(13.9)

Substituting Eq. (13.9) into Eq. (13.7) results in

\[
\begin{align*}
    r_{\text{ua}}(z) &= r_{1} m(z) + \alpha \Delta z(z) \\
\end{align*}
\]  

(13.10)

where

\[
\begin{align*}
    m(z) &= -\frac{2\mu_{1}}{\gamma} \int_{0}^{z} \frac{c_{0}(\xi) d\xi}{(1 + \gamma z)^{1/2} (r_{f} - \beta_{0} \xi)^{2}} + 2\mu_{1} \int_{0}^{z} \frac{c_{0}(\xi) d\xi}{(1 + \gamma \xi)(r_{f} - \beta_{0} \xi)^{2}} \\
\end{align*}
\]  

(13.11)

and

\[
\begin{align*}
    \Delta z(z) &= -\frac{2\mu_{1}}{\gamma} \int_{0}^{z} \frac{c_{0}(\xi) \xi d\xi}{(1 + \gamma z)^{1/2} (r_{f} - \beta_{0} \xi)^{2}} - 2\mu_{1} \int_{0}^{z} \frac{c_{0}(\xi) \xi d\xi}{(1 + \gamma \xi)(r_{f} - \beta_{0} \xi)^{2}} \\
\end{align*}
\]  

(13.12)

in which \( m(z) \) and \( \Delta z(z) \) indicate the lateral magnification and the longitudinal defocusing distance. Substituting Eq. (13.9) into Eq. (13.8) yields

\[
\begin{align*}
    r_{\text{ua}}(z) &= D(z) r_{1}^{3} + F(z) r_{1}^{2} \alpha + C(z) r_{1} \alpha^{2} + S(z) \alpha^{3} \\
\end{align*}
\]  

(13.13)

where

\[
\begin{align*}
    D(z) &= -\frac{\mu_{1}}{\gamma} \int_{0}^{z} \frac{c_{2}(\xi) d\xi}{(1 + \gamma z)^{1/2} (r_{f} - \beta_{0} \xi)^{4}} + \mu_{1} \int_{0}^{z} \frac{c_{2}(\xi) d\xi}{(1 + \gamma \xi)(r_{f} - \beta_{0} \xi)^{4}} \\
\end{align*}
\]  

(13.14)

\[
\begin{align*}
    F(z) &= \frac{3\mu_{1}}{\gamma} \int_{0}^{z} \frac{c_{2}(\xi) \xi d\xi}{(1 + \gamma z)^{1/2} (r_{f} - \beta_{0} \xi)^{4}} - 3\mu_{1} \int_{0}^{z} \frac{c_{2}(\xi) \xi d\xi}{(1 + \gamma \xi)(r_{f} - \beta_{0} \xi)^{4}} \\
\end{align*}
\]  

(13.15)

\[
\begin{align*}
    C(z) &= \frac{3\mu_{1}}{\gamma} \int_{0}^{z} \frac{c_{2}(\xi) \xi^{2} d\xi}{(1 + \gamma z)^{1/2} (r_{f} - \beta_{0} \xi)^{4}} + 3\mu_{1} \int_{0}^{z} \frac{c_{2}(\xi) \xi^{2} d\xi}{(1 + \gamma \xi)(r_{f} - \beta_{0} \xi)^{4}} \\
\end{align*}
\]  

(13.16)

\[
\begin{align*}
    S(z) &= \frac{\mu_{1}}{\gamma} \int_{0}^{z} \frac{c_{2}(\xi) \xi^{3} d\xi}{(1 + \gamma z)^{1/2} (r_{f} - \beta_{0} \xi)^{4}} - \mu_{1} \int_{0}^{z} \frac{c_{2}(\xi) \xi^{3} d\xi}{(1 + \gamma \xi)(r_{f} - \beta_{0} \xi)^{4}} \\
\end{align*}
\]  

(13.17)

in which \( D(z), F(z), C(z) \) and \( S(z) \) represent the distortion coefficient, the field curvature and astigmatism coefficient, the coma coefficient and the spherical aberration coefficient, respectively.

If the plane of \( z=Q \) in figure 13.1(1) is considered as the image plane of a lens, one is interested
in the beam spreading due to the accelerating field and the space charge effect in this plane. In this case, the beam spreading produced by the field is given by

\[ r_{\text{ef}}(Q) = r_f + 2 \frac{r_f - r_b}{\rho - 1} (1 - \rho^{1/2}) \]  

(13.18)

It is obvious that \( r_{\text{ef}}(Q) = r_b \) when \( \rho = 1 \). The beam spreading caused by the space charge effect is determined not only by the position \( z \) but also by the ray \( r_p(z) \), i.e. \( r_r \) and \( \alpha \). Substituting \( r_r \) for \( r_r \) and \( \beta_0 \) for \( \alpha \) yields a maximum value of the beam spreading. In the image plane of \( z = Q \), the beam spreading due to the first order aberration is given by

\[ r_{\text{if}}(Q) = r_m(Q) + \beta_0 \Delta z(Q) \]  

(13.19)

Unfortunately, the coefficients \( m(Q) \) and \( \Delta z(Q) \), which are determined by Eqs. (3.11) and (3.12) when \( z = Q \), cannot be evaluated analytically. For the same reason the maximum beam spreading in the image plane due to the third order aberration is calculated by

\[ r_{\text{sf}}(Q) = D(Q) r_f^3 + F(Q) r_f^2 \beta_0 + C(Q) r_f \beta_0^2 + S(Q) \beta_0^3 \]  

(13.20)

in which the coefficients \( D(Q) \), \( F(Q) \), \( C(Q) \) and \( S(Q) \) cannot be evaluated analytically either.

The field aberration \( r_{\text{ef}}(Q) \) is independent of the beam current \( I \). Figure 13.1(2) shows the dependence of the relative field aberration \( r_{\text{ef}}(Q)/r_b \) on the accelerating and decelerating fields, in which we suppose that an electron beam segment with \( V_1 = 30 \) kV, \( Q = 150 \) mm, \( r_b = 0.1 \) μm, \( \beta_0 = 0.5 \) mrad varies from the decelerating field \( 0.2 < \rho = V_2/V_1 < 1 \) to the accelerating field \( 1 < \rho < 3.5 \). It is seen that the field strongly alters the electron beam shape. The beam is compressed when \( \rho < 1 \) and expanded when \( \rho > 1 \).

