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Electrostatic Breakdown at the Nanoscale

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by

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Executive summary

This thesis investigates electrostatic breakdown in gases at the micro and nanoscale. Electrostatic breakdown, commonly referred to as arcing, is a problem in many applications. Just like an electric shock hurts on your finger, it can damage mechanical systems to the point where they are unusable. Understanding electrostatic breakdown is thus important to prevent such damage. An attempt is made to simulate electrostatic breakdown in multiple dimensions using a Particle-in-Cell computer model. Electrostatic breakdown classically is governed by two principles: first *electron avalanches*, the rapid multiplication of free electrons due to an applied electric field. Secondly *secondary emission*, the emission of free electrons from the surface of an electrode due to incoming ions. An investigation of existing literature reveals that at the small scale, secondary emission is increased compared to breakdown at a larger scale. It has been shown that this increase is not only due to incoming ions, but also the electric field plays an important role. Researchers have proposed an exponential relation between the emission of electron and the electric field. However, electrons can also be emitted without any ions reaching the electrode. These effects have not been included in existing literature.

Since the fine details of this increase are not entirely known as of yet, a flexible computer model could allow the introduction of various hypothesized relations in order to investigate their effect. By implementing the model in multiple dimension, also an attempt can be made at investigating the effects of the geometry of the system on the process of breakdown. The model is implemented in the programming language *Python*. A Particle-in-Cell method discretizes the domain in cells. At the corners of each cell, the electrical potential and electric field are solved using the Poisson equation for electrostatics, a direct result of electromotive Coulomb forces between charged particles. A discrete form of Poisson equation is solved using a linear system of equations that is first transformed using an LU-decomposition to find the solution using one forward and one backwards substitution. The solution for the electric field is then used to determines the motion of the particles inside the domain, since the electric field imposes a net force on each particle. The updated distribution of charged particles throughout the domain is then used to update the electric field once more. This alternating process repeats itself to simulate the motion of the particle in the domain.

Inside this framework, collisions between particles are implemented since these collisions are the main principle that initiate electrostatic breakdown. *ionization*, the process in which a neutral gas particle is struck by a high energy electron and breaks up into an ion and an electron, is modelled to incorporate the avalanche multiplication of electrons. At the electrode surface, both the classical theory and the updated theory on surface electron emission have been implemented to reproduce the results of both experimental and theoretical research on the topic. This validation of the model shows that all the important aspects are incorporated and thus the model is ready to be expanded for use with other hypotheses that describe electron emission from the electrodes. The effects that emerge from the geometry of the system have not yet been investigated, but as the model is fully two dimensional, this can be achieved in future work on this topic. Some initial simulations show the tendency of breakdown to occur at a larger distance then strictly required, since the classical theory predicts an energetic optimum at a separation of around $10\,\mu\text{m}$ between the electrodes.

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Introduction

1.1. Introduction

To come to a thorough understanding of the phenomenon of electrostatic breakdown, the first step is to understand what it entails and where this knowledge can be applied in a practical situation. When any system is exposed to electric fields and potentials, whether they are applied from the outside or generated within the system itself, there is the possibility that current will flow within the system. More often than not, it is actually desired to design such an electrical system for all kinds of applications. The whole field of electrical engineering is based on this, and mechanical systems often need electronic components to function. In some cases however, especially when systems get smaller and smaller, there is the possibility that these electrical effects negatively affect the system. The main problem is short-circuiting. When current flows in a place that it shouldn't, a variety of defects can occur. Generally the most damaging effects occur due to overheating which causes permanent changes in the form of melting or rupturing [42]. A study by Strong [44] clearly illustrates damage in a MEMS device caused by electrostatic breakdown of the air in between two differently charged electrodes. Figure 1.1 shown below depicts the damage.
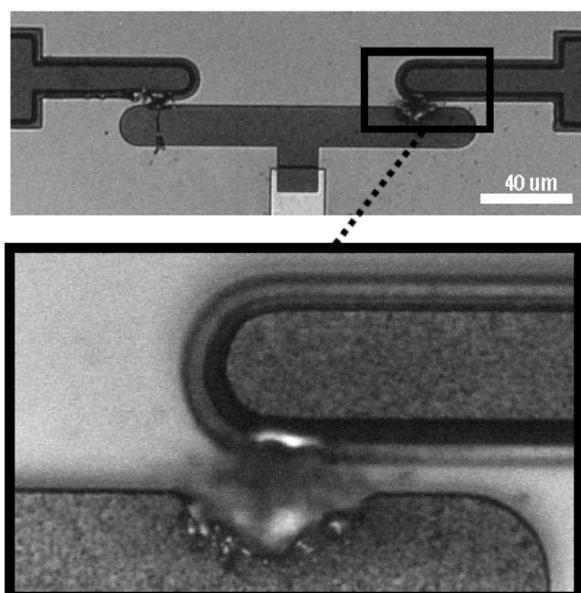
Figure 1.1: Two charged electrodes with a electrically floating conductor in between. The inset clearly shows damage on both sides of the air gap [44].

A short-circuit can be caused by for example contamination of the device with dust or water. The contaminant then acts as a conductor through which current can flow in an alternate path. Also without contaminants, a short can occur. This happens when materials, that are generally considered as insulators, become conducting due to loading of the system. In semiconductor devices, controlling the electrical conduction of the material is the essential operating principle, but when the limits are pushed, junctions can become unstable and breakdown can occur [6].

In MEMS and NEMS technology, which are the focus of this work, devices generally consist of conducting geometries separated by atmospheric air or sometimes other gases for special purposes [27]. Under the right (or rather the wrong) circumstances the surrounding gas can become conducting, and cause the flow of current; this is electrostatic breakdown, the actual topic of this thesis. These prerequisites together form the field of gas discharge physics and are the foundations of electrostatic discharge. This thesis will further focus on the physical effects that come into play and how these can be modelled to be able to predict the conditions under which breakdown occurs.

1.2. What is breakdown?

As previously stated in the introduction, when electrical charge rapidly moves from one location to the other, there is the possibility that a vulnerable system will be permanently damaged. Electrostatic breakdown focusses on insulating gases that become conductive when breakdown occurs. To assist the reader in visualizing breakdown; lightning is a gigantic form of electrostatic breakdown. And for instance when you get an electric shock when you are approaching a doorknob, the small spark you see between your finger and the object is governed by the same physical principles. The all cases the mechanism relies on an electric field being applied to the gas. In the case of lightning and electric shocks, either the cloud or the person has built up electric charge that creates the electric field. Commonly, two conducting sides, the electrodes are considered at given electric potentials, with in between them a gap containing a gas. The behaviour of conductive gases and formation thereof is called plasma physics. Simply stated, a medium is electrically conductive when there is a sufficient amount of free charge carriers. In a gas, where all particles are freely moving already, this manifests itself as the presence of a sufficient number of ions and free electrons as oppose to neutral gas molecules. The interpretation of the word 'sufficient' will be discussed later in a detailed description of gas and plasma behaviour. The formation of free charge carriers is governed by ionisation and recombination. A neutral gas particle can become ionised and decompose into a positive ion and an electron. This aids the formation of a spark. The reverse process, an ion and an electron combining into a neutral molecule, is called recombination. Recombination removes charge and therefore inhibits the formation of a spark. The rate of these two processes together determine the degree of ionisation in a gas. During a breakdown event, the degree of ionisation will rise exponentially until a conductive channel is formed between the electrodes. Through this channel an electric current will flow until the potential drops or some other prerequisite is removed.

1.3. How can breakdown be predicted?

To predict electrostatic breakdown, the process of ionisation must be quantitatively described. A very brief explanation of will be given to give the reader some insight in the process. This short introduction of physical effects is by no means extensive enough to capture all of the nuances, and is applicable is specific cases only. Despite the shortcomings, a basic understanding of this section will allow the reader to grasp the fundamental processes that occur during breakdown. This will prove extremely useful during the rest of this work, in which the concept explained here will remain of great importance.

1.3.1. Basic physical principles

To introduce the different types of electrostatic discharge, some fundamental physical effects must be described. The most important are electron avalanches and secondary electron emission. They are explained individually and when combined will allow the representation of the different mechanisms that can occur.

Electron avalanches

Consider a single electron free to move in space. It is exposed to an external electric field. Since the electron is charged, it will accelerate in the field. After it has gained a significant amount of energy from the applied field, suppose it collides with a neutral particle. An ionisation event takes place. The neutral particle loses an electron and now constitutes of an ion and an electron as displayed in Figure 1.2a.

(a) Ionization event graphically displayed.   (b) Electron emission event graphically displayed.
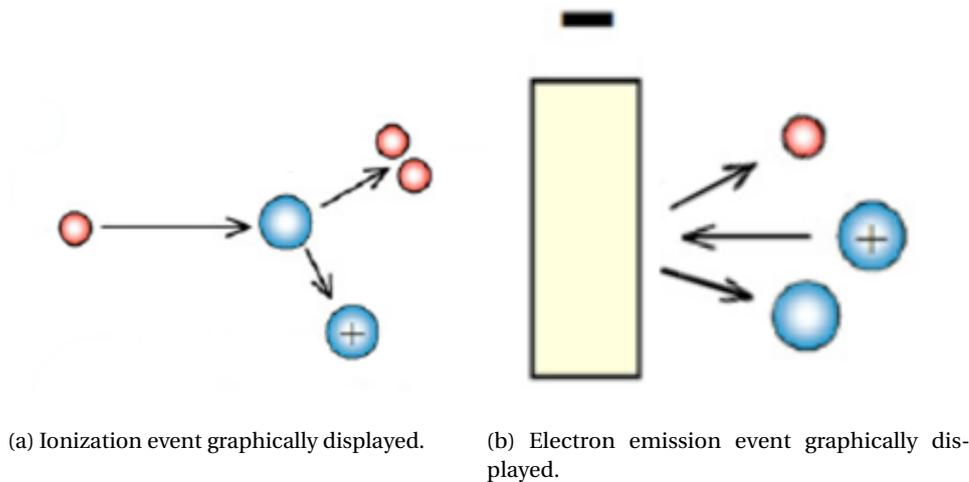
Figure 1.2: Important effects displayed. Electrons depicted in orange, atoms in blue. Positive ions are shown as atoms with a plus sign.

Since the original electron is still present, at this point there are two electrons, which will both again be accelerated in the external field. The ionisation process continues and every ionisation event produces a new electron. The result is a so called 'avalanche' of electrons, as shown in Figure 1.3 . In a practical system these electrons will reach the positive electrode, and the ions that are produced will move towards the negative electrode.

1.3.2. Secondary emission

When a particle hits a solid, it will transfer its kinetic energy to the material it collides with. The energy transferred to the material can be sufficient to emit another (secondary) particle, see Figure 1.2b. In this context the most influential variant of this process is the emission of one or more electrons when an incident ion hits the surface of the anode. Due to the chaotic nature of this process it is commonly regarded as being stochastic, and the process is quantified by the expected number of emitted electrons per incident ion.

1.4. Types of electrostatic discharge

In the introduction the word electrostatic breakdown was used. The words *breakdown* and *spark* imply a violent behaviour that happens suddenly. The broader term *electrostatic discharge* is used to describe the flow of electricity through gases, even when the flow is very small or happens locally. Discharges can be characterized in four main types: *glow discharge, corona discharge, streamer*
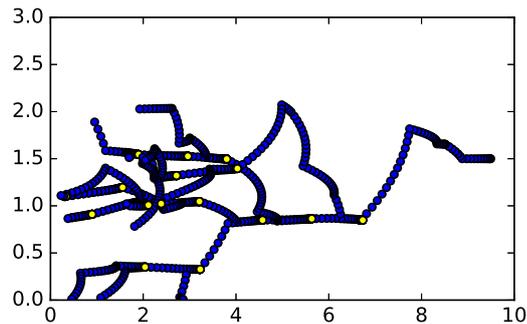
Figure 1.3: The avalanche effect, with electrons in blue and positive ions in yellow.

discharge and *Townsend discharge*. Of these, in the latter two, the dielectric breaks down all the way between the electrodes, causing a spark, incorporating high current and heat. Glow and Corona discharges on the other hand are not accompanied by high currents and heat generation. They can be maintained over longer periods of time and do not damage the device per se. A real world example of glow discharge are glowing advertising lighting tubes.

Electrical discharge can occur in different forms, depending on the dominant mechanism. The prevalance of each mechanism depends on the pressure, the applied potential, and the geometry. Each of these will be briefly described here

1.4.1. Glow discharge

To illustrate the principle of a glow discharge, we again consider the situation of two parallel plates with an electric field in between them. When there is a voltage applied, a random electron originating by photo-ionization or cosmic radiation, can initiate an electron avalanche in the gas. The produced positive ions and electrons will reach the negative and positive electrode respectively. These electron avalanches result in a measurable current and produce sufficient amounts of photons to produce visible light. A criterion for a glow discharge is that the ohmic resistance of the external circuit must be high, in order to keep the current from rising indefinitely until the system fails. Using this principle, glowing tubes are fabricated for the use of commercial lighting. An example can be seen in Figure 1.4.

1.4.2. Corona discharge

In the basic parallel plate configuration, the electric field generated is uniform (neglecting boundary effects at the edges of the plates). However, when the electric field generated by the applied potential is not uniform, different effects can be observed. The easiest way to obtain non-uniform electric fields is by altering the geometry. To demonstrate corona discharge, consider a conducting tube, with a conducting wire running through it coaxially. An applied voltage between these two will generate a radial electric field which will fall off with $1/r$ from the wire. Since a minimal electric field is necessary to accelerate the electrons sufficiently and form an avalanche, electron avalanches can only occur in the region where the electric field is strong enough, i.e. near the wire in the centre. The result is a similar glow as in a glow discharge, but in this case the process does not rely on the external resistance of that circuit. In practice this type of discharge can be seen on high voltage systems such as power lines, especially in spots with sharp features that enhance the electric field.

1.4.3. Streamer discharge

The previously explained glow and corona discharges are both stable phenomenon that can be sustained for longer periods of time. Streamer discharges are generally not stable and can cause system failure. Whenever an electron avalanche propagates towards the anode, the front of electrons

Figure 1.4: 'Neon sign' using the physical mechanism of a glow discharge to generate photons. Reprinted from *Brite Lite Tribe*, 2017, Retrieved June 13, 2017 from `https://britelitetribe.com/products/pineapple`. Copyright 2017 by Brite Lite Tribe.
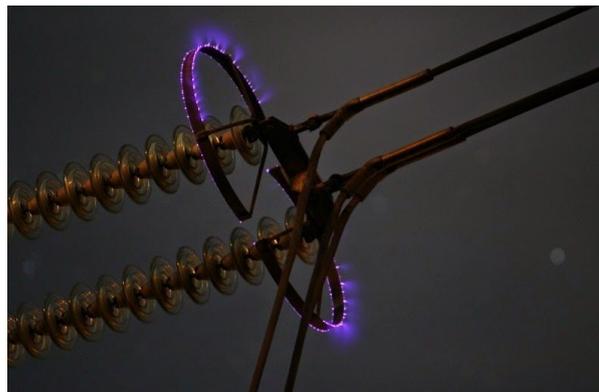
Figure 1.5: Corona discharge around a high voltage power line. Reprinted from *Electrical Concepts*, 2017, Retrieved June 13, 2017 from `http://electricalbaba.com/advantage-disadvantage-corona/`. Copyright 2017 by Electrical Concepts.

leaves behind the formed ions in it's wake. The moment the electron front sinks into the anode and is registered as an electric current, the ions still retain the shape of the original avalanche because they are orders of magnitude heavier and thus slower. This so called *ionic trail* now forms a channel of space charge that deforms the original electric field. When the multiplication of the avalanche is sufficiently large the electric field can be transformed significantly. In this case, a second avalanche in close proximity will be attracted towards the original avalanche and they will merge together. The ionised channel has now been extended slightly, and due to the recurring of the above, the channel extends itself towards the cathode, opposite the propagation direction of an electron avalanche. When the ionised channel reaches the cathode, the current can increase until the resistance of the external circuit is reached.

1.4.4. Townsend discharge
Townsend breakdown is most commonly seen at small length scales. Referring back to the section about glow discharge, the production of source electrons is explained by stray electrons originating
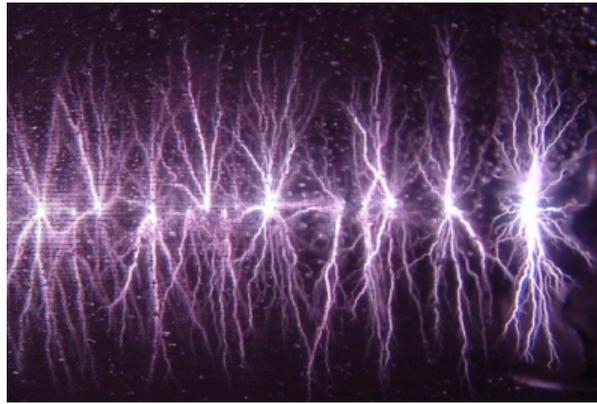
Figure 1.6: Formation of streamers [48].

by for example photo-ionization or cosmic radiation. However one of the requirements for a glow discharge is that the external resistance is high. When the resistance of the external circuit is not extremely high, secondary emission can play a significant role. The positive ions will, upon reaching the negative electrode, have the ability to free an excess electron located at the surface of the electrode material. This electron then acts as a source for the avalanche effect in the same manner as would happen in a glow discharge. Contrary to a glow discharge, in this case the current can rise indefinitely and a spark is formed.

1.4.5. Focus of this work

Since the field of gas discharge is vast and involves numerous mechanisms that can individually determine the breakdown potential, it is not feasible to analyse breakdown for all regimes, and essentially the different types of breakdown as elaborated on before. Because we are interested in discharges between electrodes on small length scales, Townsend's mechanism of initiating breakdown, is seen to be teh focus of this work. At a later stadium it will become clear why this is the most effective approach and some interesting similarities will show between the classical theory and the new theories that can predict breakdown outside of the region where the accepted theory is applicable.

1.5. History of breakdown research

1.5.1. Early experiments in atmospheric air

In the year 1889, Friedrich Paschen published his research titled: 'Ueber die zum Funkenübergang in Luft, Wasserstoff und Kohlensäure bei verschiedenen Drucken erforderliche Potentialdifferenz' [34]. In his research he investigated the electrostatic breakdown behaviour of different gases and gap distances. This work is still widely considered as one of the founding papers of the subject of gas discharges. Paschen used spheres of different radii as electrodes and by increasing the voltage until a spark occurs. The breakdown voltage could be found for a wide variety of situations, by changing the gas, the pressure or the radii of the spheres.

In line with what other researchers at the time had already found [2] [37], experiments in air at atmospheric pressure resulted in a linear behaviour of the breakdown voltage with the gap distance. A necessary condition for this however was that the radius of each sphere must be larger than the gap distance between the two. This puts a lower bound on the configuration of the experimental setup, in order to maintain the ability to model the system as two infinite parallel plate electrodes separated by the same distance d. From the experimental data obtained by the aforementioned researchers, a relationship can be found between the gap distance, and the voltage required to initiate breakdown. With d ranging from 0.01 cm to 1.5 cm, a linear relation was found. This relation

is generally described as the *breakdown strength*, and in air was found to be 3 V/μm.

Since this is essentially a minimum requirement for the electric field strength, this conclusion already indicates that the occurrence of electrostatic breakdown is dependant on the electric field instead of the voltage applied.

1.5.2. Varying the gas pressure

A second part of the experiments conducted by Paschen, involved varying the pressure. Since it was known at the time already that the process of breakdown relied on the gas particles, it was a reasonable assumption that varying the molecular composition and/or the pressure would influence the behaviour of the test system. When modifying the pressure, a similar result was obtained as when modifying the gap distance. The same linear behaviour was found which resulted in the assumption that the breakdown properties of a gas depend on pressure and distance in the same way, therefore up until this day, many graphs considering breakdown voltage use a combined variable pd on the horizontal axis.

1.5.3. Breakdown at low values of pd

At lower values of pd, measurements indicated the voltage required to achieve breakdown did not converge to zero. Instead, a plateau was observed at a combined value $pd \approx 1\,\mathrm{Pa\,m}$. This corresponds to a distance of around 10 μm at atmospheric pressure. Further lowering of the combined variable increased the voltage again to very high values. A physical explanation behind this observation was first attempted by Townsend [46]. Townsend argued that positive ions, produced in ionisation events in the gas, could strike the negative electrode and set free new electrons. The free electrons then provided a source for new avalanches, and the avalanches in turn provide new positive ions to start the cycle all over again. If then the amount of charged particles changed from the start of the cycle to the end of the cycle, a high number of repeating cycles would always result in the number of charged particles decaying to zero or increasing exponentially, depending on the parameters of the system. Very shortly stated, this meant that if the amount of positive ions generated by a single avalanche exceeded the amount of positive ions needed to emit one electron from the electrode, breakdown would occur.

Going back to the observation that the breakdown voltage increases at lower pd values, this physical explanation relies on the fact that the number of positive ions produced by an avalanche depends on distance, pressure and the electric field. Even if the exact relation between an electron avalanche and the variable pd is unknown, it is reasonable to assume a positive correlation between the two. The consequence of this is that at low values of pd, a high electric field, and thus voltage is needed to produce sufficient positive ions in a single avalanche.

1.5.4. Paschen's law

From the obtained data a very well known empirical relation between the required voltage, V_B and pd was constructed. Paschen's law was first formulated by Townsend [46] in 1915, who introduced ionisation coefficients α and β, which describe the ionisation rate by electrons and positive ions respectively. As mentioned before Townsend also introduced a parameter to quantify the number of emitted electrons for each incident cation, denoted by γ_se. The breakdown voltage is then given by

$$V_\mathrm{b} = \frac{Bpd}{\ln\left(Apd\right) - \ln\left(\ln\left(1 + \frac{1}{\gamma_\mathrm{se}}\right)\right)}, \tag{1.1}$$

where A and B are constants that were determined to fit the relation to the available experimental data. This relation has been plotted in Figure 1.7, where it can be clearly seen that there is a minimum breakdown voltage, and further lowering of the variable pd increases the required voltage again. Another peculiar thing that should spring to attention is that (1.1) goes to infinity when the
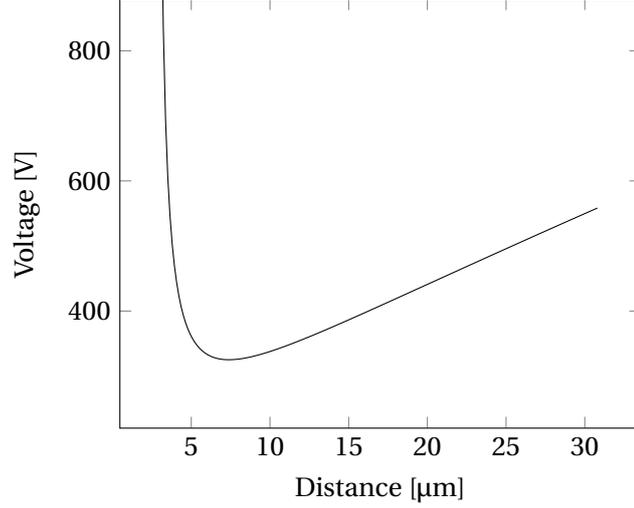
Figure 1.7: Schematic of Paschen's curve

denominator approaches zero. This perfectly captures the behaviour as described because there will be a value of pd low enough that the avalanche effect can not manifest itself at all and that any particle inside the domain will just be diffused at one of the electrode in the end. It is however not feasible in the sense that this model predicts that it would not be possible to obtain breakdown when the electrode are moved closer and closer together.

1.5.5. Minimum breakdown potential

To extract more information from Paschen's law, it makes sense to have a more in depth look at the minimum predicted value of the breakdown voltage and the corresponding value of pd. A minimum for this curve can be found by taking variations of pd which give us

$$\frac{\partial V_{\mathrm{b}}}{\partial pd} = \frac{B\left[1 + \ln\left(\ln\left(1 + \frac{1}{\gamma_{\mathrm{se}}}\right)\right) - \ln\left(Apd\right)\right]}{\left[\ln\left(Apd\right) - \ln\left(\ln\left(1 + \frac{1}{\gamma_{\mathrm{se}}}\right)\right)\right]^2} \tag{1.2}$$

and by setting the expression equal to zero. Using the fact that $B \neq 0$, the resulting expression

$$\ln\left(Apd\right) - \ln\left(\ln\left(1 + \frac{1}{\gamma_{\mathrm{se}}}\right)\right) = 1 \tag{1.3}$$

will return a value for pd, dependant on the secondary emission coefficient γ_{se}. For common values of the parameter γ_{se}, the variable pd lies in the order of $1\,\mathrm{Pa\,m}$. The minimum breakdown voltage in Paschen's curve for air is found to be $327\,\mathrm{V}$. This Paschen's minimum represents the energetically optimal pd value for which a spark will be formed.

1.5.6. Long path breakdown

In practice the energetic minimum means that an arc can take a longer path then the shortest distance between the electrodes. According to Townsend, this was experimentally observed by Carr (reference unknown to current author). The effect was reported by Townsend [46, p. 352]. These measurements have shown that, in the case of parallel plate electrodes, the arc may be observed at the edge of the plates where it is free to assume a longer path that is energetically more efficient. In the experiments of Carr, this was negated by using parallel plate electrodes with an insulating ring in between that acts as a separator and prevents a longer breakdown path at the same time. These observations indicate that breakdown is strongly affected by the geometry of the system. This is also one of the main topics of interest of this work, the effect of geometry on breakdown.

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Literature

2.1. Determination of research question

To achieve a clear perspective on work that has been done regarding breakdown in gases, a well defined problem must be stated and bounds must be set to the scope of the investigation. Once this has been done it will thereafter by possible to follow a more clear-cut path through literature without unintended sidetracks and keeping the final objective in mind. Returning to the barest problem statement that can be distilled from the introductory part, the aim is to narrow down this problem statement to end up with a manageable research objective. Another part of precisely determining and limiting the problem is explaining the need for a 'solution' to the problem at hand.

2.1.1. Problem statement

In essence, when stating the goal in a problem form, where then the goal is to 'solve' the problem, we find the following: Electrostatic breakdown is not well understood at the nanoscale. This in itself is simply a statement, not implying any positive or negative meaning to it. By including the information that a better understanding of the phenomenon is desired, there already is more meaning to this statement. Rewording the previous statement results in the following: It is desired to achieve a better understanding of electrostatic breakdown at the nanoscale.

2.1.2. Ratification of breakdown research

Now that it has been determined what the problem is in its broadest sense, an elaboration has to be made on the importance of the topic. As described in the introduction, MEMS and NEMS are the main fields where electrostatic breakdown is of great interest. In such devices, an everlasting search for smaller dimensions pushes the limits of what can be achieved. One very important advantage of MEMS and NEMS is that they can utilize certain physical effects that are actually negligible at the macroscale because many aspects do not scale similarly with the lengthscales that are involved. One example of this is the scaling of eigenfrequency when the system dimensions decrease. Consider the bending beam in Figure 2.1. Assuming the beam itself massless its eigenfrequency can be determined by

$$\omega_\mathrm{n} = \sqrt{\frac{k}{M}} \tag{2.1}$$

with

$$k = \frac{3Ewh^3}{12l^3} \tag{2.2}$$

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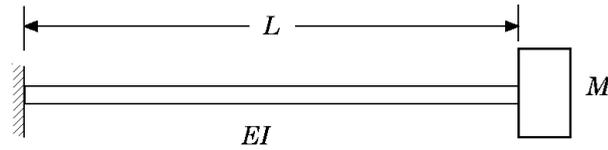
Figure 2.1: Transverse beam with point mass at tip

and w,h and l specifying the width, height and length of the beam respectively. If then all dimensions of the system are scaled by a factor of S, we can substitute all parameters denoting length by their value times S. Thus the new bending stiffness becomes

$$k_S = \frac{3ESw(Sh)^3}{12(Sl)^3} = S\frac{3Ewh^3}{12l^3},$$

(2.3)

while the mass M scales by a factor of S^3. Substituting in the equation for ω_n reveals how scaling by a factor of S will affect the eigenfrequency of the beam

$$\omega_{nS} = \sqrt{\frac{Sk}{S^3M}} = S^{-1}\sqrt{\frac{k}{M}} = S^{-1}\omega_n.$$

(2.4)

We have now established an inverse relationship between the size of the system and its natural frequency. This is a very basic example of how scaling a system may cause a change in behaviour due to separate scaling of certain properties. This change of behaviour can be very beneficial in exploiting certain effects to utilize them in for example a sensor. Tying in tot the topic of sensors, other benefits of small scale devices are their low power consumption, unobtrusive placement and low material cost. This does however require a viable production process, because low material cost can easily be negated by costly fabrication methods.

This description of all the advantages of MEMS and NEMS also has its result in the real world. They are used in a wide range of commercial products such as piëzo controlled nozzles in ink-jet printers, accelerometers in products ranging from cars to smartphones to radio controlled toys and micro mirrors in projection beamers, as shown in Figure 2.2.
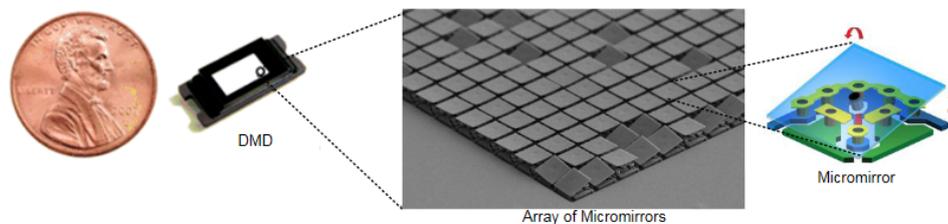
Figure 2.2: Digital Micromirror Device (DMD), the mirrors can tilt using an electric current. Reprinted from *TI DLP® Pico™ Technology for Gaming / Pachinko Applications*, by V. Thakur, 2015, Retrieved July 5, 2017 from `http://www.ti.com/lit/wp/ssiy002/ssiy002.pdf`. Copyright 2015 by Texas Instruments.

Returning to the topic of electrostatic breakdown, it already becomes a more obvious threat to such devices. The micro mirror depicted in Figure 2.2 relies on a voltage between the substrate and the mirror, thus providing an electrostatic pull force. The substrate has two separate electrodes, and by applying a bias voltage the mirror will flip towards the one that results in the highest electrostatic pull force. Removing the bias voltage but still retaining the base voltage, the mirror will stay in the position it is in already due to the fact that the mirror already is closer to the active electrode. Since the electrostatic pull force is given by

$$F = \frac{\epsilon A\Phi^2}{2d^2},$$

(2.5)

the quadratic dependence on d, the distance between the electrodes, indicates that the pulling force of the closely spaced set of electrodes is dominant and therefore will retain the position like before.

Since this system includes electrodes at different voltages, with a dielectric between them, all the main building blocks for electrostatic breakdown are present. This necessitates an analysis to confirm that the system parameters are not such that electrostatic breakdown can occur, and if required the system can be optimized to obtain better behaviour with regard to electrostatic breakdown. Besides this example there are many more practical applications where it could be critical to asses the system whether it will be prone to breakdown problems during the design phase.

As shown, the practical applications for MEMS and NEMS are vast and further miniaturization will always be one of the main goals in this area. One of the issues that must be tackled to continue this development is electrostatic breakdown and therefore a thorough understanding will drive MEMS and NEMS forward.

2.1.3. Limiting the scope

The goal of gaining a better understanding of electrostatic breakdown at the nanoscale is very broad. In principle electrostatic breakdown is a possibility in any system where there are electric potential differences, and some material that is a dielectric, i.e. not electrically conductive. Even that description is already limiting the broadness of this topic because breakdown can occur even in a perfect vacuum, where there are no molecules or atoms present between the electrodes at all. Because the mechanisms for breakdown are vastly different in solids, fluids and vacuum, it is not feasible to study all of them together.

Since the goal of this work is focussed on MEMS technology, it is reasonable to narrow down the topic so that it is applicable to most commonly occurring MEMS and NEMS devices. In the semiconductor industry, solid breakdown is of greatest importance, because a closed semiconductor gate is closed due to a solid dielectric that is preventing the signal from passing. In Micro Electro Mechanical Systems however, as is in the name, their mechanical nature results in them consisting of solids parts with liquid or gaseous media in between them.

In microfluidics, the field of research where microscale devices are used to specifically manipulate liquids or gases to assure proper mixing or sensing of biological molecules, electrical breakdown can occur in liquids. This type of breakdown is not included in this thesis and further focus will remain on gaseous breakdown.

The subset of small scale systems that maintain after elimination of the previously specified ones is also the largest set. The ease of use of systems that operate in a chamber with a gas that can easily be evacuated or pressure regulated makes them the largest group. Removing even more of the necessary precautions one can design a device to operate in air at atmospheric conditions.

Since MEMS systems that operate in gases are of great interest, the physics involved will be thoroughly analysed. These processes will in principle be applicable to any gas mixture and variable pressures, but a slight gravitation towards atmospheric air in this work allows for effective explanations that are easier to understand without losing generality.

Concluding this section, the problem of electrostatic breakdown is narrowed down so that it is applicable to small scales mechanical systems that consist of solid components operating in a gas. This heavily reduces the breadth of the topic while still maintaining applicability to a large group of MEMS and NEMS.

2.2. Historical perspective of nanoscale research

Continuing the literature research on the topic as it has been meticulously described in the first part of this chapter, the research must be placed in a historical perspective. Doing so makes the history a guide from which new directions of research naturally emerge.

The history of electrostatic breakdown has been described already, and the remaining part of the literature research focusses specifically on the small scale. Classical theory started with researchers, of which Friedrich Paschen is the most well known, initiated a series of experiments to determine the breakdown voltage required to obtain breakdown between two electrodes. Their work was highly integrated with radiation research in the 19th century. It was for instance observed that irradiating the gas between two electrodes could be a method to trigger breakdown [46][45]. These efforts in the field of electromagnetism and also combined with the discovery of the electron and elementary particle physics, allowed for a physical explanation behind the experimental observations. This theory, as it has also been described in the introduction of electrostatic breakdown, agreed with the experiments and it was generally accepted. In the 1940s, Meek published research on the failure of Paschen's law at large values of the product pd [31]. These led to new studies investigating breakdown at these large values. A new mechanism was discovered which relied more on a local high electric field.

A couple of years after, in 1948, Germer and Haworth experimentally explored the other limit of Paschen's Law [13] [14] [15]. In their work it was for the first time that the significant deviations from the established theory were actually thoroughly investigated and given a reasonable explanation for the cause [14]. They reported observed breakdown voltages as low as 50 Volts in air, even though Paschen's Law predicts a minimum breakdown voltage that is significantly higher: slightly above 300 Volts. It is here that new interest was sparked towards breakdown at the nanoscale. In the 1950s a couple of studies investigated this anomaly until interest in the topic largely died out around ten years later.

With the advent of MEMS and NEMS, there was again a new driving force to develop the theory of breakdown in cases where Paschen's Law is not applicable. The current investigation in existing literature will advance in chronological order, and focus specifically on those papers that have topics regarding electrostatic breakdown in gases at small gap electrode spacings. After discussing these publications, and their shortcomings, the literature study will gravitate more towards alternative methods that incorporate multidimensional analysis of breakdown.

2.3. Detailed overview of existing literature

This section will elaborate on papers that specifically work on breakdown at very small length scales, as they form the main topic of this work. For historical reasons investigation of breakdown at decreasing length scales emerged from breakdown research in general. Therefore papers are selected that expose flaws, or better said, expand the applicability of general breakdown theory, which is in the community mostly synonymous to 'Paschen's curve', 'Paschen's Law' and 'Townsend breakdown'. The publications aiming at small scale breakdown are mainly aimed at the physical effects, in which generally the simplest possible geometries are assumed.

2.3.1. Earhart, 1901

At the very start of the 19th century, even before Paschen's Law was formulated in its common form, Earhart presented an experiment in which he measured the breakdown voltage at small gap distances [9]. The experimental setup consisted of a planar electrode and a spherical one, which had a large radius compared to the gap distances investigated (2.5 cm compared to several µm). The distance was measured using an interferometer, and varied from 0.3 µm to 110 µm. The fringes obtained using the interferometer were counted and the gap distance was deduced from the amount of fringes and the wavelength of the used light. From the very low values a linear relation is seen and at 5 λ the value exhibits a plateau until a gap distance of 16 λ, where λ is the wavelength of the light which is 590 nm. After the plateau, again a linear relation is observed but at a different proportionality constant. In the original paper of Earhart, the results are interpreted as two straight lines with each their specific proportionality constant. The existence of some kind of air film is hypothesised as an explanation for the observations. It is proposed that the air film that is formed at small distances has the air in a

certain 'state' in which it has a higher resistance to electric breakdown. The thickness of this layer is said to be $0.9\,\mu m$ but the nature of this film and the requirements for its presence are not discussed. In short, this was one of the first experimental evidences that shows the behaviour of electrostatic breakdown at very low distances, and its differences compared to Paschen's Law. The theory that is proposed however is unsatisfactory and the research was not followed up with more experimental results confirming the data.

2.3.2. Germer and Haworth, 1948

It took almost 50 years before investigation of the topic really accelerated. In 1948 Germer and Haworth published a short paper in which they mention their own experimental research, but mainly propose a new physical mechanism for breakdown that could clarify the behaviour at these lengthscales [14]. Paraphrasing the paper: "When a positive ion, formed in the air or upon the anode surface by an electron which was drawn out by the field, approaches the cathode the field is appreciably increased by its presence. Since the field was already almost strong enough to draw out electrons, this further increase at once elicits a second electron." This sentence states that the presence of an ion can alter the electric field due to its own charge. The proposition holds that the local increase in electric field could be sufficient to draw an electron away from the cathode and into the gas by the force of the field. In the same time period related research is published by the same authors investigating damage to electrodes when they are continuously moved closer together [15].

2.3.3. Kisliuk, 1954

Following up on the research of Germer and Haworth, Kisliuk [24] zooms in on the emission of electrons from the cathode. The hypothesis that more and more electrons are emitted from the cathode when the separation is decreased, must therefore depend on some variable that changes when de gap distance d is varied. As was also already suggested by Germer and Haworth, the increased electric field that follows from a closer electrode spacing, is the most probable actor that influences the emission of electrons. It is mentioned that if this emission depends on the electric field alone, the pd scaling that is generally used will not holds for the small separations that occur in nanoscale systems. Kisliuk also introduces the cathode fall layer, which is a layer near the cathode where the electric potential drops off rapidly. The importance here is that the layer is supposed to incorporate increased electric fields, and therefore could enhance the emission of electrons from the cathode. A derivation is done to determine the electric field at the cathode which is based on work by Mackeown [29]. Using the number densities of positive ions and electrons separately, Poisson's equation is formulated as follows:

$$\frac{\mathrm{d}^2 V}{\mathrm{d}x^2} = -4\pi\rho = -4\pi\left(\frac{j_\mathrm{i}}{v_\mathrm{i}} - \frac{j_\mathrm{e}}{v_\mathrm{e}}\right). \tag{2.6}$$

Equation (2.6) denotes the electric potential as V, x as the spatial coordinate, j_i and j_e as the positive ion and electron current density respectively. These current densities are divided by the respective velocities to obtain the charge density in space for both species. In the paper of Mackeown it is then assumed that within this layer that is being analysed, no collisions occur as long as its thickness is less then one mean free path. This assumption is questionable especially because the thickness of the layer is unknown but also because of the stochastic nature of the process which would result in half the collision frequency when half the distance is considered, instead of a discrete transition to zero. Following the derivation however, it can thus be stated that the current densities are constant. Also the equations of motion are given by the author as

$$\frac{1}{2}m_\mathrm{i}v_\mathrm{i}^2 = Vq, \tag{2.7}$$

$$\frac{1}{2}m_\mathrm{e}v_\mathrm{e}^2 = (V_\mathrm{c} - V)q. \tag{2.8}$$

Which relates the kinetic energy of the particle to the energy obtained from traversing a potential difference V. This allows for a substitution of (2.7) and (2.8) into (2.6) with the result being

$$\frac{\mathrm{d}^2 V}{\mathrm{d}x^2} = -4\pi \left[j_\mathrm{i} \left(\frac{m_\mathrm{i}}{2Vq} \right)^{1/2} - j_\mathrm{e} \left(\frac{m_\mathrm{e}}{2(V_\mathrm{c} - V)q} \right)^{1/2} \right]. \tag{2.9}$$

Using more substitutions for the values and also integrating the equation once, they solve the equation for the ratio between positive ion current and electron current, denoted by x, with J the total current density.

$$E_\mathrm{c}^2 = 7.75 \times 10^5 V^{1/2} J\{x\left[(1845m_\mathrm{i})^{1/2} + 1\right] - 1\} \tag{2.10}$$

The result is that a fraction of 0.07 of the total current is constituted of positive ions, and the other 93% made up of electrons. The reasoning on why the value of E_c can be substituted as $5 \times 10^9\,\mathrm{V\,m^{-1}}$ is not entirely clear, except for a mention on the Fowler Nordheim equation. The conclusion of this previously found ratio between positive and negative particles however signifies that a high amount of electrons is emitted from the electrode compared to a relatively small fraction of positive inbound ions. Even though the presented ratio gives insights in the behaviour of electron emission, the nature of the emission is still untouched upon. The use of a cathode fall as a layer of high electric field near the cathode is doubtful. From several other authors [47] [40] the nature of the cathode fall layer, or cathode drop, lies in the existing glow discharge that must already exist for this layer to form.