The space charge aberrations are directly proportional to the beam current \( I \). Figure 13.1(3) was made by numerically calculating Eq. (13.19), in which we see the relative first order aberration \( r_{\text{if}}(Q)/r_b \) decreases with the increase of the voltage \( V_2 \). The conditions for figure 13.1(3) is the same as those for figure 13.1(2). In the image plane \( z = Q \), the beam spreading due to the first order aberration \( r_{\text{if}}(Q) \) is always less than \( r_b \) when the current is lower than 30 nA, and always greater than \( r_b \) when the current higher than 400 nA in the considered beam energy range. If the angular distribution of the considered beam is Gaussian, the third order space charge aberrations should be taken into account. In this case one has to evaluate the coefficients determined by Eqs. (13.14), (13.15), (13.16) and (13.17) numerically. However, if the angular distribution of the beam is uniform, all space charge aberrations higher than three order are equal to zero since the coefficients in Eq. (13.3) \( c_{2i} \) \((i = 1, 2, 3, \ldots) = 0 \).

### 13.3 Evaluation of Coulomb effects in high brightness electron sources

#### 13.3.1 Coulomb effects in vicinity of Schottky emitter

The high brightness Schottky emitter has been modeled as figure 2.1. We are now at the position to calculate the statistical Coulomb interactions in the emitter. The numerical method described in section 3.4 has to be used to perform this evaluation since the beam in the source region is in an accelerating field.

The energy spread due to the Boersch effect is calculated by
\[ \Delta E_{\text{Boe}} = \frac{1}{\int r_i(z) \text{d}z} \left[ F_{\text{r}}[r(z), V(z), I] \right] \text{d}z, \quad \frac{\text{d}V}{\text{d}z} = V_i \left[ 1 + \frac{1}{L - z_i} \right], \quad \rho = \frac{V}{V_i} \]  

(13.21)

where the beam shape \( r(z) \) is determined by Eq.(2.2), the beam potential distribution \( V(z) \) is assumed to be linear, and the energy spread function \( F_{\text{r}}[r(z), V(z), I] \) is given by Eq.(3.50).

The expression of evaluating the trajectory displacement blur \( d_{\text{tra}} \) in Eq.(3.51) should be modified since we now intend to calculate the blur referred to the image plane \( z = L - L_i \) of the extractor lens, not to the object plane \( z = z_i \). Based on the model presented by Barth, Jansen derived this expression. It is

\[ d_{\text{tra}} = \frac{2}{L} \left[ \frac{2(L - z_i - z)}{V(z)} + 1 \right] \left[ F_{\text{r}}[r(z), V(z), I] \right] \text{d}z \]  

(13.22)

where the angular deflection function due to the trajectory displacement effect \( F_{\text{r}}[r(z), V(z), I] \) is still determined by Eq.(3.53).

Based on the emission model of figure 2.1 and the calculation models of Eqs.(13.21) and (13.22), we can evaluate the statistical Coulomb effects in the vicinity of the emitter from two approaches. One is to vary the object of the extractor lens and the other to change the current of the emission. As seen from figure 13.2, the first approach is used to observe the variation of the Coulomb effects with the modelling of figure 2.1 and the second to evaluate the influence of the Coulomb effects on the obtainable current. In both evaluations, the final results depend on several emitter parameters. Based on a practical Schottky gun (XL-FEG), the typical values of these parameters are: the angular current density \( J_a = 0.4 \) mA/sr, the emission current \( I = 200 \) mA, the virtual source diameter \( d_v = 20 \) nm, the tip electric field \( E_t = 5.10^8 \) V/m, the tip radius \( R_t = 0.8 \) \( \mu \)m, the extractor voltage \( V_e = 5 \) kV, the object position \( z_i = R_s = 0.8 \) \( \mu \)m and the distance from the tip to the extractor \( L = 0.5 \) mm. One of these parameters varies around its typical value will result in a variation of the statistical Coulomb interactions in the vicinity of the source.

For the first approach described in figure 13.2(1), the magnification \( M \), the image distance \( L_i \), and the focal distance of the extractor lens \( f \) vary with the object position \( z_i \) or the tip electric field \( E_t \). This results in the changes of the beam shape \( r(z) \) and the potential distribution \( V(z) \), and further causes the variation of the energy spread \( \Delta E_{\text{Boe}} \) and the trajectory displacement blur referred to the image plane \( d_{\text{tra}} \). Figure 13.3 shows the computational results in terms of this approach. In the calculation of figure 13.3 we

![Fig.13.2 Two approaches to evaluate the statistical Coulomb effects in the vicinity of the Schottky emitter: (1) changing the object of the extractor lens and (2) changing the current of the emission.](image)

141
assume that when one of the emitter parameters changes, all other parameters are fixed at their typical values mentioned previously. The statistical Coulomb effects in figure 13.3 were evaluated with FW50 measurement by using the ANALIC program. We see from figure 13.3 that the energy spread due to the Boersch effect $\Delta E_{\text{Boe}}$ changes slightly with both the tip electric field $E_z$ and the object position $z_t$. The value of $\Delta E_{\text{Boe}}$ is around 0.2 eV. This value is close to the intrinsic energy spread (0.3 ~ 0.4 eV) of an usual Schottky gun. This means that the energy spread caused by the Boersch effect in a Schottky gun with the normal parameter values depends slightly on the modelling of the emitter. Together with the intrinsic source energy spread, the energy spread due to the Boersch effect $\Delta E_{\text{Boe}}$ will deteriorate the resolution of an electron beam instrument, especially, a chromatically limited system. The trajectory displacement blur referred to the image plane ($z=L-L_e$) $d_{\text{tra}}$, varies greatly with the tip electric field $E_z$ and also strongly with the object position $z_t$. This is because the trajectory displacement effect varies strongly with the position of an observed image plane. In the emitter model of figure 2.1, the image distance $L_e$ described as Eq.(2.3) depends strongly on both the object position $z_t$ and the object potential $V_1 (=E_z z_t)$. At the typical values of $E_z=5.10^8$ V/m and $z_t=0.8 \mu$m, $d_{\text{tra}}$ is about 3.6 nm. This value is much smaller than the source virtual diameter $d_0=20$ nm. Accordingly, the trajectory displacement effect in the vicinity of the emitter is in fact not a significant factor. Both increasing the tip electric field $E_z$ and making the tip sharper (decreasing the tip radius $R_e$) can reduce the trajectory displacement blur $d_{\text{tra}}$, with which the energy spread due to the Boersch effect only increases slightly.