2.3.4. Boyle & Kisliuk, 1955

shortly after the initial publication where the cathode fall layer forms the main cause of electron production, Boyle and Kisliuk publish a detailed paper that specifically aims at the deviations seen from Paschen's Law [5]. The backbone of the presented results is formed by the hypothesis that the emission of electron from the cathode, which is already acknowledged in Paschen's Law, is influenced by the spatial distribution of electric charges in the domain. Restating Paschen's Law there is included a parameter γ_se which quantifies the amount of secondary emission from the electrode,

$$V_\mathrm{b} = \frac{Bpd}{\ln\left(Apd\right) - \ln\left(\ln\left(1 + \frac{1}{\gamma_\mathrm{se}}\right)\right)}. \tag{1.1}$$

By replacing the parameter γ_se by a new coefficient of electron emission, the previously proposed method of emission by space charge could be superposed onto the secondary emission to obtain an effective emission coefficient. To obtain the effective yield of electrons per incident ion, the derivation of Boyle and Kisliuk is analysed here. The starting point of the derivation is what is named by the authors as the empirical form of the field emission equation:

$$j_\mathrm{e} = A\mathrm{e}^{-B/E}. \tag{2.11}$$

By then writing the electric field as a sum of two components, namely one for the applied field $\mathrm{E_A}$, and one for the electric field due to positive ions, $\mathrm{E_+}$, (2.11) can be expanded. This expansion however assumes $\mathrm{E_+} \ll \mathrm{E_A}$, which is not validated as of this mention.

$$j_\mathrm{e} \approx A\mathrm{e}^{-B/\mathrm{E_A}}\mathrm{e}^{B\mathrm{E_+}/\mathrm{E_A^2}} \tag{2.12}$$

Since the applied field is constant the first part of the expression is shortened and the relation becomes

$$j_e \approx j_0 e^{BE_+ / E_A^2}. \tag{2.13}$$

Using the assumption that the electric field induced the positive ion is directly proportional to the current flow induced by the same ions, $E_+ = C j_+$, and introducing $j_+ = G j_e^n$, the equation can again be rewritten. The validity of both the assumptions is critical and they are hard to verify at this point. In the new equation a large part can be summarized in a constant again, it then becomes

$$j_e \approx j_0 e^{M j_e^n}, \tag{2.14}$$

with $M = BCG/E_A^2$. The crucial next step is the expression of $\gamma = j_e / j_+$, which is the ratio of the electron current density over the positive ion current density. Since these quantities are considered over the same electrode area, the current density ratio is the same as number ratio. Thus this is exactly what was sought, namely the number of electrons emitted for each incident ion. Since relations for j_e and j_+ are both determined, γ can also be found. Omitting the basic algebraic steps that were taken, the final result is

$$\gamma = K e^{-B/E_A}. \tag{2.15}$$

In this expression K is constant but depends on the unknown parameter n. Since B is also a constant, the same one as introduced at the start of the derivation, in the equation for the field emission, this new relation could provide a means to extend the applicability of Paschen's Law by using this enhanced formulation for the electron emission instead of the previously used constant γ_{se}. As a conclusion the authors propose that future experimental results could be used to confirm their theory if they are in agreement. There is however no proposed method to differentiate secondary emission from field emission, which are two effects that strengthen each other.

2.3.5. Osmokrovic, 1994

At the advent of Micro electromechanical systems, scientist and engineers suddenly had found a new application electrostatic breakdown. It is therefore at the time of around 1990, that new research was published on deviations of Paschen's law and the physical explanation behind this. In a 1994 paper by Osmokrovic [33], electrostatic breakdown is classified using different value of pd for which certain mechanisms are dominant. It is stated that any form of breakdown relies on the avalanche process, and that the method of creation of source electrons is differentiating. According to Osmokrovic, at large value of pd, Meek's streamer mechanism is dominant. The dominant source of electrons is then given by bulk processes in the gas, such as photo ionization and ionization by positive ions. If the largest part of electrons are formed at the cathode, the Townsend mechanism is characterising the breakdown, and Paschen's law can be applied. The next mechanism stated is vacuum breakdown. It is supposed to appear 'when the inter electrode gap becomes smaller than the mean free path of electrons'. This would mean electrons can only produce new electron by collisions after travelling the distance of the mean free path. This statement can only be true if the energy acquired within one mean free path is too little to induce an effective collision and produce another electron. According to the author, thermal instabilities of the electrodes cause evaporation of the material. This evaporated material then accelerates the avalanche process in a way that is not specified. The paper then continues to mathematically investigate breakdown. To follow their line of thought the presented derivation will be followed. The presented mathematical analysis depends on three parameters:

- α, the number of ionization collisions per unit distance in the direction of the electric field

- η, the number of electrons recombining per unit distance in the direction of the field

- γ, the number of electrons generated from each avalanche

This last parameter γ, according to the author denotes the number of electrons generated as a result of one avalanche in the gas. The problem with this definition is that the 'size' of an avalanche is undetermined, which will obviously affect the number of electrons produced. In the rest of the text however it seems like the more common definition of γ is used, which is the number of electrons generated per ion that is incident on the cathode.

Using the coefficients as mentioned, two criteria are presented, one for Streamer breakdown and one that should predict breakdown for the Townsend mechanism. First the criterion for streamer breakdown is

$$\int_0^d (\alpha - \eta)\mathrm{d}x = 10.5, \tag{2.16}$$

for which no rationale is given and especially the number 10.5 remains inexplicable for the current author. The expression that is integrated over the domain, $(\alpha - \eta)$ is in the simple case of constant electric field not a function of the spatial dimension x, thus it evaluates to

$$(\alpha - \eta)d = 10.5. \tag{2.17}$$

Since $(\alpha - \eta)$ denotes the net multiplication per unit length, the final expression can be visualised as an electron, starting at the cathode, moving towards the anode and on its way performing ionization events. According to (2.16) this single electron must perform 10.5 ionizations while traversing the whole domain to attain breakdown. This would result in a total number of electrons arriving at the anode of

$$N_e\Big|_{x=d} = \mathrm{e}^{10.5} \approx 3.63 \times 10^4. \tag{2.18}$$

This does not give more insight in the relation, so it will now be considered further at this point. For Townsend breakdown which is prevalent for smaller pd values the following criterion is presented:

$$\gamma \int_0^d \mathrm{e}^{\int_0^x (\alpha - \eta)dx} \alpha dx = 1, \tag{2.19}$$

of this criterion, no elaboration is given. As determined in the section of the streamer breakdown, this equation considers the number of electron produced at position x, multiplies it with α, and integrates over the domain. Since the inner integral evaluates to $(\alpha - \eta)x$, the factor of α is probably supposed to drop out when the outer integral is determined. In this case however there is an issue with η, which is included in the exponential but not in the other term. If for the moment η is set to 0, the outer integral can be determined and results in

$$\gamma \mathrm{e}^{\alpha d} = 1 \tag{2.20}$$

This equation does provide us with reasonably useful information as here, the number of electrons produced by an avalanche (the exponential) is inversely related with the number of electron emitted from the electrode. The product of these production rates must equal a minimal value to facilitate breakdown.

The remaining part of the paper presents experimental results that are claimed to match the mathematical model, but essentially is aimed towards differentiating between the different underlying mechanisms instead of really looking at the quantitative analysis. A numerical curve is plotted in their results but there is no mention of the relation between their criteria, involving the parameters α, η and γ, and the plotted curve, which uses pd for the product of pressure and distance and V for the voltage.

2.3.6. Radmilović-Radjenović & Radjenović, 2008

Since the start of the 21st century, researchers from the Institute of Physics Belgrade have worked on breakdown of gases from a viewpoint of plasma physics and simulation. Of a number of papers they have published on this topic, one specifically addresses a theory that could be used as an analytical expression to predict breakdown below Paschen's minimum [38]. In the paper, the governing equations are determined and solved analytically. One of the first statements made, is on the separated scaling of the variables p and d. In the original Paschen's law, they are considered as one variable pd. Because the small scale effects are hypothesized to depend on the electric field, these effects scale with the parameter d, because the gap distance determines the electric field for a given voltage. Since the electric field does not scale with the pressure this relationship does not hold when these effects come into play. Starting again from the principle that the bulk process is governed by electron avalanches, the authors reckon a similar equality as (2.20) to be governing the process. It is stated that field emission becomes important at high electric fields and aims to re-purpose γ to a parameter including field emission from the cathode, which will then be a function of the electric field. It is presented to have the following form:

$$\gamma = Ke^{-D/E}. \tag{2.21}$$

In this relation K and D are constant. In this form a low electric field provides a highly negative exponent which means the resulting γ is low. When the electric field reaches a critical value D, the exponent will attain a value on the order of unity and thus γ will rise to a value determined by K. According to the authors, the value of D can be found by

$$D = 6.85 \times 10^7 \frac{\Phi^{3/2}}{\beta}. \tag{2.22}$$

Herein Φ is the work function of the electrode material in eV and β is the field enhancement factor, a measure of influence of local roughness on the electric field. For the source of this expression they reference their own material published earlier [39]. In this other work the authors present the Fowler-Nordheim equation for field emission.

$$j_{\text{FE}} = \frac{1.54 \times 10^{-6} 10^{4.52\Phi^{1/2}} (\beta E)^2}{\Phi} e^{-\frac{6.53 \times 10^9 \Phi^{3/2}}{\beta E}} \tag{2.23}$$

This equation is used to determine the current density of field emission. It somewhat resemble the equation for γ, but this would only work out if the first part of the equation is a constant. Another problem here is that j_{FE} denotes a flow of charge per unit time, whilst γ is a coefficient. Since the coefficient defines the emission of charge on incoming charge, they do not compare in physical quantities. The current j_{FE} has a finite value whenever there is an electric field applied to an electrode, and in comparison to γ, does not require incoming particles to exist.

The paper continues with the breakdown condition

$$\gamma(e^{\alpha d} - 1) = 1, \tag{2.24}$$

Which is different from the one derived from the criterion presented by Osmokrovic [33]. The -1 that is included here is an addition that takes into account the original electron that initiated the avalanche. The number of electron newly created in such an avalanche is denoted by the amount at the 'end' of the avalanche, $e^{\alpha d}$, deducted by the initial amount, 1.

Substituting (2.21) into (2.24) the result is

$$Ke^{-D/E}(e^{\alpha d} - 1) = 1, \tag{2.25}$$

which can be rearranged to obtain

$$\mathrm{e}^{\alpha d} = \frac{1}{K}\mathrm{e}^{D/E} + 1. \tag{2.26}$$

Since field emission is dominant when $E > D$, and k is much larger than unity, the first term on the right hand side is much smaller than 1. Taking the natural logarithm on both sides transforms the righthandside into the form $\ln(1 + x)$, on which we can use a Taylor expansion as follows:

$$\ln(1 + x) = x - \frac{x^2}{2} + \frac{x^3}{3} - \frac{x^4}{4} + \dots \tag{2.27}$$

The authors then opt to use only the first term in this Taylor series expansion, and remain with the following

$$\alpha d = \frac{1}{K}\mathrm{e}^{D/E}. \tag{2.28}$$

The author then uses a relationship for α found from another publication [26]

$$\frac{\alpha}{p} = A\mathrm{e}^{-Bp/E}. \tag{2.29}$$

In this case A and B are again constants that depend on the composition of the gas. (2.28) and (2.29) can be combined to eliminate α,

$$Apd\mathrm{e}^{-Bp/E} = \frac{1}{K}\mathrm{e}^{D/E}. \tag{2.30}$$

Equation (2.30) now has only E, p and d as parameters, and can be rewritten to find E as a function of p and d.

$$E = \frac{D + Bp}{\ln(ApdK)} \tag{2.31}$$

This is then taken further to breakdown voltage by using the constant field assumption, thus allowing the substitution of

$$V_{\mathrm{bd}} = dE = \frac{d(D + Bp)}{\ln(ApdK)} \tag{2.32}$$

This relation for the breakdown voltage elegantly illustrates the separate scaling of p and d. What the authors fail to mention, is that this expression has the same fundamental flaw that is present in Paschen's Law as well. When either one or both of the variables p and d are decreased continuously, the voltage required for breakdown becomes infinite. In reality it is however clearly infeasible to create systems that are not susceptible to breakdown at all. Care must however be taken to not disprove a method without knowledge of its limitations. More on this later.

2.3.7. Go & Pohlman, 2010

Recently a study by Go & Pohlman [16], attempted to unify the classical Paschen's law with the newly developed breakdown criterion by Radmilovič & Radjenovič. Using the same building blocks, they develop the breakdown criterion as a function of p, d and V. Using (2.25) and (2.29) without requiring field emission to be dominant, they find that

$$K\mathrm{e}^{Dd/V}\left[\mathrm{e}^{Apd\mathrm{e}^{-Bpd/V}} - 1\right] = 1. \tag{2.33}$$

Which includes a nested exponential, and thus can not be solved analytically. Without providing a numerical method to solve the presented equation, the authors continue with the observation that γ now solely depends on ion enhanced field emission. This would mean that at large gaps, the low
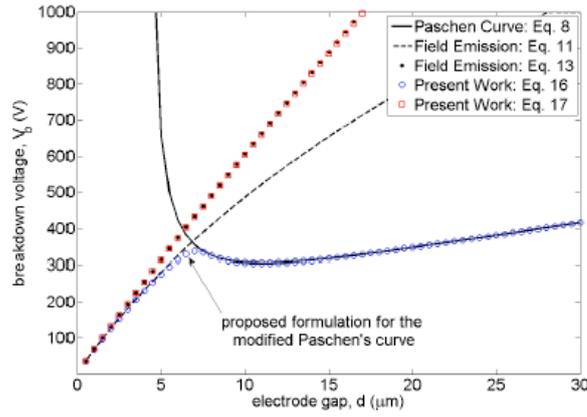
Figure 2.3: Blue dots representing the modified form of Paschen's curve by numerically solving (2.34) [16].

electric field would result in γ being much lower as compared to the constant value that represents secondary emission. If these different effects are independent of one another, a simple summation of their contributions can lead to an effective value for γ [35]. This then allows to replace γ by the summation term of both secondary emission and ion enhanced field emission

$$\left(\gamma_{\text{se}} + K e^{Dd/V}\right)\left[e^{Apd e^{-Bpd/V}} - 1\right] = 1. \tag{2.34}$$

A numerical solution to this curve perfectly resembles Paschen's curve at larger distances, and incorporates the lowering of the required voltage at small distances. The curve produced by the authors is shown in Figure 2.3. This curve now represents the behaviour of the system when ion enhanced field emission is accounted for. Just like the small gap distance condition presented by Radmilovič & Radjenovič, the breakdown voltage will also tend to infinity when the distance approaches zero.

2.4. Limitations of described papers

All the described papers have one thing in common. They approach electrostatic breakdown as a problem that involves one spatial dimension. This also involves keeping the electric field a scalar, which in reality should be described by a three dimensional vector at every point in space. From a physics point of view, these assumption make sense since the physical effects that are involved are generally present independent of the dimensionality of the system. Using the simplified case many conclusions can be drawn on the behaviour. These conclusion are however not always applicable in engineering when systems rarely comply to the limitations imposed on theoretical investigations. Also care must be taken for certain descriptions of processes which can not exist or behave differently for varying the number of spatial dimensions.

As an example consider the electric field induced by a single point charge. The electromotive force at a radius r from this particle since the force will be 'divided' over the area of the sphere around the particle with radius r. In 3D this results in a spherical shell with area $4\pi r^2$, which relates to the r^{-2} dependence found in Coulomb's law. When the problem is reduced to a 2D setting, mathematically the surface will become a line element, which equals the circumference of a circle: $2\pi r$. This now means that the electromotive force between two particle will only drop off by r^{-1}. Taking this even further two a one dimensional case, the mathematics will reveal that the force does not depend on the distance at all, since there are only two points in space that are defined by moving a distance r from a predetermined point. In a 1D system this would result in considerable forces between particles even if they were infinitely far apart. The implication of this example is that mathematically correctly reducing the dimensionality of the system, will result in non-physical effects that can never

be experienced in the real world. Care must be taken regarding the dimensionality of the whole system, or components thereof.

In existing literature some general assumptions are commonly made, and it is important to identify those and learn if they are indeed justified. Also they could be perfectly suitable for certain method described, but will not hold if certain expansions or changes are made.

2.4.1. Scalar electric field assumption

In our three dimensional world, a force is determined by a magnitude and a direction. This means that a force can be completely described by either a magnitude and a unit vector with three elements, or a vector with three elements. Note that even in the first situation, there are three independent variables, since the unit vector includes a constraint (magnitude is unity), which means only two of the three components are independent. Remembering that an electric field is nothing more then a force per unit charge, it can be concluded that the electric field at any location in space must be described by a vector.

In papers on electrostatic breakdown, often times the electric field is reduced to a scalar value. This means the field must always point in the same direction throughout the whole system. Justification of this assumption is often found in the geometry considered. When two infinitely large parallel plates are used as the electrodes, the electric field will certainly direct itself so that the vector always points perpendicular to the surface of the electrodes. When the plates have finite dimensions however, the electric field can not be represented by a scalar value any longer at the edges. From the research of Paschen [34], a very suitable method method of creating parallel plate geometries in practice was devised. By using two spheres of a radius that is large compared to the distance between them, the small section where they approach most closely, can be considered a parallel plate geometry for all intents and purposes. In the regions further from this centerline the electric field will not be scalar, but this is outside of the region of interest anyway.

2.4.2. Constant electric field assumption

A second, not less frequent assumption, is the one of constant electric field. At first glance this might sound similar to the previous section, but there is a significant difference between *scalar* and *constant*. When applying the scalar electric field assumption and a parallel plate geometry, it seems a sensible step to use a constant electric field. When two electrodes are sitting at a potential of V_I and V_{II} respectively, and are a distance d apart, the scalar and constant electric field can be determined by

$$E = \frac{V_I - V_{II}}{d}. \tag{2.35}$$

This does however only work if the system does not contain any other charges. Any charge (ions, electrons) between the plates will influence the electric field. Therefore even if the electric field can be considered a scalar, the value can still depend on the location inside of the domain due to space charge. In plasma physics this effect is very important since it studies the coupling between motion and concentrations of charges and the electric fields generated.

2.4.3. Inherent difficulties of analytical methods

Analytical method have proven to be provide simple and elegant solutions to certain problems. One of the main difficulties however is that they are very hard to apply to many non-trivial problems. Finding the important effects requires many assumptions, and finding analytical solutions often requires approximations, like dropping higher order terms and linearisation.

2.5. Alternate methods

Instead of going the conventional route of analytical solutions of physical effects, other techniques can be used. Splitting the process in two steps, first the determining of the important effects and finding quantitative relations between important parameters, secondly finding a solution as function of the parameters. Determination of important effects can occur using a top-down approach, or a bottom-up approach. A top-down method would involve observations of the real world, that can be captured by formulations. An example would be the observation that an electrode emits electrons when a strong electric field is applied. Using this knowledge we would then develop a relation expressing the amount of emitted electrons as a function of the electric field. A bottom-up approach would start at the 'bottom', which is the very small scale. By establishing the governing equations for elementary particles, the same behaviour should emerge that is observed in the real world.

2.5.1. Continuous description of charge densities

Using the Poisson equation, the electric field can be determined from the charge density inside the domain. The equation for an electron avalanche allows a solution for the charge density as a function of the ionization multiplication which is in itself a function of the electric field.

$$\frac{\mathrm{d}n}{\mathrm{d}x} = \alpha n, \tag{2.36}$$

where n is the number density of the electrons. Simultaneous solving of these two equation would result in a solution for the charge density, which would go to infinity in the event of breakdown.