For the second approach described in figure 13.2(2), the beam shape $r(z)$ determined by Eq.(2.2) varies with the emission (current $I$ and angular current density $J_\phi$) through the initial condition $\alpha_i$, thereby resulting in the changes of the energy spread $\Delta E_{\text{Boe}}$ in Eq.(13.21) and the trajectory displacement blur $d_{\text{tra}}$, in Eq.(13.22). Figure 13.4 presents the computational results in line with this approach. In the evaluation of figure 13.4, when the current $I$ or the angular current density $J_\phi$ alters around its usual value, all other parameters remain at the typical values mentioned previously. We see that both $\Delta E_{\text{Boe}}$ and $d_{\text{tra}}$ increase with the emission current $I$ or the current density $J_\phi$. This can be easily understood. The energy spread $\Delta E_{\text{Boe}}$ is still around 0.2 eV, and the trajectory displacement blur $d_{\text{tra}}$ is still much smaller than the virtual source diameter $d_0$, even at a higher current of 350 $\mu$A, $d_{\text{tra}}$ is only 4.8 nm.

Fig.13.3 Influence of the emitter modelling on the statistical Coulomb interactions. $R_e=0.8 \mu$m.
13.3.2 Coulomb effects in whole region of electron sources

A complete electron source equipped with a Schokky gun is already modeled as figure 2.2, in which three of the four apertures are cutting the beam. The third aperture $D_3$ is a real aperture used to select the beam current to the column.

In the model of figure 2.2, the virtual source is used to replace the real source in order to evaluate the optical performance including the Coulomb effects in a complete optical column conveniently. The virtual source model is characterized by the virtual source size $d_0 = 20$ nm, the half opening angle $\alpha_0$ defined as Eq. (2.4) and the image distance of the extractor lens $L_s$ determined by Eq. (2.3). Another important characteristic of a virtual source model is that the beam in the whole source region is equipotential. The value of the potential is equal to the extractor voltage $V_e$.

With the virtual source model, the energy spread due to the Boersch effect and the trajectory displacement blur referred to the virtual source can be respectively evaluated by

$$\Delta E_{Boe} = \int_0^p F_{Boe}(r(z), V_e, I(z)) dz \quad (13.23)$$

and

$$d_{tra} = \int_0^p z F_{tra}(r(z), V_e, I(z)) dz \quad (13.24)$$

where $p$ is the object distance of the source lens, as shown in figure 2.2. The energy spread function $F_{Boe}(r(z), V_e, I(z))$ and the angular deflection function $F_{tra}(r(z), V_e, I(z))$ are determined by Eq. (3.50) and Eq. (3.53), in which the beam shape $r(z)$ and the beam current $I(z)$ are now determined by the aperture sizes $D_1$, $D_2$, $D_3$ and $D_4$. The functions $F_{Boe}$ and $F_{tra}$ can be used to observe the distributions of the statistical Coulomb effects along the $z$-axis. Figure 13.5 shows these distributions. This figure was evaluated with the following conditions. Aperture sizes are $D_1 = D_2 = 400 \mu$m, $D_3 = 500 \mu$m, $D_4 = 1$ mm. The apertures and source lens are positioned at the places shown in figure 13.5. The extractor voltage is $V_e = 5$ kV, and the virtual source diameter $d_0 = 20$ nm. The emission current and the current density are $I = 200 \mu$A and $J_e = 0.4$ mA/sr, i.e. the half opening angle $\alpha_0 = 0.4$ rad. The beam current between the first aperture and the second aperture is 153 $\mu$A, between the second aperture and the third aperture 44 $\mu$A and behind the third aperture 11 $\mu$A.

As seen from figure 13.5 that the energy spread distribution due to the Boersch effect decreases rapidly with the increase of the position $z$. This explains that the Boersch effect occurs mainly in the vicinity of the virtual source. However, the angular deflection distribution decreases slowly with the
increase of the position $z$. This means that any beam segment at position $z$ has a contribution to the trajectory displacement blur $d_{\text{tra}}$. We see that no jumping in both the function $F_{\text{Boe}}$ and the function $F_{\text{tra}}$ occurs although the beam current $I_e$ has a jumping in different beam segments. This is because the beam segments run at the Holtsmark regime, in which the statistical Coulomb effects are directly proportional to the beam current $I_e$ and inversely proportional to the beam radius $r(z)$, and the power of the current is two times smaller than that of the radius, as can be seen from Eq. (3.50) and Eq. (3.53).

The real aperture $D_3$ controls the beam current to a practical electron beam column. Figure 13.6 presents an investigation how the aperture size $D_3$ (or how the column current $I_e$ behind $D_3$) influences the statistical Coulomb effects in the source region. The computational model of figure 13.6 and the concerned parameter values are the same as figure 13.5. We see that the energy spread $\Delta E_{\text{Boe}}$ due to the Boersch effect in the whole source region is almost independent of the column current $I_e$. This means that the beam segment between the aperture $D_3$ and the source lens makes a negligible contribution to the total energy spread in the whole source region. Accordingly, the energy spread in the source is mainly produced in the region in front of the aperture $D_3$, especially, in front of the aperture $D_1$. In the considered source region, the total energy spread is about 1 eV. This value should include the intrinsic energy spread of the source since we now utilize the virtual source model. However, the beam segment between the third aperture and the source lens has a contribution to the trajectory displacement blur referred to the virtual source plane $d_{\text{tra}}$. It is seen that $d_{\text{tra}}$ increases with the Column current $I_e$ when the beam segment behind $D_3$ varies from the pencil beam regime to the Holtsmark regime. After that, $d_{\text{tra}}$ does not increase any more with the current $I_e$ since in the Holtsmark regime the increase of the beam current counteracts that of the beam radius, as mentioned previously. The trajectory displacement blur in the whole source region is still much smaller than the virtual source diameter no matter how to change the column current. Accordingly, compared to the Boersch effect, the trajectory displacement effect does not play a significant role in the whole source region.
13.4 Evaluation of Coulomb effects in ion beam projection systems

The charged particle projection systems are already modeled as figure 2.7. The configurations of the projection systems, for the examples of ALG-1000†, SCALPEL† and A-LPHAX†, are similar to each other. For this reason we here only consider the evaluation of Coulomb effects in the ALG-1000 ion beam lithography prototype, which is being built for the goal of a resolution at and below 0.18 μm with the current higher than 1 μA. The focal distances of the first lens and the second lens in this model are \( f_1 = 630 \text{ mm} \) and \( f_2 = 470 \text{ mm} \), so the total column length is \( l = 2200 \text{ mm} \). The aperture is positioned in the plane of the crossover of the beam, and the beam semi-angle at the crossover is \( \alpha_c = 40 \text{ mrad} \), the diameter of the crossover \( 2r_c = 6.3 \text{ μm} \) and the potential in the crossover plane \( V_c = 200 \text{ kV} \). The beam potential in the mask and wafer planes are supposed to be 10 kV and 150 kV. For the ion particles the beam segments \( S_1 \) and \( S_2 \) are in an accelerating space, and the segments \( S_2 \) and \( S_3 \) in a decelerating space. The beam current I can be adjusted from 1 μA to 20 μA.

We intend to investigate three problems for the optical model of ALG-1000 system illustrated in figure 2.7. (1) How do the accelerating and decelerating fields in the column affect the focussing of the beam in the wafer plane? (2) Does the Boersch effect influence the resolution of the system? (3) Does the trajectory displacement effect influence the resolution of the system?

To simplify the investigation of the problems and to make the following discussion clearer, we assume that 1) the lenses \( L_1 \) and \( L_2 \) in the column of figure 2.7 are the thin lenses, thereby ignoring the influence of the lens fields, 2) the \( S_1 \) and \( S_3 \) beam segments are the cylindrical segments and \( S_2 \) and \( S_3 \) the half-crossover segments, and 3) the mask object is imaged onto the wafer perfectly before the accelerating and decelerating fields as well as the Coulomb effects are considered. These assump

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**Fig.13.7 Influence of the accelerating and decelerating fields in ALG-1000 ion beam lithography prototype on the focussing of the beam in wafer plane.**

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145
tions are shown in figure 2.7 and figure 13.7(1). The beam angle $2\alpha$ in figure 13.7(1) is $10 \mu$rad, and the crossover half angle $\alpha_0$ in figure 2.7 40 mrad for the ALG-column. Accordingly, the size of the mask object $d_1$ is 50.4 mm and the size of the wafer image $d_2$ is 37.6 mm.

Figure 13.7(1) shows the ideal imaging of the ion trajectories before the acceleration of the field is taken into account. However, figure 13.7(2) and figure 13.7(3) indicate the real ion trajectories under the acceleration. The trajectories are obtained by solving the ray equation described as Eq.(2.1), in which we suppose that the field distribution $V(z)$ is linear from the mask to the wafer. The potential in the mask plane is 10 kV, in the crossover plane 200 kV and in the wafer plane 150 kV. We see from figure 13.7(2) that a very serious defocussing occurs when the accelerating and decelerating fields are included. The focussed plane is moved from the wafer in figure 13.7(1) to the front of the wafer in figure 13.7(2). The defocussing distance is 345 mm and the defocussing size $W_{\text{foc}}$ on the wafer is 3.8 $\mu$m. The accelerating and decelerating fields cause not only the defocussing of the beam but also the contraction of the beam. We see from figure 13.7(3) that the original trajectory (broken line) without the influence of the fields contracts towards the axis. The maximum contraction $\Delta_{\text{max}}$ on the wafer is 3.5 mm and 4.5 mm for $\phi 50$ mm and $\phi 60$ mm masks respectively.

The defocussing and contraction produced by the fields can be corrected by adjusting the focal distances of the lenses $L_1$ and $L_2$. By means of the correction, the field defocussing should be reduced as low as possible, otherwise, the resolution of 0.18 $\mu$m may be challenged for the ALG-column because five percent of the defocussing size $W_{\text{foc}}$ is still larger than the expected resolution 0.18 $\mu$m. If we consider the alignment problem of a lithography system, the more accurate correction for the defocussing and contraction, say, with an accuracy of $10^{-5}$, is required.

The ionic species used in the ALG-1000 system are $H^+$ and $He^+$, which are produced by a duoplasmotron source or multicusp source. Including these ionic species, figure 13.8 shows the dependencies of the energy spread caused by the Boersch effect $\Delta E$ on the beam current $I$ for the ALG-column of figure 2.7. The energy spread in the four beam segments $S_1$, $S_2$, $S_3$ and $S_4$ were

---

**Fig.13.8 Energy spread due to the Boersch effect $\Delta E$ in the ALG-1000 system in the cases of $H^+$ beam (1) and $He^+$ beam (2).**
independently evaluated by using the numerical method described in Eq. (3.45) and Eq. (3.50). The curve with marker is the total energy spread of the column, which is a linear summation of the four individual energy spreads. In this evaluation, the impact of the accelerating and decelerating fields $V(z)$ on the beam shape from the mask to the wafer $r(z)$ is not considered, and the field distribution $V(z)$ is assumed to be linear.