2.5.2. Numerical solving of the equations

As mentioned, analytical solution can be very difficult to find. Many numerical method have been developed to solve differential equation by discretization and computer solving. This does not supply a solution in term of elementary mathematical functions, but the shape and magnitude can be obtained.

2.5.3. Solving Equations of Motion for all particles

The motion of each gas particle inside the system is governed by simple Newtonian mechanics. Any particle will accelerate in the direction of the net force that is applied to it. To model electrical charge in such a system the force acting upon a charge can be determined using the Coulomb force. This will result in a net force acting on a particle that will determine its movement. To accurately model collisions in this case one would have to model short range interaction between particles by adding to the Coulomb force a possible short range force when a collision event occurs. For every particle there will be a governing equation, which can all together be put into a large system using a state-space formulation. Since the force acting on a particle depends on the degrees of freedom of every other particle, this will be a very dense system, that will be very expensive to solve. This difficulty in solving can be visualized by realising that every particle has a 'link' with every other particle. Figure 2.4 illustrates the problem by showing a number of particles and shows the number of links that have to be determined. By adding one more particle to the system, a new link must be made to every other particle that was there beforehand. This means the difficulty of the problem scales with the number of particles n with $n!$, which becomes very costly if a suitable number of particles is used.

2.6. Existing literature on numerical methods

In the past researchers have employed numerical methods on many physical problems. In mechanical engineering, a great interest in computational solutions to mechanical problems has led to the development of finite element methods. In solid mechanics, one could also attempt to solve the
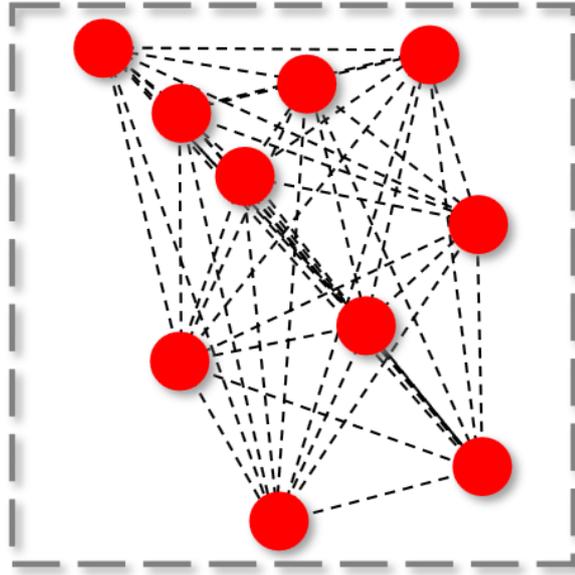
Figure 2.4: Interactions between particles are very costly to determine. Reprinted from *Introduction to Particle-in-Cell Methods in Plasma Simulations.*, by C. Ren, 2011, Retrieved Mar 31, 2017 from `http://hedpschool.lle.rochester. edu/2011SummerSchool/lectures/Ren.pdf`. Copyright 2011 by University of Rochester.

equations of motion for all elementary particles that constitute a solid to determine its behaviour. To overcome the computational difficulties that arise in *many-body systems*, which is a common term for, as the name implies, system with many independent degrees of freedom, the domain can de divided into larger sections. These larger sections are subject to the same governing equations but since they are much fewer in number, computation is justifiable. Naturally, the size of the elements in which the domain is dicretized greatly influences the accuracy of the result. This is a trade-off between speed and accuracy.

In electrostatic breakdown, where the governing physics are very different, similar techniques could be used. As mentioned before however, the greatest difference compared to mechanics is the existence of long range forces. In mechanics, the behaviour of a single element will be fully determined by the ones that are directly attached to it. This means that the number of 'interactions' that must be calculated for each element is bound and remains on the order of unity.

2.6.1. Finite difference method

The finite difference method can be applied to many fields of research. Essentially the finite difference method relies on discretization of any domain, and attempting to satisfy the governing equations at locations that are a finite distance apart. The discretization allows the derivatives in the governing equations to be written in a discrete form. Without going into too much detail, the *central finite difference* equation gives the discrete derivative of function $f(x)$ at discrete locations x_i as

$$f'(x_i) = \frac{f_{i+1} - f_{i-1}}{2\Delta x}, \tag{2.37}$$

with Δx being the distance between two locations. This method can be expanded to partial and higher order derivatives to solve many differential equations.

In electrostatic breakdown, the finite difference method has been employed to solve the governing equations by Georghiou [12]. Also, the finite difference method can be used as just one component of the analysis, as it is also used within the hereafter following Particle-in-Cell method.

2.6.2. Particle in Cell method

In plasma physics, electrostatic forces are important to the collective behaviour of gas particles. This means that the plasma physics community has developed possible methods that could be of use in breakdown problems [18]. The electrostatic force cause that long range forces are important and that one would have to solve a dense system of equations to determine the motion of particles. Solving the electric field (Poisson equation) using a finite difference method would be an interesting method since that eliminates the need to determine interaction force between locations that are not adjacent. The problem in using the finite difference method lies however in the fact that particles are not stationary. At every time step the locations of particles are updated and to then again find the electric field, the system of equations must be updated to accommodate for the change in locations.

The solution is found in a separate treatment of the electric field and the particle motion [4]. By keeping the points where the electric field is solved fixed, the finite difference method can still be applied. The charge of the individual particles is then mapped to these fixed points by a weighing that depends on the distance to the point. After a solution has been found with the finite difference method, the electric field is known on these fixed locations. By mapping the electric field back to the locations of individual particles, the total force acting upon them can be found. Updating particle positions and velocities, a new distribution is found for the charge density in the domain. Returning to the beginning of the process, the electric field is again solved and updated. By repeating the described steps the simulation advances and thus shows the behaviour of the system in time. This numerical method thus provides an interesting option for analysing a system of gaseous charged particles, because of the ability to scale the number of particles without exponentially increasing the computational difficulty of the problem.

2.7. Possible new research strategies and opportunities

After the analysis of existing literature, there are several methods and elaborations that have not been explored as of yet. Also it is important to remember the applicability of the theory in multidimensional settings, so that analysis of real life systems is possible. Some interesting possibilities have are described in more detail below.

2.7.1. Write α as a function of vector electric field

The assumption of scalar electric field does not hold for arbitrary geometries. To extend the theory an interesting option could be to write the ionization coefficient α as a vector. This means ionization can be introduced in multiple dimensions, depending on the direction of the local electric field. This method however requires the integration over the domain in multiple dimensions.

2.7.2. Including γ as a summation term and solving system PDEs

From literature it can be concluded that there are different effect contributing to the emission of electrons from the electrode, whether they are dependent on incoming particles or only rely on the electric field. To properly include these effects the total emission of electrons can be determined as a function of the electric field. Just like Go & Pohlman have attempted [16] with secondary emission and ion enhanced field emission, it might prove very interesting to also introduce a source of emitted electrons that does not involve incoming ions. This does however provide a difficulty with the breakdown criterion, since it classically is given by a relation that determines if there will be more electrons generated in every cycle of individual avalanches. Including a field emission current that does not involve incoming ions would lead to a time dependence, which complicates things significantly [8]. As of yet, there have been no such attempts (to the authors knowledge). This probably is largely due to the fact that it would be a very difficult feat to establish the breakdown criterion with the inclusion of time.

2.7.3. Including γ as a summation term and solving particle EOMs

To include this combined emission coefficient one could attempt to set up a full system of equations determining the motion of particles and iteratively solve the system to determine behaviour of charges. This is already much further away from a simple criterion for breakdown and also the removal and creation of particles would change the size of the system on every iteration. As a thought experiment, this strategy is interesting but in practice the sheer complexity would be too much to handle in any situation.

2.7.4. Fluid dynamics simulation techniques

In fluid dynamics, a continuous approach can be taken to study behaviour of liquids and gases. Using a continuous approach for gaseous particles, their motion can be described using the momentum equations that are known as Navier-Stokes equations [10]. Similarly by disregarding the viscosity of the gas, Euler's equations provide a similar description of fluid flows. Both methods result in a continuous field that specifies a flow of the given species. If electromotive forces could be included into this continuous description of the particle densities, the behaviour of electrically charged gases could be described. The electric field would then be incorporated as a body force that varies along the domain. In the field of fluid dynamics, one of the first to look into such descriptions was Hannes Alfvén [1]. He is considered the founder of a field called Magnetohydrodynamics, studying the behaviour of fluids that contain electrical charges. These studies combine the Navier-Stokes equations with the Poisson equation to provide a simultaneous solution of them. Application of this theory are found in plasma problems, but there are certain limitations due to the continuum hypothesis. In MHD, the implementation of electromotive forces into the fluid equations requires a current flow to be specified as a field. This results in a current flow being written as a function of the local electric field, using Ohm's law. A current flow in such a system then relies on the conductivity of the fluid in a classical sense. Also, fluid motion is assumed to be slow compared to the flow of current, whilst in breakdown systems the electrical current and the motion of particles are directly related since the particles are the carriers of the electrical current.

3

Deeper into the physics

To obtain a very thorough understanding of all the effects that are relevant for this work, the most sensible method is to start at the basics and elaborate on the physical effects for different parts of the system. This chapter give all of the required framework to grasp the effects that are significant and also certain effects that are not significant will be elaborated upon to prove that they are unrelated to certain aspects of electrostatic breakdown.

3.1. Kinetics of gases

To start this chapter off, the qualitative and quantitative behaviour of gases must be understood so that useful statements can be made. The main postulate of kinetic theory states that 'matter', independent of it's state, is not continuous and indefinitely divisible. Instead matter is composed of a finite number of particles that may or may not directly interact with each other. Most commonly these particlse that constitute matter are molecules, atoms, ions and electrons.

In principle different kinds of particles can be combined within one system, but a prerequisite for application of the theory is that the number of individual particles is large enough to be regarded as stochastic processes. In a solid, the individual particles, where the definition of a particle can be determined by the observer to suit specific needs, have a strong interaction and are not allowed to displace beyond small vibrations. In a liquid the particles are free to move past each other but they still significantly attract and repel their close neighbours. In the case of a gas the particle spacing is a lot larger which results in freely moving particles that only interact when they are very close together compared to the average spacing.

3.1.1. Statistical analysis

Continuing the focus on gases, a suitable method must be found to characterize the behaviour of such a system comprising a gas. Commonly when considering a system of individual bodies, we strive to predict their behaviour from initial conditions and governing equations. In the case of a gas it is however an infeasible thing to attempt. Even a tiny $1 \, \text{cm}^3$ cube of the air that we live in contains a staggering 1×10^{19} particles moving about. Instead of tracking all of those particles individually and determining their motion, it is more sensible to limit our quantitative analysis of properties to statistical averages. The first thing to consider is a gas in equilibrium, and determine its characteristic properties. Let us consider a single gaseous particle, it possesses a position and momentum. As long as no forces are acting on this particle, it moves in a straight line. A particle modelled as a hard sphere, can then be modelled to interact with another particle when the two of them collide. When they collide both of the particles will attain a new direction of travel and velocity. Their combined momentum however is unchanged. Therefore if the momentum and position of the particles was
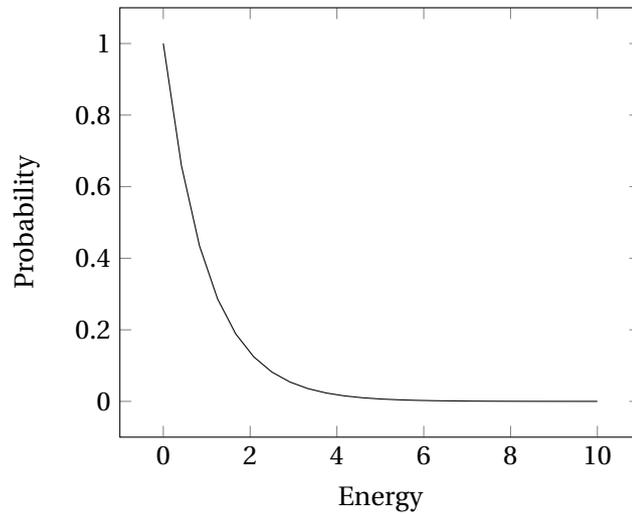
Figure 3.1: The Boltzmann distribution with arbitrary units

randomly determined before the collision, it will still be random after the collision. This results in the momentum distributions of a large number of particles remaining the same even if there are collisions between them.

3.1.2. Velocity distribution

In the previous paragraph it was stated the the total momentum of a system of particles does not change due to internal interaction. The distribution of momentum and position states among the individual particles however can change. At each point in time, each particle will possess a certain energy. Looking at the same thing from another perspective, it can be stated that for a given amount of energy, there is a certain chance of a particle being in that state. In a gas that is in equilibrium, this distribution of a particle having a certain energy, was developed by Boltzmann. The Boltzmann distribution denotes for an ensemble of particles, the probabilities of a particle being in a given state E. The number of particles n at a given energy is given by

$$n(E) = A\mathrm{e}^{-E/kT},\tag{3.1}$$

where the possible states are given by E. The ratio of E over kT acts as a scaling factor for the particle energy. The constant k is Boltzmann's constant and relates energy to temperature. In the kinetic theory of gases temperature is related to the average kinetic energy of the particles by $\overline{E} = \frac{1}{2}kT$. A graphical representation of eq. 3.1 is given in 3.1.

To obtain the occupied energy states per unit volume the density of states must be included. The energy of the particle is related to the magnitude of the velocity by $E = \frac{1}{2}mv^2$. This allows us to rewrite Eq. 3.1 as

$$n(v) = A\mathrm{e}^{-mv^2/2kT},\tag{3.2}$$

A particle moving in three dimensional space will have a magnitude of the velocity and a direction. Therefore the total movement of the particle must be projected on each orthogonal direction. Using the theory of k-space, we can multiply the chance of a particle moving in a certain direction with the chance of it having a certain energy. Considering the velocity vector of the particle as having a known magnitude v but unknown direction, the velocity vector can lie anywhere on the sphere with a radius of v. The surface area of this sphere is given by $4\pi v^2$, so therefore the probability density for the velocity is given by
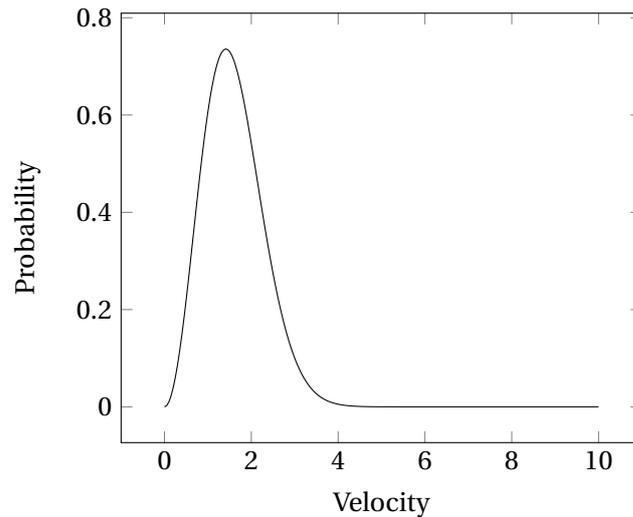
Figure 3.2: The Boltzmann distribution with arbitrary units

$$f(v) = 4\pi v^2 A e^{-mv^2/2kT} \tag{3.3}$$

where v is the scalar magnitude of the velocity. This equation can then be normalized to obtain the constant A because the integral over all probabilities must equal 1. The obtained final form of what is called the Maxwell-Boltzmann distribution, is the following

$$f(v) = 4\pi \left(\frac{m}{2\pi kT}\right)^{3/2} v^2 e^{-mv^2/2kT}. \tag{3.4}$$

The distribution now has obtained the form illustrated in Figure 3.2. Note that the energy axis is given in arbitrary units.

3.1.3. Boyle's Law

Instead of the velocities of gas particles, it is also interesting to determine some of the bulk properties. What comes to mind as characterizing many gases is Boyle's Law, also known as the ideal gas law. First a short mention on what makes a gas an ideal gas. The main assumption has already been done in this case: namely that particle are considered as hard spheres that only interact when they collide. Another important thing is that the distance between two particles is large compared to their radius, the volume of a gas is determined by the motion of the particles, not by the volume of the particles themselves. If a collision occurs the particles can interchange momentum and change the velocities (in both magnitude and direction). The ideal gas law has been determined experimentally thus it is give below in the form that it is most readily known.

$$pV = NkT \tag{3.5}$$

In words it states that pressure items volume equals the number of particles times the constant k times temperature. The implication of this relation that will prove to be most important is the proportionality between the pressure p and the number of particles in the system N. Doubling the pressure at constant volume requires the number of particles inside that volume to double by means of generation or inflow through a boundary.

3.1.4. Diffusion

When there is a gradient of concentration (number per unit volume) the particles in an area of higher concentration will move towards an area of lower concentration, thus diminishing the gradient. The

diffusion equation can be written as

$$J = -D\frac{d\varphi}{dx} \tag{3.6}$$

Which holds for the one dimensional case. In multiple dimensions it must be written using the gradient operator. The diffusion flux J is proportional to the difference in concentration varied in the spatial direction. A proportionality constant D is a constant relating the two.

As mentioned the flux J tends to even out the concentration gradient. Therefore it might be useful to investigate the temporal behaviour of diffusion, which can be captured in a differential equation.

$$\frac{\partial\varphi}{\partial t} = D\frac{\partial^2\varphi}{\partial x^2} \tag{3.7}$$

Here the change in the concentration over time is related to the second derivative of the concentration in the spatial coordinate.

3.2. Behaviour of Charges

The physical particles that constitute a gas are generally assumed to only interact with one another when the distance between them becomes zero, i.e. the particles have a direct elastic collision. Particles however can also posses an electric charge. Such a particle is called a charged particles or sometimes just as 'charge'. Electric charge is expressed in the SI unit of Coulomb [C]. Since charges generally have a quantized value of charge, another common way to denote an amount of charge is the *elementary charge*, which is often denoted e or q. A conversion between elementary charge and SI units is given by $q = 1.6 \times 10^{-19}$ C.

3.2.1. Charged Particles

To start this section on the forms in which electric charges exist, Bohr's model of the atom will be considered. The Bohr model states that an atom is made up of a nucleus, with electrons occupying 'circular' paths around the nucleus, see Figure 3.3 for a simplified graphical representation of an atom. The number of electrons that the atom contains depends on the type of atom, and is also directly related to the elementary particles inside the nucleus. The nucleus contains a set of neutrons and protons. The number of elementary particles inside the nucleus determines the type of atom, which fill up the periodic table of elements. Every proton has a positive charge of one elementary charge q, therefore the nucleus is positively charged. Around the nucleus a cloud of electrons creates the negative charge of an atom. Again, each electron has a negative elementary charge q. At this point it might be interesting to mention some of the dimensions and masses in an atom. The total size of an atom is generally on the order of 1 Å, whilst the nucleus is a mere 1 fm to 10 fm (femtometer), around a factor of 10 000 smaller. The mass of a small atom, that would generally make up a gas, is around 10^{-25} kg, where the mass of an electron is again much smaller, with the same factor of around 10 000. The rest mass of an electron $m_e \approx 1 \times 10^{-30}$ kg. This also implies that the general mass of a gaseous ion $m_i \approx 1 \times 10^{-25}$ kg.