It is found from figure 13.8 that the $\Delta E$ curve for $S_2$ segment overlays that for $S_3$ segment. This implies that the energy spread due to the Boersch effect is mainly produced in the crossover region and the contribution from the beam segment far away from the crossover is negligible. The energy spreads in the $S_1$ and $S_4$ beam segments are more than one order of magnitude lower than those in the $S_2$ and $S_3$ beam segments. For the $H^+$ beam, the total energy spread is lower than 1 eV, and for $He^+$ beam lower than 2 eV. Ideally speaking, these values do not influence the resolution of the ALG-1000 system. This argumentation can be explained by a simple evaluation. Suppose that the energy spread caused by the Boersch effect $\Delta E=2$ eV, the chromatic aberration coefficient of the second lens $C_{\alpha}=10 \text{ m}$ (much larger than the usual), the beam landing energy on the wafer $E_w=150 \text{ keV}$ and the beam landing half angle $\alpha_w=5 \mu\text{rad}$. Substituting these values into equation $d_{\text{ch,w}}=C_{\alpha} \alpha_w \Delta E/E_w$ yields $d_{\text{ch,w}}=0.67 \text{ nm}$. Here, $d_{\text{ch,w}}$ is the chromatic aberration blur due to the Boersch effect in the wafer plane. However, if the deflection effects of the edge ray caused by the field acceleration and the statistical trajectory displacement are considered, the landing angle of the outer ray $\alpha_w$ will increase rapidly, thereby increasing the chromatic aberration blur due to the Boersch effect.

It is found that the trajectory displacement effect really influences the resolution of the ALG-1000 system. Figure 13.9 presents this evaluation. The resolution $W$ on the wafer of the ALG-1000 ion beam lithography system is defined as:

$$W=2\delta_{\text{stock}}=2f_z \Delta\alpha_{\text{stock}}, \quad \Delta\alpha_{\text{stock}}=|\Delta\alpha_2-\Delta\alpha_3|$$

(13.25)
This definition only considers the stochastic position blur due to the trajectory displacement effect without including the influence of the Boersch effect and the space charge effect. In which δ_{stoch} expresses the position uncertainty (the stochastic blur) on the wafer due to the total statistical angular deflection Δξ_{stoch} in the S_i and S_j beam segments^{7,8}, and Δα_1 and Δα_2 are the statistical angular deflections in the S_2 and S_3 beam segment respectively. Accordingly, to evaluate the resolution W requires to calculate the statistical angular deflection Δα_2 and Δα_3. Because S_2 segment is in the accelerating field and S_3 segment in the decelerating field, we have to use the numerical method to compute Δα_2 and Δα_3. These calculations have been performed by using the ANALIC program for two ionic species (H^+ and He^+) and two measurements (FW50 and FWHM), as shown in figure 13.9 for the results of the computation.

As seen from figure 13.9 that the statistical angular deflection in the S_2 segment Δα_2 is larger than that in the S_3 segment Δα_3 no matter which ionic species or which measurement is considered. This is different from the evaluation of the energy spread in these segments. The deviation of the two statistical angular deflection Δα_2 and Δα_3 determines the resolution W in terms of Eq. (13.25). When the ALG-1000 system operates at the He^+ beam current higher than 1.2 μA or the H^+ beam current higher than 2.5 μA, it is found that the expected resolution of 0.18 μm can not be obtained. Note that this observation is only based on the evaluation of the statistical angular deflection in the S_2 and S_3 beam segments. For a practical system, the stochastic blurs produced in S_i and S_j beam segments even in the beam segments in front of the mask should be included. If the field defocussing size and the space charge effect are further considered, we are forced to draw a conclusion that it is difficult to reach the goal of a resolution at and below 0.18 μm with the current higher than 1 μA for the ALG-1000 lithography system, especially, when the He^+ beam is used.

13.5 Approximate two-particle dynamics

The mechanical problem resulted from the interaction of two charged particles is referred to as two-particle dynamics. Many investigations of physical phenomena are based on the two-particle dynamics. The basic subject of which is to solve the relation between the relative position of the two particles and time. Under the assumption of the complete collision of the two particles, the solution of this relation can be easily found by studying the motional asymptote of the two particles. Unfortunately, the collision of the two particles is usually incomplete in many cases of practical applications. One may use the numerical computation or the power series expansion and so on to solve the relation between the relative position and time in the case of the incomplete collision. However, the expressions of these solutions are usually too complicated to be used to calculate the further problems based on the two-particle dynamics conveniently. A very typical example of the problem is explicitly found in the evaluation of the statistical Coulomb

Fig.13.10 Unperturbed trajectories of a test particle A and a field particle B in the laboratory system.
interactions in particle beams. Jansen summarized the achievements of Ref. [13, 14, 15 and 16] and developed the theory of an extended two-particle approximation. The power series expansion method is used in Ref. [3] to calculate the relation between the relative position of the two particles and time. Because there exists a logarithmical term in the expression of the relative position versus time, this makes it impossible to calculate the trajectory displacement effect in particle beams analytically.

A new calculation method of the two-particle dynamics, approximate two-particle dynamics, is discussed in this section for simplifying the evaluation of the statistical Coulomb interactions. Based on the approximate two-particle dynamics, a series of concerned formulas of the displacements of the velocity and relative position of the test particle were derived by following the approach in Ref. [3]. The derivation and the obtained formulas are reported in Ref. [17]. In the rest of this section we only present the approximate solution of the relation between the relative position of two particles and time for an incomplete collision of particles. In order to compare with Ref. [3] and to simplify the expressions concerned, the notational system of Ref. [3] is utilized in this section. When quoting the formulas in Ref. [3], we shall use the symbol of J(*, ., .). For instance, J(6.5, 3) denotes the equation (6.5, 3) in Ref. [3].

Figure 13.10 describes the case in which a test particle A is moving at a unperturbed velocity $v_t$ along the beam axis (z-axis) and a field particle B is passing the x,y-plane of the laboratory system at a unperturbed velocity $v_r$. The angle between $v_t$ and $v_r$ is $\alpha$. An orbital plane C is spanned by the relative unperturbed velocity vector $v = v_r - v_t$ and the relative unperturbed position vector $r = r_r - r_t$. In figure 13.10, the beam parameters are indicated by the current $I$, the potential $V$, the mass of particle $m$, the length of a beam segment $L$, the position of the crossover plane $S_c = L_c / L$, the position of the image plane $S_i = L_i / L$, the radius of the crossover $r_c$ and the radius of the cylindrical beam $r_0$. The geometrical variables of determining the relative velocity and position of the particles are represented by $\xi = \{r, b, \psi, \Phi\} (\Phi = \psi - \phi)$ for the crossover beam segment or by $\xi = \{r, b\}$ for the cylindrical beam segment.

Other important parameters about time are the flight time of a particle $T_f$ in the beam segment, $T_i = L / v_z = L(m/(2 eV))^{1/2}$, the initial time $t_i$ and final time $t_f$ of the interaction, $t_i = S_c T_f$ and $t_f = (1 - S_i) T_f$. Here, time $t = 0$ means the moment that the field particle passes through the x,y-plane in figure 13.10.

According to the dynamical laws, the two-particle relative position $r(t)$ is determined by

$$\rho^2 \left( \frac{d\rho}{dt} \right)^2 + \rho^2 \left( \frac{d\theta}{dt} \right)^2 + \frac{2}{\rho \sqrt{q}} = 1 \quad (13.26)$$

$$\rho^2 \left( \frac{d\theta}{dt} \right) = 1 \quad (13.27)$$

in which the relative position $r$ and time $t$ are scaled by

**Fig. 13.11** Comparison between different solutions of the relative position versus time in the case of nearly complete collision ($T > 3.5$ and $v_t \neq 0$).
\[
\rho = \frac{r}{d_i}, \quad \tau = \frac{t}{t_s}, \quad d_i = \frac{J}{\sqrt{mE}}, \quad t_s = \frac{J}{2E}
\] (13.28)

where \( E \) is the particle energy and \( J \) the angular momentum. The quantity \( q \) is an important parameter and calculated by

\[
q = \frac{4J^2E}{C_0^2m}, \quad C_0 = \frac{e^2}{4\pi\varepsilon_0}
\] (13.29)

Substituting Eq.(13.27) into Eq.(13.26) yields

\[
\frac{d\rho}{d\tau} = \frac{H(\rho)}{\rho} \text{sign}(\tau - \tau_p)
\] (13.30)

where

\[
H(\rho) = (\rho^2 - \frac{2\rho}{q} - 1)^{1/2}
\] (13.31)

\( \tau_p \) in Eq.(13.30) is the scaled time of perihelion passage. Eq.(13.28), Eq. (13. 29), Eq.(13.30) and Eq.(13.31) exactly describe the relation between the relative position \( r \) and time \( t \) in the case of the crossover beam segment model with the initial relative velocity \( \mathbf{v}_i = \mathbf{v}_0 - \mathbf{v}_n \neq 0 \). In the case of the cylindrical beam segment model with the initial relative velocity \( \mathbf{v}_i = \mathbf{v}_0 - \mathbf{v}_n = 0 \), the relative position \( r(t) \) is determined by

\[
\left[ \frac{d\rho}{d\tau} \right]^2 + \frac{1}{\rho} = 1
\] (13.32)

Now the relative position \( r \) and time \( t \) are scaled by

\[
\rho = \frac{r}{d_i}, \quad \tau = \frac{t}{t_s}, \quad d_i = \frac{C_0}{E}, \quad t_s = \frac{m^{1/2}C_0}{2E^{3/2}}, \quad \nu_s = 2\sqrt{\frac{E}{m}}
\] (13.33)

To solve the relation between the relative position \( \rho \) and time \( \tau \) determined by Eq.(13.30) and Eq.(13.32) needs the knowledge of the initial conditions of the interaction. The descriptions about the relative motion of two-particle including the initial conditions of this motion can be found in Ref.[3,17]. After having determined the initial conditions, we can calculate the total energy \( E \) and the angular momentum \( J \) in Eq.(13.28), Eq.(13.29) and Eq.(13.33). With \( E \) and \( J \) the quantity \( q \) in Eq.(13.29) can be determined by

Fig.13.12 Comparison between the accurate solution and the approximate solution of the relative position versus time in the case of weak collision (\( T < 3.5, q \gg 1 \) and \( \nu_s \neq 0 \)).
\[ q = \left( \frac{m b v_i^2}{2 C_0} \right)^2 \left( 1 + \frac{4 C_0}{m v_i^2 r_i} \right), \quad b = (b_x^2 + r_i^2 \sin^2 \Phi)^{1/2} \]  

(13.34a)

where \( v_i \) and \( r_i \) express the modulus of the vector \( v \) and \( r \) at the initial conditions. For the asymptotic condition \( r_i \to \infty \), Eq. (13.34a) becomes

\[ q = q_e = \left( \frac{m b v_i^2}{2 C_0} \right)^2 \]  

(13.34b)

Integrating Eq. (13.30) results in

\[ |\tau - \tau_p| = T(\rho) = H(\rho) + \frac{1}{\sqrt{q}} \ln \left( \sqrt{\frac{q}{1+q}} \left( H(\rho) + \rho - \frac{1}{\sqrt{q}} \right) \right) \]  

(13.35)

and integrating Eq. (13.32) yields

\[ |\tau - \tau_i| = T(\rho) = \sqrt{\rho} \sqrt{\rho - 1} + \ln(\sqrt{\rho} + \sqrt{\rho - 1}) \]  

(13.36)

where \( \tau_i \) is the scaled initial time.

Eq. (13.35) and Eq. (13.36) specify the scaled time \( \tau \) as a function of the scaled separation of the particles \( \rho \). One has to calculate the inverse function of \( T(\rho) \) for a practical application, however, it is impossible to find an analytical expression of this inversion without introducing approximations. On the other hand, the expressions of the inversion obtained by using the numerical method (J(6.6.5)) and the power series expansion (J(6.7.4)) or (J(6.9.9)) are so complicated that one is not able to calculate the further problems based on these inversions analytically. For this reason, we suggest using approximate formulas to take the place of the inverse function of Eq. (13.35) or Eq. (13.36).