For now it can simply be stated that two charges that are both positive or both negative repel each other, and that two charges with different sign attract each other. The atom is then stable because of the attraction between the cloud of electrons and the nucleus. The total charge of the atom under consideration is then zero of the number of protons equals the number of electrons. Instead of the atom having a neutral net charge, it can also 'lose' an electron, a process called ionization. The atom itself is now positively charge by an amount q, and a free electron is formed with charge $-q$. A positively charged atom is in practice called a positive ion, or cation. This implies that ions can also have negative charge, which is true. A negative ion, or anion, is created when a neutral atom
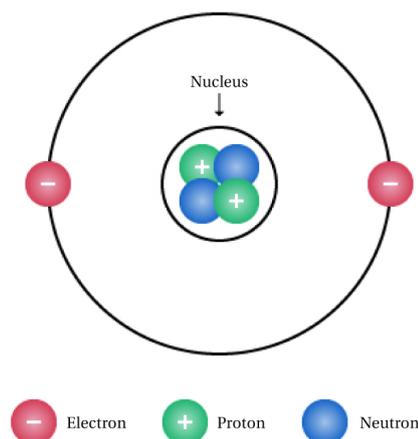
Figure 3.3: Bohr's model of the atom, depicting a Helium atom with two electrons, two protons and two neutron. Reprinted from *Atomic Theory II: Bohr and the Beginnings of Quantum Theory*, by Adrian Dingle, Anthony Carpi, 2003, Retrieved July 16, 2017 from `http://www.visionlearning.com/en/library/Chemistry/1/Atomic-Theory-II/51`. Copyright 2017 by VisionLearning Inc.

obtains an extra electron, and becomes negatively charged. Both types of ions can also exist in a more extreme form, when multiple electrons are surplus or missing. Due to the great charge that these ions have, they tend to occur less frequently because they also require more energy to be created, and will likely regain the surplus or deficit of electrons if there are free electrons in the vicinity. This process is called recombination, and can be seen as the opposite of ionization. Both processes will be quantitatively analysed later, but to do so the quantitative analysis of the attracting and repulsion between charged particles must be determined.

3.2.2. Coulomb's Law

The determination of the aforementioned attractive or repulsive force between two charged particles, was investigated by Coulomb in the end of the 17th century. He discovered that the force between charged spheres was proportional to the amount of their charge, and inversely proportional to the square of their distance.

$$F = \frac{Q_1 Q_2}{4\pi\epsilon d^2} \tag{3.8}$$

It is this force that acts between any two charges, no matter their distance apart. The force will however become negligible rapidly when d is increased, due to the quadratic scaling. At a later stadium, during the development of a model of electrostatic breakdown, a suitable manner must be found to model these Coulomb forces in the system of particles without overly increasing the complexity involved in scaling such a system.

3.2.3. Electric fields

If instead of determining the force between two interacting charges, another useful method could be to try and determine a field, that quantifies the force that would work on some *test charge* if it were at that location, under the influence of another charge at a given location. If this could be achieved it would be possible to determine the force at any given location that is induced by this reference charge. Because the electromotive force F depends also on the value of the test charge, it is natural to divide this value out to obtain a force per unit of charge. This field, the electric field $\mathbf{E}(\mathbf{r})$ in units of Newton per Coulomb [$N\,C^{-1}$], then allows us to find the force acting on a particle with charge

q at location $\mathbf{r}$ by using the fact that $\mathbf{F} = q\mathbf{E}(\mathbf{r})$, where now the force and electric field are vectorial quantities that denote the direction of the force and electric field respectively.

3.2.4. Movement of charged particles
For this section an electron will be taken as a charged particle to determine its motion. Assume that the electric field $\mathbf{E}$ is known. The electric field now acts on this electron by applying a force on it,

$$\mathbf{F} = -q\mathbf{E}, \tag{3.9}$$

since the charge of the electron is $-q$. The classical Newtonian equation of motion allows us to relate the electric field to the movement of the electron.

$$m_e\dot{\mathbf{v}} = \mathbf{F} \tag{3.10}$$

$$m_e\dot{\mathbf{v}} = -q\mathbf{E} \tag{3.11}$$

It is seen that the electron, as expected, accelerates opposite the direction of the electric field due to its negative charge, and the acceleration is proportional to the field. The kinetic energy of a particle can be determined using the formula

$$E = \frac{1}{2}m_e\mathbf{v}^2, \tag{3.12}$$

in which the energy E and the electric field $\mathbf{E}$ must not be confused. Also note that $\mathbf{v}^2$ denotes a vector squared, which implies the dot product of $\mathbf{v}$ with itself, or equivalently, the square of the magnitude of $\mathbf{v}$. Assuming at the moment that the electron does not undergo any collisions and start from rest, the energy it obtains from a constant electric field $\mathbf{E}$ can be determined as a function of time.

$$E(t) = \frac{1}{2}m_e\left[\int_0^t -\frac{q}{m_e}\mathbf{E}\mathrm{d}t\right]^2 \tag{3.13}$$

If the electric field can be considered static, there is no dependence on t and the energy can be simplified to

$$E(t) = \frac{1}{2}m_e\left[-\frac{q}{m_e}\mathbf{E}t\right]^2 = -\frac{1}{2}\frac{q^2}{m_e}\mathbf{E}^2t^2 \tag{3.14}$$

3.2.5. Ionization
Several mechanisms can cause the process of ionization. As mentioned before ionization is the process wherein a neutral atom or molecule obtain or loses one or more electrons. This process also incorporates a change in electric charge of the atom, forming an ion. The most commonly occurring process of ionization is induced by collision events. Whenever an atom or molecule is struck by some quantity of energy, this event can overcome the energy required to change the state of the atom or molecule. Common means of collisions are by electrons, other atoms or molecules, or high energy photons are other forms of radiation. Another interesting method of ionization is what is known as field ionization. The methods of ionization will be discussed in separate sections.

Electron impact ionization
An electron, such as the one described in the previous section, can obtain kinetic energy from moving in the electric field $\mathbf{E}$. Once this electron has obtained significant energy from the field, a collision with a neutral atom could be such that one of the electrons from the electron cloud of the atom is 'knocked' out of its orbit and become a free electron in the gas. By denoting a neutral atom by
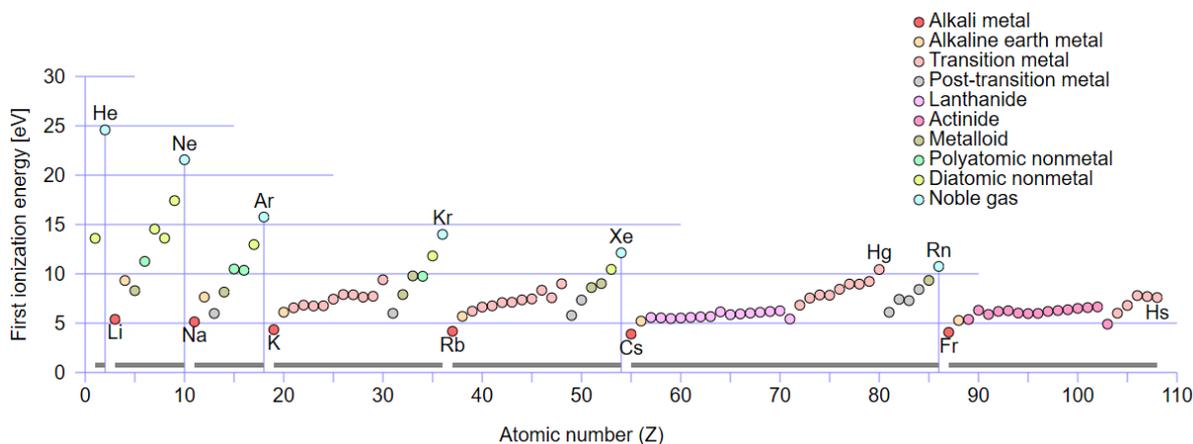
Figure 3.4: Energy required to ionize an atom of given atomic number. Reprinted from *Ionization energy*, by Sponk, 2011, Retrieved Mar 11, 2017 from `https://en.wikipedia.org/wiki/Ionization_energy`. Copyright 2011 by Sponk.

A, a positive ion by A^+, and an electron by e^-, the process can be shown in the form of a chemical equation

$$A + e^- \rightarrow A^+ + 2e^- \tag{3.15}$$

The original free electron must then have sufficient energy to maintain free itself, and surplus energy to break the bonding of the second electron that is removed from its orbit. A physical analysis of this process involves in depth quantum mechanics and wave functions, which are rather incomprehensible to present here. In physics, many models have been developed to determine the *ionization cross section* of this process [21], [22]. The ionization cross section denotes the area within which the two particles must pass each other to achieve an effective collision. Another way to look at ionization is by the energy required to accomplish this emission. If the required energy is called I, one can argue that the cross section depends on the excess energy of the electron compared to the required energy I. Thus

$$\sigma_i(E) = C_i(E - I), \tag{3.16}$$

which states the ionization cross section as a function of the electron energy. The ionization potential I is a dependant on the element, its values can be viewed in

This relation does not provide any useful information when the energy of the electron is less then the ionization energy. The ionization cross section does not mean much in itself since the probability of a collision is not determined. In a later stadium, where the frequency at which ionization occurs is important, this will be elaborated.

Electron capture ionization
It is also possible for an atom to capture an electron and become negatively charged. The difficulty with this type of ionization however is the this core of this process involves only two particles. A third particle is required to achieve this type of ionization to ensure a balance of energy. This type of ionization could thus only occur if there is a suitable manner to release this energy.

$$A + e^- \rightarrow A^- + x \tag{3.17}$$

Ion impact ionization
If an electron with sufficient energy can ionize a neutral molecule, it is reasonable to suspect that ions can accomplish the same. Ions can also be accelerated in an electric field and since they are
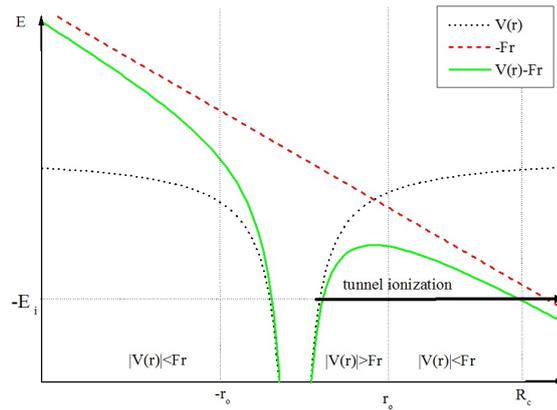
Figure 3.5: The quantum mechanical potential of an atom in an external electric field. Reprinted from *Tunnel ionization*, by A. Talebpour, 1998, Retrieved Mar 16, 2017 from `https://en.wikipedia.org/wiki/Tunnel_ionization`. Copyright 2017 by A. Talebpour.

much bigger than electrons, one would conclude that the probability of them inducing an ionization event is larger compared to electron impact ionization. It is however due to this very fact that ions are not successful in liberating electrons from a neutral particle. An electron and an ion travelling the same distance through a constant electric field obtain the same amount of kinetic energy from this field. Because the ion is larger however it will be much less likely to be able to travel this distance without experiencing a collision with another gas particle, in which it loses part of its kinetic energy to this other particle. It is for this reason that the ionization in electrostatic breakdown is generally considered to be caused by electron impact ionization.

$$A + A^+ \rightarrow 2A^+ + e^- \tag{3.18}$$

Field ionization
In field ionization, the ionization is induced by the electric field surrounding the atom. Inside an atom the electron is attracted to the nucleus by the Coulomb force. If there is an electric field applied from an external source, **E**, this electric field exerts an electromotive force on the electron. Assuming the Bohr model of an atom, the circular orbit of the electron around the nucleus causes the electron to experience a varying force depending on the 'side' of the nucleus it is located. When the field is strong enough, this force exerted by it can exceed the internal force that keeps the atom stable and ionization can occur.

Tunnel ionization
Even at a lower electric field then the threshold field as described in the section of field ionization, ionization can occur. From quantum mechanics, it is known that electrons, instead of having a determined location, are characterized by the probability of them being at a given location. This implies that there is always a chance of an electron appearing at any location. As seen in Figure 3.5, whenever the potential barrier is thin enough, an electron can tunnel through this barrier and appear on the other side. This process, called quantum tunnelling, is an effect that proves to be of importance at high electric fields.

Associative ionization
This type of ionization was discovered by Hornbeck and Molnar [20]. It was shown to occur when there are atoms present in an excited state. Two atoms, of which one must be in an excited state, are

able to combine into a larger positive ion, and a free electron is released. This principle is then given by

$$A + A^* \rightarrow A_2^+ + e^-. \tag{3.19}$$

This process requires two particles as the input so is therefore highly likely to occur. Also the required energy is significantly lower than the energy required for impact ionization. The produced ions are known as molecular ions, since the consist of multiple atoms combined.

Photoionization
Photoionization can be viewed as a form of impact ionization. The photon must have sufficient energy to ionize the atom by having an energy above the ionization energy I. For a quick analysis it is found that a photon in the spectrum of visible light, with a wavelength of 500 nm has an energy of

$$E = \frac{hc}{\lambda} \approx 2.5 \, \text{eV}. \tag{3.20}$$

This is generally too little compared to the ionization energies which are found in Figure 3.4.

Chemical ionisation
Ionization of a molecule or atom can also depend on a chemical reaction. In gases, chemical ionization requires the presence of suitable reagents. These reagents must posses the correct atomic structure to be in a state where they are specifically available for ionization. In electrostatic breakdown, the chemical composition of the atoms and molecules involved, do not generally lend themselves for this type of ionization. If other gases than air are used, they are noble gases such as Argon or Xenon.

3.2.6. Recombination
All ionization processes that were elaborated on before, could be reversed to remove ions and free electron from the gas. These reverse processes are together named as recombination. Since the process of recombination is no different than for ionization, it is more interesting to look into the rate at which recombination occurs.

Dissociative recombination
From the section of associative ionization, it was found that molecular ions can be produced in a gas at relatively high rates. This process can also be reversed and the prerequisites for it are only for a molecular ion and a free electron to meet each other. Due to the fact that 'normal', ineffective collisions between two particles are much more common as compared to effective collisions, the rate of dissociative recombination is very high.

Electron-Ion recombination
Electron-Ion recombination is a very complicated subject characterized by various form of recombination [19]. Examples are Radiative Recombination(RR), Dielectronic Recombination (DR)and Three Body Recombination (TBR). To simplify this theory and make it applicable for the case of electric breakdown, the decay of electrons can be determined in time by

$$\frac{dn_e}{dt} = -\beta n_e n_+. \tag{3.21}$$

The rate of recombination, denoted by the time derivative of the concentration of electrons, is proportional to the concentration of electrons and concentration of ions. If the initial condition $n_e = n_+ = n_e^0$ holds,

$$n_e = \frac{n_e^0}{1 + \beta n_e^0 t}. \tag{3.22}$$

β here is the *recombination coefficient*, which is given in volume per unit time.

Electron losses to boundaries

In the event of breakdown, interaction between charged particles and the electrode surface play an important role. It must not be forgotten that these effects prove to be a significant factor in the removal of charged particles from the system. Interaction between the boundaries and particles will be explained in a specific section.

3.3. Solid-Gas interaction

This section will focus on all possible forms of interaction between the solids that form the electrodes of the system and at the same time provide the boundary. The nature of an electrode will be discussed and the influence of the electric field on the electrodes is analysed.

3.3.1. Electrodes

In electrostatic breakdown, the electrodes consist of a conducting material that exists at a certain electrostatic potential. The electrostatic potential is measured in the SI unit of Volts and denotes the difference in electrical potential between two points. In this description an imported notion is the included word *difference*. An electrical potential always needs two points and the potential difference between the two points is defined by the amount of work required to move an electric charge from one point to the other. $1\,V$ thus equals one $1\,JC^{-1}$. If the electrodes are assumed to be perfect conductors, there is no electrical potential between any two points within that electrode. This means an electrode can be described by one number for its electrical potential. Because electrical potential denotes a difference between two points, there must be a reference to which other potentials can be related. In the case of two 'points', which are actually electrodes with a finite size, the most common method is to set the potential of one the points to zero. The electrical potential of the other point will then be given by V and immediately denotes the potential difference between those two locations.

The electrode at zero is also called reference electrode, negative electrode, ground or cathode. The other electrode then is the positive electrode, or also called anode. A potential like this must be generated somehow, and this its origin can be found in Coulombs law in subsection 3.2.2. If an electrode, which can be referred to as the anode is charged with a charge of $1\,C$, it exerts a force on any other charge. The other electrode also has a level of charge, but for now can be taken to be at $0\,C$, this one is now the cathode. Due to Coulombs law this second electrode does not exert any force on other charges. The work required to move a charge from the cathode to the anode is now found by the force working on the charge and the path that it travels along. The force working on the charge is found by Coulombs law, but the path taken is still unknown. To continue the notion of a *conservative* force is required. A conservative force has the property that it depends only on location, and not on velocity or acceleration. This also has the implication that the required work depends only on the starting and final location and is independent of the path taken. The electromotive Coulomb force has this property and thus the work is not dependent on the path. Using these relations and properties the work required for moving a charge from the anode to the cathode can be found by integrating the Coulomb force over the distance from the anode to the cathode.

External circuitry

The energy required to bring and maintain the electrodes at these electrical potentials must come from an outside source. In electrical circuitry the source is commonly a chemical battery cell. Such a cell can transport electrical charge from one location to another and therefore introduce the described potential difference between these locations. In electrical engineering, a differentiation is made between two ideal sources: ideal voltage source and ideal current source. In practice any source will be a combination of both. An ideal voltage source is an electrical source that will maintain a given potential difference between two points without compromise. If charges are moved, removed or extra charges are added to the system an ideal voltage source will respond infinitely fast by moving
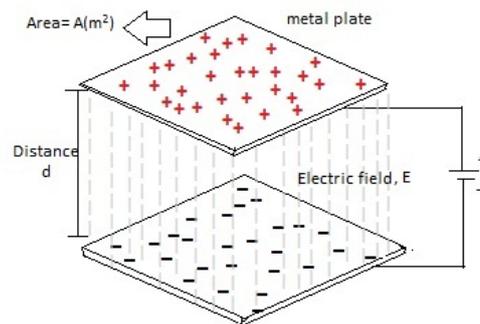
Figure 3.6: Parallel plates capacitor system with external voltage source. Reprinted from *Capacitance and Charge*, 2015, Retrieved June 3, 2017 from `http://www.electronicshub.org/capacitance-and-charge/`. Copyright 2017 by Electronicshub.org

charges until the imbalance is removed.

An ideal current source will move electrical charge independent on the work that is required to do so. This means that moving, removing or adding charges to the system will alter the voltage.

If an ideal current source were hooked up to two electrodes, the voltage would increase until breakdown conditions are attained. At that point however, the conducting gas will let the current flow and this will drop the voltage. Due to a decreased voltage the gas will conduct less easily and will lead to an increase in voltage again. The final result of this is a stabilized voltage at which exactly the amount of current flows through the gas as 'specified' by the ideal current source. This phenomenon is what has been described in the introduction in subsection 1.4.1 and is a form of gas discharge.

An ideal voltage source, which has way better semblance to practical electrical sources such as batteries, behaves differently. If the voltage is sufficient to cause breakdown, the gas will become more conductive and current flows through from one side to the other. The voltage source immediately restores the balance to maintain the voltage and thus the gas will become more conductive than before. This process does not stabilize like in the case of a current source, but here the current will keep rising indefinitely.

As touched upon, practical sources behave more like ideal voltage sources, and thus are prone to breakdown.

3.3.2. Particles impacting the electrodes
Returning to the interactions between the electrodes and the gas, difference mechanisms of interaction are found. These effects are all methods which interchange charge between the electrode and the gas. Interactions in which no charge is transmitted to not influence electrostatic breakdown and in those cases are related to kinetic gas theory instead. Hereafter some of the most significant processes are described in which particles strike the electrode.

Neutralizing of ions

In electrostatic breakdown ions are generally positively charged, thus atoms that are missing one electron. Positive ions are attracted towards the cathode due to the electrostatic force and will eventually collide with the solid material. The cathode itself contain a surplus of electrons due to its electrostatic charge. Thus when a negatively charged ion reaches the cathode, it can recombine itself with an electron sitting at the surface of the material. This electron is now removed from the cathode so indirectly there is a flow of current into the cathode (note the sign convention, an electron leaving the cathode means current towards the cathode). The neutralized particle diffuses back into the gas

according to the laws described in section 3.1.

For negative ions a similar process can occur at the anode. Their surplus electron can be transmitted to the anode from which it can flow into the material. The neutral atom again mixes into the gas where it behaves as a regular particle [18].

Adsorption of electrons
For electrons the process is almost the same as for ions. Electrons are attracted by the anode because there exists a 'shortage' of electron at that location. Again, this process involves wave functions to completely describe but the essence is that the anode acts as a perfect sink for incoming electrons.

3.3.3. Emission due to fields
This section regards the electrodes as they are exposed to an electric field **E**. The electrons in the lattice material of the electrode are susceptible to the electric field that exists in the system. If the field pulls on the electron with sufficient force, there is a chance that they will escape into the gas. The most important mechanisms of this process will be described with the aid of some graphs depicting the potential as a function of location.

First a situation is considered where there is no electric field applied in the system. The black line in Figure 3.7 shows what can be simply stated as the energy an electron needs to posses in order to (most likely) exist at that specific location. Inside the material and very close to it, the electron does not require any energy and can move around freely. To get further from the solid material the electron needs to have a certain energy level. The energy level denotes by the dotted line signifies the energy requires to completely release from the material, and is equivalent to the work function of the electrode material in this case. The work function is defined as the minimum work required to remove the electron from the surface. Also shown besides the vertical axis is the energy distribution of the electrons. At room temperature the energy levels of all the electron inside the material are distributed around a mean value called the Fermi level. The width of this distribution is determined by the temperature and the energy level of all electrons converges to the Fermi level when the temperature is lowered to absolute zero.
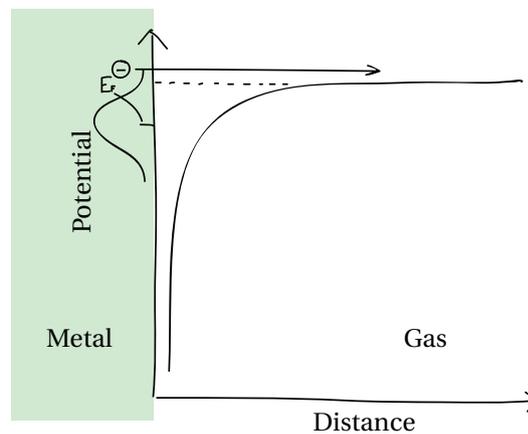
Figure 3.7: High energy electron emitted from the surface.

Thermionic emission
Directly following up on the previous section where the distribution of energy levels was explained, thermionic emission comes in. The energy distribution function of the free electrons inside the solid becomes wider when temperature is increased. In Fermi-Dirac statistics the distribution function is given by:
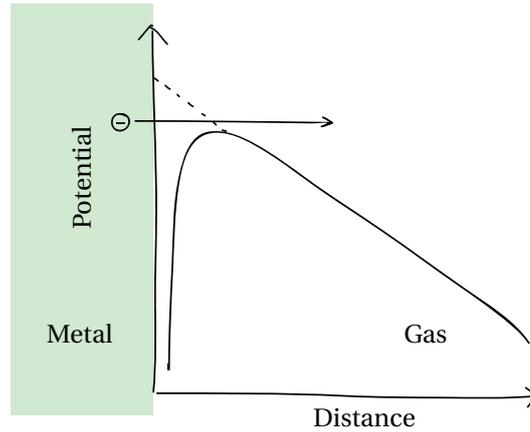
Figure 3.8: The Schottky effect reduces the barrier seen by an electron.

$$f(E) = \frac{1}{1 + e^{(E-E_f)/kT}} \tag{3.23}$$

In Fermi-Dirac statistics, due to the Pauli exclusion principle only one electron can occupy a certain energy state. Therefore the distribution function as depicted in **??** is not an accurate representation. To be more precise, one can determine the chance that a given quantum energy state will be occupied by an electron. The important message here is that a high temperature increases the chance of the high energy levels to be occupied. Figure 3.7 depicts an electron that is emitted from the solid material because it has one of the low probability energy states that is sufficient to break free.

Experimental observations from Richardson [41], enabled the construction of a simple formula to find the emission of electrons from a solid as a function of the temperature. He proposed the following function

$$j = AT^2 e^{-W/kT}, \tag{3.24}$$

where j is the current density, and further involves a constant A, the temperature T, the work function W and Boltzmann's constant.

Schottky emission

When an electric field is applied at the surface, the potential drops off with increasing distance from the electrode. This will reduce the energy that an electron is required to have in order to escape the material [36]. A visual representation is given in Figure 3.8. A common measure of this increase in emission is the perceived change in the work function, ΔW. This change is naturally a function of the applied field and given by [25]

$$\Delta W = \sqrt{\frac{e^3 E}{4\pi\epsilon_0}}. \tag{3.25}$$

This can then be used in conjunction with Richardson's law to develop a relation for the current density of emission. It must be noted that due to the nature of the expression, the dependence of j on E is not very large.
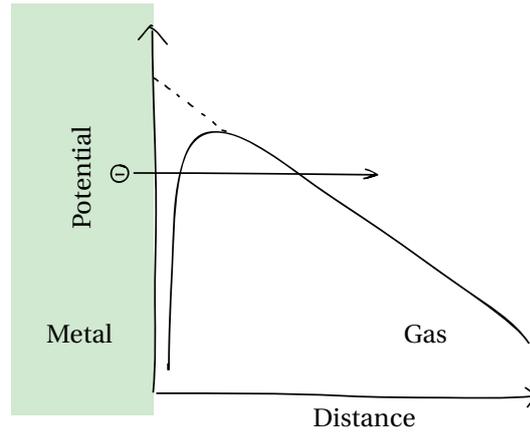
Figure 3.9: In field emission a particle can pass through a potential barrier.

Fowler Nordheim tunnelling

At higher electric fields, the barrier experienced by the electron in the material does not become much lower, and thus the Schottky effect stabilizes. With increasing field, the potential barrier does become thinner. An effect that can not be neglected at electric fields on the order of $1 \times 10^8 \, \text{V m}^{-1}$. In quantum mechanics, an elementary particle can tunnel through a potential barrier, even when its energy is not sufficient to classically do so Figure 3.9.

In reality the width of the barrier is dependant on the energy of the electron, which makes it a triangular or sawtooth shape. To illustrate the effect, a rectangular barrier will be considered in one dimension. In Figure 3.10, the space is divided into three regions. In region (I), the electron is free to move and the potential $V = 0$. Region (II) has a non-zero potential of height $V = V_0$. Region (III) again has a potential of 0. To execute this analysis the Schrödinger equation must be solved. Starting with the Schrödinger equation in a time independent form

$$-\frac{h^2}{8m\pi^2}\nabla^2\psi + V\psi = E\psi. \tag{3.26}$$

Here the wavefunction ψ contains all physical information of the system, and therefore fully defines it. Also, V is the energy potential, and E is the energy of the particle. The width of the barrier is d Writing this equation in one dimension

$$-\frac{h^2}{8m\pi^2}\frac{\text{d}^2\psi}{\text{d}x^2} = E\psi, \tag{3.27}$$

allows us to use the substitution

$$\kappa^2 = \frac{8m\pi^2 E}{h^2}, \tag{3.28}$$

which will make for a very elegant solution of the ordinary differential equation (3.27). The result is

$$\psi_\text{I}(x) = Fe^{i\kappa x} + Ge^{-i\kappa x} \tag{3.29}$$

in which F and G are integration constants to be determined by the boundary conditions of the system. The same equation holds for region (III) but here we will use the integration constants P and Q This equation must hold on both the left and right side of the potential barrier. Inside the potential barrier, it is known that $V_0 > E$, since the essence of tunnelling lies in the fact that the particle has a
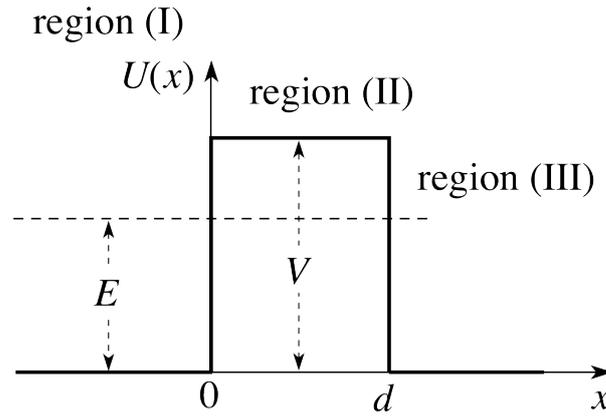
Figure 3.10: Electron tunnelling through a potential barrier. Reprinted from *Reflection and transmission at steps and barriers*, 1996, Retrieved June 11, 2017 from `http://www.physics.brocku.ca/PPLATO/h-flap/phys11_1.html`. Copyright 1996 by Open University.

lower energy than the barrier. In that case the total potential of the particle is written as $E - V_0$. Also solving the Schrödinger equation for region with integration constants U and V, we obtain three wavefunctions. To find the total solution we use the conditions that the wave functions and their first order derivatives must be equal at the interfaces. Thus

$$\psi_{\text{I}}(0) = \psi_{\text{II}}(0), \qquad \frac{d\psi_{\text{I}}}{dx} = \frac{d\psi_{\text{II}}}{dx}, \qquad (3.30)$$

$$\psi_{\text{II}}(0) = \psi_{\text{III}}(0), \qquad \frac{d\psi_{\text{II}}}{dx} = \frac{d\psi_{\text{III}}}{dx}, \qquad (3.31)$$

Of the two missing constants, boundary conditions, one can be found by the input of the particle at the left. fact that there is an incoming particle at the left towards the barrier, and no incoming particle from the right towards the barrier. The transmission coefficient can be found by the remaining coefficient Q, which denotes the part of the wavefunction that comes through the barrier.

In the end the probability for the electron to tunnel through the barrier is approximated by [3]

$$T \approx \frac{16E(V_0 - E)}{V_0^2} e^{-2\kappa W}. \qquad (3.32)$$

Most importantly, the probability of tunnelling is seen to depend on the height of the barrier, but especially on the width of the barrier, W. This probability does provide insight in the mechanics of this effect, but a translation must still be made to find an emission current density as a function of the electric field. For these a set of equations have been developed to roughly estimate this emission of electron from a solid into vacuum (gas) under the influence of an electric field [11] [32]. Solving the following integral allows the conversion between probability and current density, where the 'supply' of electrons in the tunnelling direction is included inside the integral . A simplified form of the Fowler-Nordheim field emission current is characterized by

$$j = \frac{AE^2}{\Phi} e^{-\frac{B\Phi^{3/2}}{E}}. \qquad (3.33)$$

Also a parameter can be included to capture local enhancement of the electric field due to the microgeometry. Small unevenness in the surface will cause increased electric field locally, and this can be included by replacing the electric field E in the equation with βE [7].
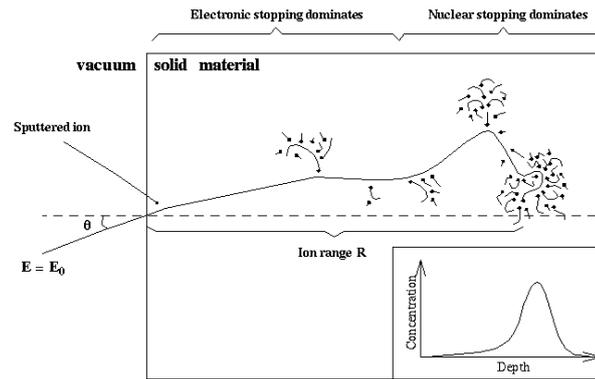
Figure 3.11: Incoming particle transferring energy to the solid material. source wiki `https://en.wikipedia.org/wiki/Stopping_power_(particle_radiation)`

3.3.4. Emission due to particles

In the theory on electrostatic breakdown, emission of electrons from the electrode due to incoming particles is of great significance. These particles are of the same nature as described in the section on particles sinking into the electrodes. Instead of only involving the incoming particle, such an event can involve more particles. Because the number of particles striking the electrodes depends directly on the processes in the gas, the surface effects and bulk effects are strongly coupled. The occurring processes are described by their origin below.

Secondary emission

The historical term for emission due to incoming particles is secondary emission. The term is not specifically aimed towards one physical mechanism and quantifies the emission of *secondary particles* as a whole. The general method in which secondary emission occurs and which is not captured in the other effects that do have a separate name, is as follows. Any particle striking the electrode a certain quantity of energy. This energy will be transferred to the lattice material which will increase temperature and also the Fermi level. The release of energy from a particle will commonly happen during a trajectory in which a particle penetrates a solid. Figure 3.11 show how far a common particle will penetrate the surface and by what forces it is slowed down. These increased values mean the other emission effects have a higher probability of occurring due to the incoming particles.

In practice the value of secondary emission is generally taken to be a parameter that includes all effects together. It's dependence on the electric field is therefore hard to describe but has been attempted in the research on electrostatic breakdown by Boyle & Kisliuk [5].

Malter effect

The influence of the Malter effect is something that is not mentioned commonly in breakdown research. The effect, first proposed by Malter in 1936 [30], describes the formation of a layer of positive charge at the surface of the cathode. The positive layer then acts as an attractor for electrons in the material and is thus supposed to aid in bringing new electrons to the surface and also increase emission. This effect might not be of much importance in electrostatic breakdown since the supply of electrons is governed by the external source and the layer might not be able to form because of the recombination of any positive particles near the cathode. The Malter effect might require an insulating layer at the surface which prevents direct recombination of positive ions and electrons, but allows the positive layer to remain stationary while creating the long range electromotive force require to pull out electrons, application for this can be found in multiplier tubes [50].
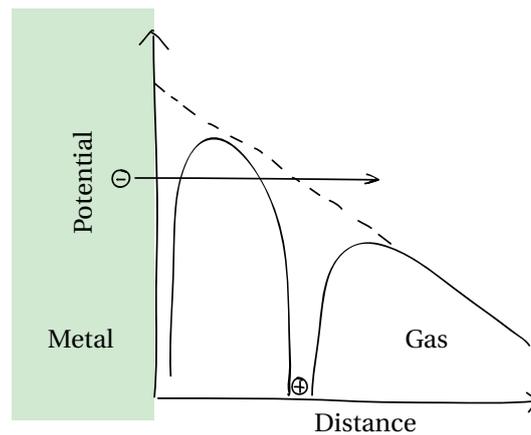
Figure 3.12: In ion enhanced field emission a positive charge deforms the potential barrier to increase probability of emission.

Ion enhanced field emission

Directly relating to the Malter effect is another proposed effect, Ion enhanced field emission [23]. In this publication Kisliuk mentions the possibility of positive ions enhancing the emission of electrons from the surface, just like the Malter effect. The difference being that there is no supposed positive layer at the cathode surface, but the ions are exerting their attractive force whilst they are being drawn towards the cathode and still moving in space. The presence of a positive ion near the surface will deform the potential seen by an electron near the surface as shown in Figure 3.12.

In this effect, time-scales are of great importance since the emission probability of a single electron is greatly dependent on the time that there is such a reduced and thinned potential barrier, which is again greatly dependent on the velocity of the incoming ion. Kisliuk does not mention the timescales involved except for a note on vacuum breakdown. It is reckoned that in vacuum breakdown, this effect is less prominent because the inbound positive ions will have great velocity and therefore will not allow the emission of electron during the short time period that they are within close proximity as to significantly alter the potential barrier. Also naturally the vacuum does not contain considerable numbers of particles so the absence of ions will logically also inhibit this behaviour.

Recently Li and Go have attempted to establish a theoretical basis for this type of tunnelling [28]. They mention that a simplified approach that was previously attempted involves the inclusion of the positive space charge in the scalar electric field that is used in the Fowler-Nordheim equation Equation 3.33 [49]. This does not however do any justice to the quantum mechanics involved. As seen in Figure 3.12, the electron can tunnel through the first barrier as the one depicted, but a lower energy electron could also tunnel through both barriers sequentially. A detailed analysis must then entail the solutions of the wave equations for both the single barrier and the double barrier, which will provide tunnelling probabilities. These probabilities must then be combined with the electron supply function which depends on the energy, to obtain the emission per unit time as a function of the location of the positive ion. To complete the analysis the motion of the ion must be accounted for by integrating this process over time starting at a point distant enough to be negligible, up until the moment the ion recombines with an electron. This all does require the assumption that the motion of the ion is slow compared to the emission of an electron. From Shafir et al. [43], the timescale for tunnelling of an electron is in the order of 1×10^{-15} s. Considering a typical speed for the ions in the order of $1 \times 10^4 \, \mathrm{m \, s^{-1}}$, the timescale characterizing the approach of an ion will not exceed 1×10^{-11} s. Another, simpler reasoning can be made considering the difference in mass between electrons and ions. The mass of a typical ion will exceed the mass of an electron by three order of magnitude, which

means that, their charge being equal, they will travel much slower.

3.4. Emergent behaviour

Previously described physical effects are limited to the elementary processes that occur. The processes of breakdown relies on the elementary processes, but just as much on the larger scale effects. At a larger scale, involving many particles, the electron avalanche is the main effect that deserves some more in depth investigation.

3.4.1. Townsend ionization

In sufficiently large gap distances and pressures, the ionization process will occur as follows. It is assumed that the gas already contains some ions and/or electrons due to background effects such as Gamma radiation or incident light. Due to the applied potential, these charged particles will be accelerated by the electric field **E**. If the field is sufficiently large, and the mean-free-path is long enough, electrons can gain energies in the range of 10 eV to 100 eV. This acquired energy allows them to initiate a second ionisation collision. The particle formed in this second collision in turn are accelerated by the field and result in more collisions. A so called avalanche-effect occurs which rapidly ionizes the gas until it is in a plasma state where the current starts to flow through an arc. This process can be quantified by determining the rate at which the ionization process happens. The rate of ionization depends on two elementary processes, which are both form of electron-neutral collisions. To clearly separate the two, one can be referred to as *ineffective collision*, and the other one as *effective collision*. An ineffective collision denotes a collision between an electron and a neutral particle, in which no ionization takes place. The number and nature of the particles remain the same before and after the collision, and there is only an exchange in momentum. The effective collision refers to an ionization event as given in subsection 3.2.5.

Since the two initial particles do not interact over a long range (remember that a neutral particle and a charged particle do not experience a coulomb force together), their collision dynamics only depend on short range interaction. In such a case, the collision is similar to scattering by hard spheres, just like a game of billiards [18]. The chaotic nature of such collisions [17], allows us to disregard the exact angles involved in the process. This means the only thing of interest is the probability of the collision being effective. This measure then fully depends on the energy of the particles involved. The collision frequency is a common measure of the occurrence of these processes. In general it is given by

$$\nu_{ne} = n_n C_e \sigma_n \tag{3.34}$$

In which n denotes the number density, C denotes the 'thermal speed', directly related to the kinetic energy, and σ denoting the *collision cross section* [18]. The collision cross section represents the overlap area in which the two particle must meet in order to achieve this collision. Studies have determined the cross section σ for both ineffective collisions, in which it is a constant, and in effective collisions, in which it depends on the kinetic energy of the incident particle [22]. Such dependences are very complicated and getting outside the scope of this work.

A simple approach could be to let the probability of a collision being effective relate to the energy with a step function. In that case, if the kinetic energy E exceeds the ionization energy IE, the collision if effective. The fraction of collisions that is effective can then be determined by evaluating the Energy distribution of the electrons from Figure 3.1 at the value of the ionization energy. Let us call this fraction τ. If it is simply assumed that an ineffective collision removes all of the kinetic energy from the electron, and it has to start all over gaining energy from the field, the travelled distance of that electron until it has an effective collision is simply λ/τ. Where λ is the mean free path of the electrons. The travelled distance between ionization event gives a very good indication of the propagation of such an avalanche. From a single electron, the number of generated electrons increases in the spatial

direction, which is important for breakdown. The parameter α, that denotes the number of collisions per unit distance, can then be used to find the number of electrons at a distance d from the starting position of the avalanche by

$$n(d) = \mathrm{e}^{\alpha d} \tag{3.35}$$

The use of these relations also however relies on the electric field being constant, since the parameter α depends on $\mathbf{E}$ locally.

4

Model

Using all of the physical effects described before, and the research that has been conducted in the past, the goal now is to build further and add something to increase knowledge and understanding of the problem. From the literature study it has become clear that most benefit can be achieved from modelling the existing effects and mechanisms into multiple dimensions. This chapter attempts to transition from the theory towards a model that will be suitable to predict breakdown. Many of the techniques that are possible candidates have been briefly discussed and a more in depth explanation will lead to the choice of the best method of modelling.

4.1. Goal

First a clear goal must be set for the model. The main goal of any model is to mimic the reality so as to gain a better understanding of the universe we live in. Modelling is especially useful if studying the 'real system' is either too expensive or if we cannot practically fabricate or observe such a system. This applies to manmade systems: a bridge is modelled and studied before it actually gets deployed to make sure it will perform as required. And for understanding physcis: modelling an isolated system of two electrons interacting is easy, setting up an experiment to do the same is something totally different. As has been discussed, for this work we would like to be able to predict the risk of breakdown in a practical system that can not be approached as being parallel plates geometries. By obtaining the locations inside the domain where breakdown is most likely to occur, changes to the system can be incorporated to prevent breakdown from occuring in the final system. By modelling the system using the specified geometry, simply imposing a voltage and evaluating the breakdown criterion at regular intervals throughout the domain, one could retrieve a map of the locations where the breakdown condition is met and mark those as risk areas. Sadly however it is not that simple. Breakdown is not a local process, so even if the electric field is very large at one specific location, it might well be possible that there is no real risk of breakdown. To find a more suitable method, several aspects have to be considered to determine the effectiveness of such a model.