For a nearly complete collision of particles (\( T = |\tau - \tau_p| \gg 1 \)), the inverse function of Eq. (13.35) can be approximately determined by

\[ \rho(T) = T \]  

(13.37)

Figure 13.11 shows the comparison between the numerical accurate solution of Eq. (13.35), the series solution of J(6.7.4) and the approximate solution of Eq. (13.37). It is seen that Eq. (13.37) fits the accurate solution well when \( T > 3.5 \). This regime is just the situation of the nearly complete collision. For the weak collision with \( T = |\tau - \tau_i| < 3.5 \) and \( q \gg 1 \), the inverse function of Eq. (13.35) can be approximately expressed as

\[ \rho(T) = 1 + \frac{2}{\sqrt{q}} \tau - \frac{T^2}{3} - \frac{T^4}{88} \]  

(13.38)

The comparison between the numerical accurate solution of Eq. (13.35) and the approximate solution of Eq. (13.38) is presented in figure 13.12, which shows that the agreement between them is good in the given regime.

The inverse function of Eq. (13.36) can be simply expressed as
\( \rho(T) = 1 + T^2 / 7 \quad 0 \leq T \leq 3.5 \)  \hspace{1cm} (13.39a)

or

\( \rho(T) = -3/4 + T \quad 3.5 \leq T < \infty \)  \hspace{1cm} (13.39b)

Eq. (13.39a) and Eq. (13.39b) can be respectively used in the calculations of the weak interactions and the half-complete collision. They are considered as the analogues of J(6.9.18) and J(6.9.9), however, the formers are simpler. The function and its derivative of Eq. (13.39) are continuous anywhere. The comparison between the approximate solution of Eq. (13.39), the numerical accurate solution of Eq. (13.36) as well as the series solution of J(6.9.9) and J(6.9.18) is shown in figure 13.13. It is obvious that the agreement between them is very good.

13.6 Conclusions

The presented theory and evaluation on the space charge aberrations in an accelerating or decelerating field is a further development of our study in chapter 4, in which the acceleration of the field is not included. The space charge aberrations in an accelerating or decelerating field result not only from the repulsion of the space charge but also from the acceleration of the field. Because of these combined influences, the expressions of the space charge aberrations are much complicated than those without taking into account the acceleration. This makes it impossible to evaluate the aberration coefficients analytically.

In the high brightness electron sources with a Schottky emitter, the trajectory displacement blur is always much smaller than the virtual source size. Accordingly, the trajectory displacement effect is an insignificant factor in the source region. Oppositely, the energy spread caused by the Boersch effect can be as approximately large as the intrinsic energy spread of the sources. The energy spread due to the Boersch effect is mainly produced in the vicinity of the emitter, therefore, the variation of the column current does not change the total energy spread substantially.

The ALG-1000 ion beam lithography system mainly suffer from the field defocussing and the trajectory displacement effect. Because of the very small landing angle of the pattern beam, the additional chromatic aberration does not influence the resolution of the ALG-column although the energy spread caused by the Boersch effect may reach around 2 eV. The accelerating and decelerating fields in ALG-column can result in considerable field defocussing and beam contraction in the wafer plane. The resolution of the ALG-1000 instrument would suffer from the field effect if more than 95% of the defocussing and contraction induced by this effect could not be corrected. The

![Figure 13.13](#)
presented evaluation shows that the stochastic position blur caused by the statistical angular deflection becomes a main challenge of the resolution of the ALG-1000 system. To improve this situation, a best approach is to optimize the systems including to change the settings of the column parameters. For instance, it is obvious that adjusting the crossover position can change the stochastic position blur because the difference of the statistical angular deflections in two half-crossover beam segments determines the resolution of the system.

Many studies of physical phenomena are based on the two-particle dynamics. A very typical example of the application of the two-particle dynamics is in the calculation of the statistical Coulomb interactions in charged particle beams. A new method, referred to as approximate two-particle dynamics, of approximately evaluating the relative position of the particles is proposed in the last section of the chapter. The values of the proposed expressions are consistent with those of the numerical accurate solution of the relative position in the cases of the nearly complete collision, the half-complete collision and the weak interactions.

References

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Coulomb Interactions in Charged Particle Optical Columns

Summary

This thesis describes our researches on Coulomb interactions in charged particle optical columns in three subjects: theoretical backgrounds, computer software and application studies.

We first report, in the theoretical subject, the systemic approach and formulation of equations for the combined evaluation of lens aberrations, statistical Coulomb effects and space charge aberrations in a complete particle optical system. This includes the optical models from a source to an universal system in chapter 2, the analytical and numerical estimations of the statistical Coulomb effects and space charge aberrations in chapters 3 and 4, and the comprehensive calculations of the lens effects and Coulomb effects in a practical optical system with different imaging modes in chapter 5.

We have developed a computer program, named ANALIC, which can be utilized to directly optimize a multi-variable particle optical system with an arbitrary number of lenses and apertures, an arbitrary mode of imaging relations and an arbitrary distribution of beam energy, taking into account the combined evaluation of the lens effects and Coulomb effects in the system simultaneously. Such a program consists of fifteen thousand lines, which includes using a large number of data transmission techniques, numerical calculation techniques and interface techniques for the realization of the multi-function of the program. This is described in chapter 6, in which the fundamentals on which the program has been developed are given, although the technical description about the program is not included.

The subject of the application studies covers the investigations which include the Coulomb effects in focussed ion beam instruments (chapter 7), the better imaging mode of a particle optical system (chapter 8), the influence of system apertures on Coulomb effects (chapters 9 and 10), the estimation of the Coulomb interactions in low-voltage scanning electron microscopes (chapter 11), the verification of our theoretical backgrounds and programs (chapter 12), and some extended researches on the space charge aberrations in an accelerating field, on the statistical Coulomb interactions in high brightness electron sources and in ion beam projection systems (chapter 13). The achievements in these studies are:

1) We found the better imaging mode in a two lens column. From the point of view of obtaining a smallest probe size and a maximum probe current simultaneously, we first draw a conclusion that the non-crossover imaging mode is better than the crossover imaging mode of a probe forming instrument no matter whether the Coulomb effects are considered or not.