4.2. Modelling considerations

One of the most important aspect of any model is accuracy. If a model does not represent the effetcs we want it to or produces different results, it is of no use. Since this work is purely theoretical, the accuracy of any model for electrostatic breakdown can not be verified experimentally. Achieving accuracy in such a case mainly relies on making sure the used assumptions have been verified by others. Another principle in modelling is Occam's razor. It states that among competing hypotheses, the one that makes the least assumptions should be favored. This principle does not claim to be a tested and true method of finding the best hypothesis or model, but it does make sense since there

are less critical points that can prove incorrect or inaccurate.

In numerical models, accuracy is directly related to cost. As explained previously, refining the discritization of a numerical solution will improve accuracy but increase computational time.

4.3. Numerical models

From the literature study, it was found that to incorporate multiple dimensions into a problem regarding electrostatic breakdown, one quickly finds numerical methods as the only viable option. The descriptions of the breakdown criterion also inherently relies on one dimensionality so a numerical method must step away from the breakdown criterion and simulate the system over time to determines its characteristics. Also disgregarding any numerical magnetohydrodynamics method since a continuous description of the charges requires the gas to be a highly collisional plasma, which it is not in the advent of breakdown. For time dependent description of the phenomenon, the Particle-in-cell method remains the only suitable option.

4.4. Particle in Cell method

From a desire to model the influence of an electric field on moving charges, the Particle-in-Cell was developed. This computational method that originates from the plasma physics community, models the behaviour of plasmas in general. When electrostatic breakdown is initiated, the system might not be in a plasma state, but the essence is that the creation of charged particles will cause interaction between the electric field and the gas, which is precisely what can be accomplished using the Particle-in-cell model. Let us start again from the Coulomb interaction force

$$F = \frac{Q_1 Q_2}{4\pi\epsilon d^2}. \tag{4.1}$$

This interaction force between all charges does not scale well when the number of charges increases, see Figure 2.4 for reference. By discretizing the domain into cells, the namesake of this method, each particle will live inside a cell. The charge of each particle can then be mapped to the corners of the cell that it sits in. After the net charge has been determined for each of corners of every cell, the final result is a grid of *nodes*, each with a specified value of charge. From here, the Poisson equation for electrostatics comes in. As seen in the chapter on physics, it enables us to find the electrical potential as a function of how charge is distributed in space. For now we will continue with the resulting values for the electrostatic field at the grid points. The field at the grid points can now be used to map back to the locations of the particles to find the force acting on them as illustrated in Figure 4.1.

Using this scheme, the simulation has essentially been split in two parts. One part handles the electric field as a function of the distribution of particles, the second part consists of a time step in which the distribution of particles in space is updated. From there the process starts over and a continous execution of this loop enables a simulation of the time dependent behaviour. This basic scheme allows us to describe the behaviour of a system of charged particles, and to specifically model electrostatic breakdown, several additions must be made to the model. First the main loop will be presented in more detail, and from there incremental additions will enable simulation of electrostatic breakdown.

4.4.1. Poisson equation

Let us start with the Poisson equation in it's general form. From there we can apply it to the case of electrostatics. It is given by: $-\Delta u = f$. This denotes an unknown field $u(x)$, of which the negative Laplacian is equal to a given field $f(x)$. If this equation holds on a domain $\Omega \subset \mathbb{R}^3$, we can also supply boundary conditions on $\partial\Omega$. On the part of the boundary where u is prescribed, Γ_D, it holds that $u = u_0$. This is the Dirichlet boundary. On Γ_N, which is the remaining part of the boundary, the
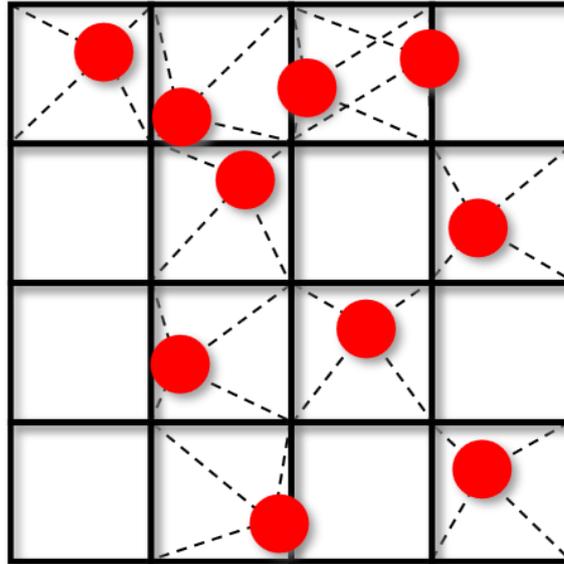
Figure 4.1: The grid acts as a stationary layer in which the electric field is evaluated. Reprinted from *Introduction to Particle-in-Cell Methods in Plasma Simulations.*, by C. Ren, 2011, Retrieved Mar 31, 2017 from `http://hedpschool.lle.rochester.edu/2011SummerSchool/lectures/Ren.pdf`. Copyright 2011 by University of Rochester.

Neumann boundary condition must be satisfied. It prescribes a value for the partial derivative of u, normal to the boundary: $-\partial_n = g$. Together these conditions can be written as follows:

$$-\Delta u = f \qquad \text{in} \quad \Omega \subset \mathbb{R}^3 \tag{4.2}$$

$$u = u_0 \qquad \text{on} \quad \Gamma_D \subset \partial\Omega \tag{4.3}$$

$$-\partial_n u = g \qquad \text{on} \quad \Gamma_N \subset \partial\Omega \tag{4.4}$$

In electrostatics, the electric field can be written as the gradient of the electric potential,

$$\mathbf{E} = -\nabla\phi. \tag{4.5}$$

Combining (4.5) with Gauss' Law:

$$\nabla \cdot \mathbf{E} = \frac{\rho}{\epsilon_0}, \tag{4.6}$$

we obtain the Poisson equation for electrostatics. Now the unknown field u is represented by the electrical potential ϕ, and the given function f is the charge density over the permittivity of free space, ρ/ϵ_0. The result is

$$\Delta\phi = -\frac{\rho}{\epsilon_0}. \tag{4.7}$$

This continuous form must then be transformed into a discretized form that can be solved numerically. To illustrate this process, a one dimensional form of (4.7) will be used. Taking the spatial coordinate to be x, it will take the form

$$\frac{\mathrm{d}^2\phi}{\mathrm{d}x^2} = -\frac{\rho(x)}{\epsilon_0}. \tag{4.8}$$

In general, the derivative of some function $f(x)$ can be approached by

$$Df(x) = \frac{f(x+h) - f(x)}{h}, \tag{4.9}$$

where h is some small value that tends to zero. If the goal is ti apply a discretization, h can take the role of the step size between discrete points. When we are limited in our choice of h for numerical reasons, a better approximation of $f'(x)$ can be given by

$$f'(x) \approx \frac{f(x+h) - f(x-h)}{2h}. \tag{4.10}$$

Extending the same method to the second derivate, it is found that

$$f''(x) \approx \frac{f(x-h) - 2f(x) + f(x+h)}{h^2}. \tag{4.11}$$

In a discrete setting, every consecutive point on the spatial axis is given an index i. The distance between x_i and x_{i+1} being Δx, we can rewrite (4.11) to

$$f''_i = \frac{f_{i-1} - 2f_i + f_{i+1}}{\Delta x^2}. \tag{4.12}$$

This now provides a set of equations, one for every discrete point denoted by index i. Combining this again with (4.8)

$$-1\phi_{i-1} + 2\phi_i - 1\phi_{i+1} = \frac{\Delta x^2}{\epsilon_0}\rho_i. \tag{4.13}$$

Rewriting this index notation to a matrix form, with the index i ranging from 1 to 5,

$$\begin{bmatrix} 2 & -1 & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & 0 \\ 0 & -1 & 2 & -1 & 0 \\ 0 & 0 & -1 & 2 & -1 \\ 0 & 0 & 0 & -1 & 2 \end{bmatrix} \vec{\phi} = \frac{\Delta x^2}{\epsilon_0}\vec{\rho} + \begin{bmatrix} \phi_0 \\ 0 \\ 0 \\ 0 \\ \phi_6 \end{bmatrix}. \tag{4.14}$$

Note that ϕ_0 and ϕ_6 are the boundary elements, that are not contained in the system as separate DOF's but are included on the right hand side. If the boundary conditions of the problem are given, the full *right hand side* of the system of equations is known. Also the matrix is fully defined, and this the problem resembles the linear algebra form

$$Ax = b, \tag{4.15}$$

with A a matrix, b a vector, and x being the sought after vector that represents the electrical potential ϕ throughout the domain. A similar system of equations can be composed in the case of a 2D or 3D system, the details of this are presented in a general manner during the implementation of the model.

This system of equations can easily be solved using a computer, which provides us with all the necessary components on the side of the electric field.

4.4.2. Particles

As mentioned, the biggest problem with simulation individual elementary particles is the vast number of interaction forces between them. But even when the individual interaction forces are not taken into account, the trajectory of each particle must be determined numerically. The description of a particle consists of it's elemental properties that are necessary for the electrostatic description, and for their motion. To start off, each simulated particle needs the following physical properties:

- mass [kg]

- charge [C]

Particles are modelled in a way that they can be treated as point-masses when determining their motion. In that case, when considering a particle, the quantities needed to fully define the state of it are either position $\mathbf{r}$, which in three dimensional Cartesian space is given by (x, y, z), or momentum $\mathbf{p}$, given by (u, v, w). Besides this an initial condition is needed for both. From Newtonian mechanics it is known that:

$$\mathbf{F} = \frac{d\mathbf{p}}{dt} \tag{4.16}$$

Since $\mathbf{p} = m\mathbf{v}$ and it is defined that acceleration $\mathbf{a} = d\mathbf{v}/dt$, the more commonly used form of Newton's Second Law is:

$$\mathbf{F} = m\mathbf{a} \tag{4.17}$$

In the setting of electrostatic breakdown, it is most useful to track the position of a particle. Therefore the momentum can be integrated twice to find:

$$\mathbf{r} = \frac{1}{m} \int_{t_0}^{t} \int_{t_0}^{t} \mathbf{F}(t) d^2 t \tag{4.18}$$

Which can be solved if it is supplied that $\mathbf{p}_0 = \mathbf{p}(t_0)$ and $\mathbf{r}_0 = \mathbf{r}(t_0)$.

4.4.3. Numerical time integration

The description above considers a continuous time situation which is not suitable for a numerical implementation since a discrete timestep Δt must be chosen to advance the simulation. Using a finite difference method for the time integration we can write the following:

$$\mathbf{a}_n = \mathbf{F}_n/m \tag{4.19}$$

$$\mathbf{v}_n = \mathbf{v}_{n-1} + \mathbf{a}_n \Delta t \tag{4.20}$$

$$\mathbf{r}_n = \mathbf{r}_{n-1} + \mathbf{v}_n \Delta t \tag{4.21}$$

$$= \mathbf{r}_{n-1} + \mathbf{v}_{n-1} \Delta t + (\mathbf{F}_n/m) \Delta t^2 \tag{4.22}$$

A timestep can now be made using the force acting on the point mass. Its new position is given by $\mathbf{r}_n$. In this case the required state variables are the previous position, and the previous velocity. This is analogous to the continuous setting where the time t_0 is shifted to the previous timestep. In that sense $\mathbf{r}_n$ is the state of the particle, and $\mathbf{r}_{n-1}$ and $\mathbf{v}_{n-1}$ are the initial conditions. In the simulation, a particle is now defined by its location r, and velocity $\mathbf{v}$. For every timestep, the scheme of (4.22) is simply used to update the state of each particle. This information is then passed back to the Poisson solver and so forth.

4.4.4. From Electrostatic potential to Electromotive force

Between the solution of the Poisson equation and the timestepping of a particle, an important translation step has been only glanced over until now. To find the motion of a particle, a force acting upon it is required. The solution of the Poisson equation however is merely a description of the electrostatic potential along the domain. Using the electrostatic potential ϕ, the first step is to determine the electric field $\mathbf{E}$

$$\mathbf{E} = -\nabla \phi. \tag{4.23}$$

Discretization of this relation also comes back to the finite difference method as shown in (4.10). This allows the electric field at grid point i to be written as (again in a one dimensional case for illustration)

$$E_i = \frac{\phi_{i+1} - \phi_{i-1}}{2\Delta x}. \tag{4.24}$$

The electric field has now been determined, but still only at the grid points that are separated at distance Δx. For a proper determination of the particle motion, the electic field must be determined at the location of this particle. Several methods can be used to accomplish this, with varying degree of accuracy and computational cost.

The simplest method would be a piecewise constant interpolation. The electric field at the location of the particle would then equal the electric field at the nearest grid point. To find the electric field more accuractely, a linear interpolation is the second option. A particle located halfway a cell would have a value of the electric field perfectly between the electric field values at the corresponding grid points. Higher order interpolations can also be used, but since the solution of the electrical potential ϕ is already only first order accurate that would not make sense.

Using the now determined electric field at the location of the particle, the force acting upon it is determined by the relation

$$\mathbf{F} = -q\mathbf{E}. \tag{4.25}$$

In this case the location of the particle is merely discretized in the sense that the representation is limited by the numerical accuracy of the computer.

4.4.5. From particle location to charge distribution
To find the charge density ρ_i that is required at the grid points, the exact same method as discussed in the previous section can be used the other way around. The charge of a particle at some location can be distributed to the nearest grid point, or its charge can be divided over the corners of the cell that it lives in. Again this affects accuracy of the model, but overall accuracy should not depend on the order of interpolation since if it does, the size of the cells is too large already.

4.4.6. Particle collisions
Now that the basic principle of the Particle-in-Cell method has been elaborated, it is time to develop some additional elements that are specifically geared towards electrostatic breakdown. Collisions are very important in electrostatic breakdown and thus must be included in the model. As mentioned, the collisional processes are very complicated even if particles are assumed to be hard spheres, and next to that ionization and recombination further complicates the matter. It is therefore that the current Particle-in-Cell model needs a simple and effective way to handle collisions specifically geared toward electrostatic breakdown. Since the movement of neutral particles is not influenced by electric fields, they can be removed from the model, which significantly simplifies the simulation. The problem then is that neutral particles are required for ionization, so they cannot be disregarded from the model completely. By referring back to the literature research and the Townsend coefficient α that is used in analytical breakdown research, a simple and elegant usage of it can be found in numerical modelling. The coefficient α signifies the number of ionization collisions an electron incurs by traveling a unit distance. Since an ionization collision occurs when the electron has gained sufficient energy from the field, this provides a treshold energy that the electron must posses before it can ionize a neutral molecule. When tracking an electron, the chance of a collision with a neutral particle simply depends on the chance of a neutral particle being in that path. This allows us to simply incorporate neutral particles as a chance of collision per unit travelled distance of an electron. Using the known travelled distance of an electron, a simple psuedo random number generator can

incur a collision, and in such a case, the momentary energy of the electron determines if the collision is effective and produces a positive ion and another electron, or if it is ineffective and transfers some of the energy of the electron to the neutral particle.

Ionisation events

An effective collision now denotes an ionization event. In such an event, an energy balance can be used to distribute the particles after the collision. Before the collision, one electron and one neutral particle constitute this isolated subsystem. After the collision, these have transformed in one positive ion and two electrons. Since the mass of the neutral particle and ion are orders of magnitude larger compared to the electrons, they are assumed to be standing still. Denoting the ionization energy of the neutral particle with E_i, we find

$$E_{e1} \rightarrow E_i + E_{e1} + E_{e2}. \tag{4.26}$$

By deducting the ionization energy from the energy of the initial electron, the energy is found that will be divided among the two resulting electrons. A simple method of distributing this energy can be accomplished by randomly assigning a fraction of the energy to one elcetron and the rest to the other. Off course this is an overly simplified representation of collisional effects, but for electrostatic breakdown it is shown to be effective in capturing the important physics. In the simulation, a simple scheme can now be used for every time step and it can be summarized as follows: First determine if electron will collide using travelled distance and collisions chance. Then determine if collisions is effective using electron energy. If it is inactive, reduce electron energy by random amount. If it is active, create new ion and new electron and redistribute leftover energy after deduction across both electrons.

4.4.7. Electrode emission and absorption

The electrodes in this system must also act as sources and sinks of charged particles. Since the background field of neutral particles is not modelled directly, the recombination of a positive ion when it hits the cathode and absorbs an electron can simply be modelled as the removal of the ion. In that case the sinking of the ion counts as an electric current between the electrodes. The sinking of electrons at the anode side also counts as electric current flowing between the electrodes. For the separate processes of secondary emission and field emission, inlucding ion enhanced field emission, a separate method has to be introduced. Analogous to the bulk process where γ can be used in modelling the ionization process, the coefficient γ can also be used in a numerical setting. Since the event of a positive ion reaching the cathode is a discrete event, a numerical simulation can simply generate an electron from the cathode if the coefficient γ is converted to a chance of emitting an electron. Using such a representation, one can investigate different expressions for γ, as they are presented in literature, to study the effects of these changes.

4.4.8. Breakdown criterion

All of the previously described elements together allow simulation of a system with a give geometry and other parameters such as the applied voltage and pressure. This does not give us any conclusive risk on breakdown, but merely describes the time dependent behaviour of the system. Since electrostatic breakdown is characterized by a rapid increase in charge carriers in the domain, this process should also occur in a simulation attempting to replicate this behaviour. The problem herein is that for every particle inside the domain, some computing power is required. This results in the required computing power per timestep being directly proportional to the number of particles. With the exponential increase in charged particles, an exponential increase in computational time will result in bad behaviour. Great care must be taken to keep the number of particles low enough to continue the simulation, but room must be given to allow an increase since that is the main operating

principle of breakdown. Since the event of breakdown itself needs not be simulated, a confirmation of the exponential increase is sufficient to determine if the initial conditions will likely cause breakdown. Since the number of particles can vary greatly in consecutive timesteps, one cannot conclude the occurence of breakdown in a couple of timesteps. Using a smoothed record of the particle concentration in time, one can confirm breakdown. To prevent false positives, the smoothing parameter must be adjusted appropriately, which is only possible once output data is available.

A method to also prevent the solving time to get out of bounds is a cap on the number of particles. This number however greatly depends on the starting conditions. Once again this is very implementation specific and such parameters must be tuned according to simulation output.

5

Particle-in-Cell implementation in Python

5.1. Python

Python is a general purpose high level programming language that is widely used in scientific computing. It is not considered as fast compared to other low level languages, but it's ability to be used as an object oriented language and the many libraries that are available for scientific applications make it very suitable for this task.

5.1.1. Generating the domain and solving the potential

To allow any useful simulation, the domain of the simulation must be programmed and *meshed*, which is the process of dividing the full domain into the discrete cells that are used in the Particle-in-Cell method. To handle generation of meshes and proper bookkeeping of the boundary conditions, *gmsh* was used. Gmsh can generate meshes from input geometries and group nodes and elements so that they can be addressed as one part in Python. This allows the user to quickly change the geometry of the boundary conditions, and providing the Python script with a robust set of mesh data that can be used to establish the system matrix. From the outputted data by gmsh, a conversion has been implemented to retrieve a list of the so called *connectivities* from the created elements. The connectivity of any node is given by the identifiers of the ones it is connected to in two dimensional space. Using this information, the system matrix is assembled by adding a row for each element, in which a column is nonzero if the elements are connected. For example consider the simple mesh from Figure 5.1. This mesh contain 9 nodes, thus the system matrix will be 9x9, For the first row, it is seen that node 1 is connected to node 5 and node 8. The first row of the system matrix thus is given by:

$$A_1 = \begin{bmatrix} 2 & 0 & 0 & 0 & -1 & 0 & 0 & -1 & 0 \end{bmatrix} \tag{5.1}$$

The full system matrix is given as

$$A = \begin{bmatrix} 2 & 0 & 0 & 0 & -1 & 0 & 0 & -1 & 0 \\ 0 & 2 & 0 & 0 & -1 & -1 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 & -1 & -1 & 0 & 0 \\ 0 & 0 & 0 & 2 & 0 & 0 & -1 & -1 & 0 \\ -1 & -1 & 0 & 0 & 3 & 0 & 0 & 0 & -1 \\ 0 & -1 & -1 & 0 & 0 & 3 & 0 & 0 & -1 \\ 0 & 0 & -1 & -1 & 0 & 0 & 3 & 0 & -1 \\ -1 & 0 & 0 & -1 & 0 & 0 & 0 & 3 & -1 \\ 0 & 0 & 0 & 0 & -1 & -1 & -1 & -1 & 4 \end{bmatrix}. \tag{5.2}$$
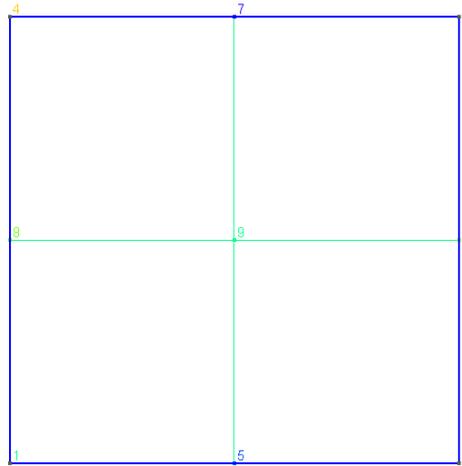
Figure 5.1: Simple square mesh with nine nodes and four cells.