2) We found the aperture effects. We first comprehensively describe the intermediate aperture effect and the aperture position effect in particle optical columns. We conclude that Coulomb effects are responsible for the aperture effects. Without the Coulomb effects only one I-d relation curve would be enough to characterize a probe forming instrument no matter where the apertures are positioned. Taken into account the Coulomb effects, the I-d line will be split into different sub-lines, which exactly record the intermediate aperture effect and the aperture position effect. In the study of the aperture effects, we have also developed the concepts of the "inaccessible area" and the "danger area".
3) We have developed a novel optimization method of a particle optical system including the evaluation of Coulomb effects. The full optimization analysis has been successfully realized for the four lens (figure 6.4) and three lens (figure 9.8) focussed electron beam instruments, the two lens focussed ion beam instrument (figures 7.1, 8.1, 10.1 and 12.8) and the low voltage scanning electron microscopes (figure 11.1), in which the combined evaluation of the lens effects and the Coulomb effects in the whole systems are considered. There are so far no reports in literature having such a complete investigation of the problem.

Coulomb Interacties in optische systemen voor geladen deeltjes

Samenvatting

Dit proefschrift beschrijft ons onderzoek aan Coulomb interacties. Het is onderverdeeld in drie onderwerpen: theoretische achtergronden, computer programma's, en applicatie studies.

Van de theorie beschrijven we de systematische aanpak en formulering van vergelijkingen voor het beschrijven van ruimteladingsberraties in een compleet deeltjesoptisch instrument. Deze formulering bevat tevens de optische modellen die gelden voor een bron maar ook voor een universeel systeem (hoofdstuk 2), de analytische en numerieke schattingen van de statistische Coulomb-effecten en ruimteladingsberraties (hoofdstukken 3 en 4), en een samenhangende berekening van de lens-effecten en Coulomb-effecten in een praktisch optisch systeem met verschillende afbeeldingstoestanden (hoofdstuk 5).

Vervolgens beschrijven we in hoofdstuk 6 het computer programma ANALIC, dat is ontwikkeld om rechtstreeks een multi-parameter deeltjesoptisch systeem met een willekeurig aantal lenzen en diafragma's, een willekeurige afbeeldingstoestand, en een willekeurige verdeling van de bundel energie te optimaliseren, waarbij tegelijkertijd het gecombineerde effect van lens-effecten en ruimteladings-effecten wordt meegenomen. Dit programma bestaat uit 15 duizend regels, en bevat een groot aantal datatransmissie technieken, numerieke rekentechnieken, en interface technieken voor de realisatie van de meervoudige functies van het programma. Tevens worden de principes gegeven waarlangs het programma is ontwikkeld; een gedetailleerde technische beschrijving van het programma wordt niet gegeven.

Dit proefschrift besluit met een aantal applicatie studies op het gebied van Coulomb-effecten in gefocussed ionenbundelmachines (hoofdstuk 7), een betere afbeeldingstoestand van een deeltjesoptisch systeem (hoofdstuk 8), de invloed van diafragma's op de Coulomb-effecten (hoofdstuk 9 en 10), de schatting van Coulomb interacties in laagspannings-elektronenmicroscopen (11), en de verificatie van onze theorie en ons programma (hoofdstuk 12). Tevens worden enkele uitgebreide studies
beschreven, van ruimteladingsaberraties in homogene velden, van de statistische Coulomb interacties in elektronenbronnen met hoge helderheid, en van ionenbundel projectiesystemen (hoofdstuk 13). De drie resultaten van deze studies zijn:

1) We hebben een betere afbeeldingstoestand gevonden voor een twee lenzen systeem. Vanuit ons streven om tegelijkertijd een zo klein mogelijke spotgrootte en een zo groot mogelijke bundelstroom te bereiken, concluderen we dat de afbeeldingstoestand zonder tussen focus beter is dan de afbeeldingstoestand met tussen focus, onafhankelijk of de Coulomb-effecten in beschouwing worden genomen of niet.

2) We hebben het diafragma-effect gevonden. Eerst beschrijven we het tussenliggend-diafragma-effect en het diafragma-positie-effect. We concluderen dat de Coulomb-effecten verantwoordelijk zijn voor deze diafragma-effecten. Zonder Coulomb-effecten is een enkelvoudige stroom versus spotgrootte curve genoeg om een bundelvormend instrument te karakteriseren, ongeacht waar de diafragma's zijn geplaatst. Echter, indien de Coulomb-effecten wel in beschouwing worden genomen splitsst deze stroom versus spotgrootte curve in verschillende deel-curven, afhankelijk van diafragma groottes en posities. In de studie van de diafragma-effecten hebben we ook de concepten van "ontoegankelijk gebied" en "gevaarlijk gebied" ontwikkeld.

3) We hebben een nieuwe optimalisatie methode ontwikkeld voor een deeltjesoptisch systeem waarin Coulomb interacties een rol spelen. De volledige optimalisatie-analyse is succesvol uitgevoerd voor een vier-lensen (figuur 6.4) en drie-lensen (figuur 9.8) gefocussed elektronen bundel instrument, voor een twee-lensen gefocussed ionenbundel instrument (figuren 7.1, 8.1, 10.1 en 12.8) en voor laagspannings-scanning elektronen microscopen (figuur 11.1). In al deze systemen wordt de combinatie van lens-effecten en Coulomb-effecten beschouwd, wat de beschrijving van dit onderzoek, voor zover bekend, uniek maakt.

Curriculum Vitae

Xinrong Jiang was born in Songyang, Zhejiang Province, P.R. China on July 13th 1957.

He enrolled at Zhejiang University, Hangzhou, China in March 1978 and received his bachelor degree in February 1982. After the graduation from Zhejiang University, he worked for the Institute of Chemical Engineering and Metallurgy, Chinese Academy of Sciences, Beijing from February 1982 to August 1983 as an engineer. He attended the Institute of Electrical Engineering, Chinese Academy of Sciences, Beijing in September 1983 and got his M.Sc. degree in physics in June 1986.

His research and teaching career as a lecturer at Zhejiang University, Hangzhou, China extended from June 1986 to April 1993. What is described in this thesis is the result of his research at the Particle Optics Group of the Faculty of Applied Physics, Delft University of Technology, the Netherlands from April 1993 to September 1996.