From this system, some of the boundaries may have a given value of the potential, this they have to be excluded from the system, and their prescribed value can be added to the RHS. Continuing with the example, suppose the left and right side of the domain are both at a prescribed potential, denoted by ϕ_i where i is the node number. This mean only nodes 5, 7 and 9 remain. The reduction of the system is also executed in python using the data provided by gmsh on the boundary conditions. The reduced system then looks like

$$A = \begin{bmatrix} 3 & 0 & -1 \\ 0 & 3 & -1 \\ -1 & -1 & 4 \end{bmatrix} \tag{5.3}$$

The nodal values that were prescribed now have to be added to the right hand side of the side as

$$\vec{\rho} + \begin{bmatrix} \phi_1 + \phi_2 \\ \phi_3 + \phi_4 \\ \phi_6 + \phi_8 \end{bmatrix} \tag{5.4}$$

In the case of no charges inside the domain, the resulting system is

$$\begin{bmatrix} 3 & 0 & -1 \\ 0 & 3 & -1 \\ -1 & -1 & 4 \end{bmatrix} \vec{\phi} = \begin{bmatrix} \phi_1 + \phi_2 \\ \phi_3 + \phi_4 \\ \phi_6 + \phi_8 \end{bmatrix} \tag{5.5}$$

If for example the left boundary, node 1, 4 and 8 were prescribed at $\phi = 1$, and the right side $\phi = 0$, the result would simply be

$$\vec{\phi} = \begin{bmatrix} 0.5 \\ 0.5 \\ 0.5 \end{bmatrix}. \tag{5.6}$$

On the other hand if the prescribed potentials were at 0, and a single unit charge would be present in the middle of the domain, at node 9, the system would be

$$\begin{bmatrix} 3 & 0 & -1 \\ 0 & 3 & -1 \\ -1 & -1 & 4 \end{bmatrix} \vec{\phi} = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}. \tag{5.7}$$
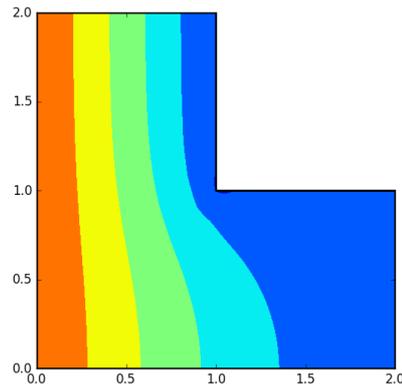
Figure 5.2: Electrical potential distribution in a domain with prescribed boundary potentials on the left and right side.

The determination of the electrostatic potential has now been generalized to any domain with arbitrary boundary conditions, and can be read and solved in Python. In Figure 5.2 the electrical potential is shown with a prescribed potential at the left and right side of the domain.

Numerical solving considerations
Since only the right hand side of the system changes every iteration, a decomposition can be applied to increase performance. An LU-decomposition was found to be useful, since the solution of the system can in that case be found using one forward substitution and one backwards substitution. This has also been implemented in the code to speed up the computation.

5.2. Including charged particles

5.2.1. Implementation details
Using the solver for the electrostatic potential, an attempt can now be made to include a charged particle and simulate its behaviour over time. First, the electrical potential must be found at the specific location of the particle. With a constant cell size denoted by Δx, and a particle at location x, the particle is known to be in cell $i = \text{floor}(x/\Delta x)$, and a *fractional remainder* is found by $\delta = (x \bmod \Delta x)/\Delta x$. However, actually it is the electric field that is being searched at the location of the particle and not the electrical potential. The electric field can be determined as the gradient of the potential. This also means if the determined electrical potential is piecewise linear, the electric field will be piecewise constant. The fact that the electric field within a cell is then constant allows us to skip the potential at the exact location of the particle and determine the electric field at its location from the potential that is determined at the corners of the specific cell. From this the local electric field is given by

$$\mathbf{E}(x) = \frac{\phi_i + 1 - \phi_i}{\Delta x}. \tag{5.8}$$

Using the scheme in (4.22), the motion of the particle can now be determined in time. For each particle only the current position and current velocity is saved. More information is not required since the acceleration is determined by the external force for every time step.

5.2.2. Demonstration and validation
A very simple example of a particle placed inside an electric field with an initial velocity is shown in Figure 5.3. It shows a top down view of a two dimensional case, with the applied electric field pushing the particle to the left, and an initial velocity directed towards the top right. At every timestep, the

location of the particle is plotted, thus larger spacing between two consecutive dots indicates a larger velocity.
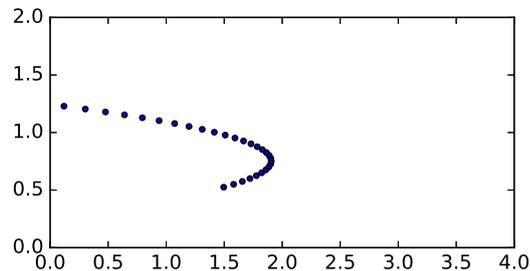
Figure 5.3: Single particle being accelerated towards the left by an external field.

If there is no applied field, a set of charged particles can be introduced inside the domain, and they will move by the force they exert on one another. This is illustrated in Figure 5.4, with one particle in blue and one in yellow. They are oppositely charged and thus are attracted towards each other by the electromotive force.

An arbitrary number of particle can now be included inside the domain, which will interact with each other and the externally applied electric field. This is the framework of the Particle-in-Cell method. From here the next step is to include particle collisions, which will allow the general particle in cell method to be used for electrostatic breakdown simulations.

5.3. Particle collisions

Interparticle collisions have been shown to be of great importance in electrostatic breakdown. By not modelling the neutral gas within the Particle-in-Cell method, the computational effort is reduced and collisions can be described without scattering dynamics calculations.

5.3.1. Electron-Neutral collisions

The implementation of electrons colliding with neutral particles uses a collision chance, as mentioned earlier. Directly after solving the equation of motion for any particle, the system determines if the specific particle will collide depending on the velocity and a given chance depending on the number density of the neutral particles, i.e. the gas pressure. If it was determined that an electron has a collision with a neutral particle, the energy of the electron is checked next. When the kinetic energy of the electron exceed the ionization energy of the neutral particle, an effective ionization event takes place. Using the principle described in (4.26), two new particle are generated. One positively charged ion with zero velocity, and another electron, with arbitrary direction, and a chunk of the total energy available for the two electrons.

5.3.2. Demonstration and validation

The implementation of collisions is best shown using a single particle, again in an applied field pushing it towards the left. At first, the ionization energy is chosen be very high. In that case the electric field is insufficient to accelerate the particle to cause an ionization event. Before the electron reaches the threshold energy, it loses part of the energy already to the neutral particles. The collisions are easily seen by the sudden changes in velocity of the particle in Figure 5.5

When the required ionization energy is lowered, the electron can attain sufficient energy and
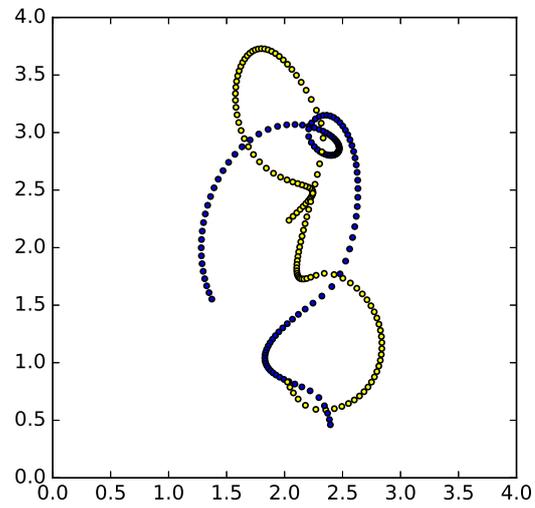
Figure 5.4: Two oppositely charged particles inside a domain with no applied electric field.
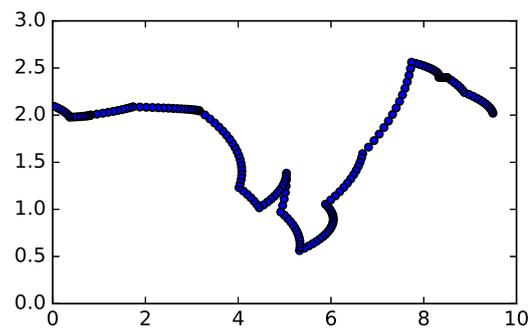
Figure 5.5: Electron losing energy to neutral particles that are not depicted here.
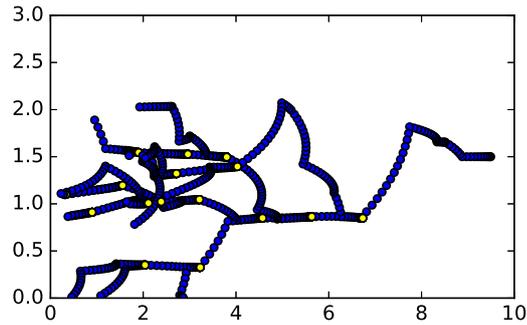
Figure 5.6: Formation of an electron avalanche, with electrons depicted in blue, and positive ions depicted in yellow.

successful ionizations take place. Figure 5.6 show the creation of an avalanche, with the electrons depicted in blue and positive ions in yellow. Some collisions are successful and create new particles, while others are not and merely dissipate energy from the electron. The yellow ions appear to be stationary due to the fact that they are much heavier than the electrons, but they do in fact move towards the right.

For an avalanche, just as predicted by the classical theory, the development also depends on the applied electric field and the pressure. Varying the pressure and electric field yields similar results to Figure 5.5 and Figure 5.6

5.4. Electrode emission

The next building block to complete the description of electrostatic breakdown using a Particle-in-Cell method is the emission of electrons from the electrode. This process is triggered by an ion reaching the electrode surface, which involves just a simple check since ions are modelled already. When an ion reaches the surface, the chance of emission of an electron is characterized by γ. The parameter γ however classically denotes the expected number of electrons emitted per incident ion. To convert from an expectation value to the probability of a certain event (i.e. the emission of one or more electron), the probability distribution is required. A sensible choice here is the Boltzmann distribution, with an average value of γ. The cumulative distribution function can can then be evaluated at discrete values (the number of emitted electrons must attain an integer value). The probability of one electron being emitted then equals a certain probability p. Using a random number generator, the computer can then induce the emission of electrons from the surface. The implementation of this allows for a more advanced description of the parameter γ, in which it depends on the local electric field, which has already been calculated anyway.

Local electric field effects
Instead of using the emission coefficient, one could directly determine the emission of electrons from for example the speed of the incoming ion and the local electric field. Also certain effects can be implemented that do not rely on a positive ion reaching the surface. A time dependent source of electrons can also be modelled as a function of the electric field.

5.4.1. Demonstration and validation

The most interesting demonstration of the implemented effect is found in a simulation of a larger system, but a simple illustration can be given by starting the simulation with a single ion that is accelerated towards the right electrode. Figure 5.7 show the ion in yellow, moving towards the surface and emitting an electron when it arrives. Note that the time intervals at which the particle location is plotted are different for the ion and the electron. The ion requires many more time steps to move a certain distance, of which some have been omitted for visual clarity.
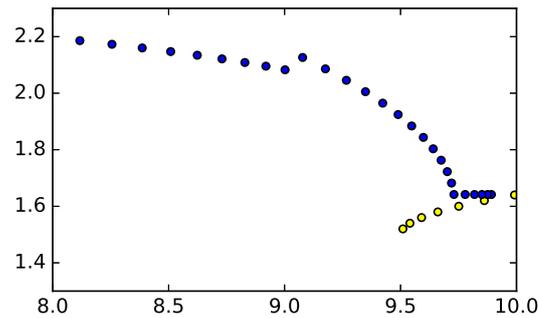
Figure 5.7: Electron emission from the electrode at the right side of the domain.

5.5. Timescales

As hinted on before, the time-scales of different processes are vastly different. It is important to investigate these differences since the time steps taken to determine the particle motion can completely alter the behaviour if chosen incorrectly.

5.5.1. Electron vs Ion motion, timescale differences

If an ion and an electron were positioned in the same electric field, the electron would travel a distance three orders of magnitude greater than the ion. This is due to the difference in mass, and complicated the modelling of the situation. Ideally, one would set the time step small enough so that the motion of the electrons is well resolved, but this does require the updating of the ion location and velocity far more often than required. One could introduce different intervals at which that equations of motion for a particle are solved, but this has not been implemented in the simulation. Simply adjusting the mass of the ions to a lower value could work, but care must be taken in that regard. Especially in a multidimensional situation, the higher inertia in reality could alter the trajectory of the ion. Also a probably even more important effect is the space charge created by the ions. As mentioned, the avalanche leaves behind the so called ionic trail. In Meek's streamer breakdown, the ionic trail alter the electric field significantly. The ionic trail would not even exist if the mass of ions and electron was taken equals, so as long as the importance of this is not verified, this is not possible method to improve performance.

5.5.2. Significance of timescales on resulting behaviour

The presence of ionic space charge inside the domain could negatively affect the performance of the model. Also the time step parameter can significantly alter the behaviour of the system. If an electron could reach the threshold energy for ionization within one timestep, the multiplication of an avalanche will become limited by the parameters of the model, which is an undesired situation.

5.6. Results of combined simulations

Now that all important building blocks of the model have been implemented in Python and are shown to be fully functional, exciting new simulation can finally be executed. The first step in this is the simulation of the classical theory, in which the nano scale adaptations are not included. To test the model, we can take a random location of Paschen's curve, and see if breakdown can be simulated. By applying 100 V at a distance of 10 μm, breakdown should not occur according to the classical theory. Because the increasing number of particles inside the domain does not really allow the graphs showing the domain and individual particle within it, the results are presented differently. In this case the domain is presented in one dimension at the vertical axis. At the bottom is the negative electrode, at the top, at 10 μm is the positive electrode. The horizontal axis now represents time.

The behaviour can then be visualised in Figure 5.8. At the starting time, 5 electrons are distributed randomly throughout the domain. Once the simulation starts running, the electrons move towards the positive electrode. The jittery behaviour that can be seen is due to the ineffective collisions that the electrons undergo to lose part of their energy. Once the electrons reach the top, they are absorbed and the simulation ends since there are no more particles inside the domain. The simulation thus now predicted that breakdown will not occur at $10\,\mu\mathrm{m}$ at $100\,\mathrm{V}$.
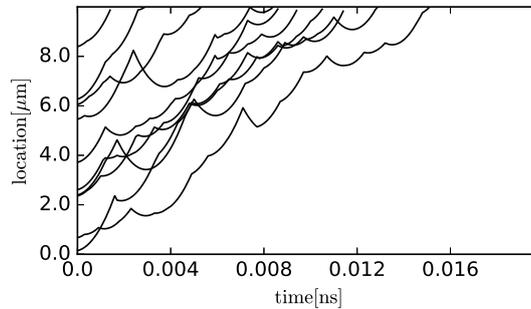
Figure 5.8: Behaviour of initial electrons at $10\,\mu\mathrm{m}$ and $100\,\mathrm{V}$.

Increasing the voltage should show the avalanche effect, so let us try the same thing but with a voltage of $250\,\mathrm{V}$. Note that this should not produce breakdown.
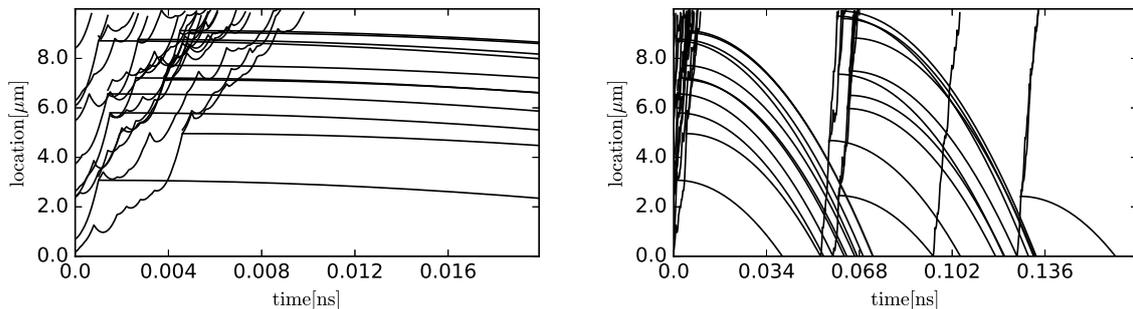
(a) Zoom on initial moments.

(b) Total simulation

Figure 5.9: Behaviour of initial electrons at $10\,\mu\mathrm{m}$ and $250\,\mathrm{V}$.

Figure 5.9 clearly shows the avalanche process once again. The slow ions produce almost horizontal lines, and slowly start moving towards the bottom. By running the simulation for a longer time, the behaviour of the ions is clearly shown, but the avalanches have been compressed to almost vertical lines. The total simulation is also shown in Figure 5.9. Clearly, all particles are removed from the domain and no breakdown occurs.

Now let us increase the voltage even more, so that the classical theory predicts breakdown should occur. The results of this simulation are shown in Figure 5.10. The number of ions generated during the avalanche process is now great enough to incur the creation of new electrons that in turn start new avalanches.

From the initial 5 electrons, the simulation contains around 500 charged particle after not even one nanosecond. This clearly indicates that the rapid increase in particle density is the start of a real breakdown event that is going to occur under these conditions.
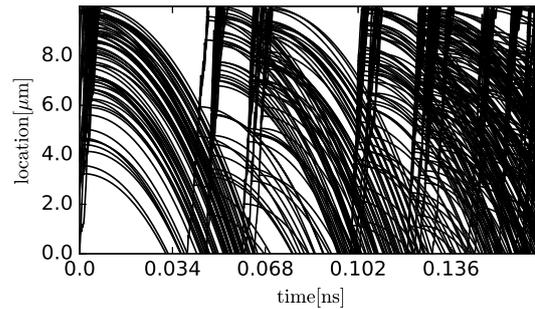
Figure 5.10: Behaviour of initial electrons at 10 μm and 400 V.

5.6.1. Charge density evolution

To get an even simpler representation of the time dependent behaviour of the system, the number of charged particles can be plotted in time. By normalizing this number with the initial number of electrons inside the domain, the influence of this parameter can be shown. The main conclusion that can be drawn from Figure 5.11 is that the number density values smooth out faster, but that in principle, initiating the simulation with one particle can be sufficient. The only thing that has be be considered is that due to the stochastic nature, using too little particles can lead to a false negative.
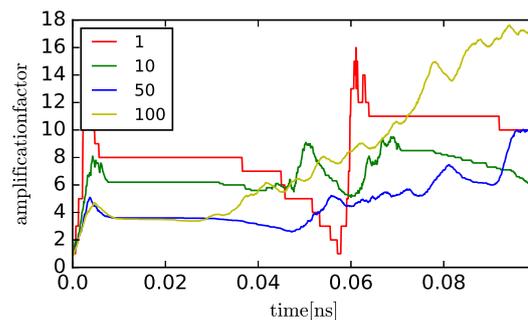
Figure 5.11: Development of the charge density as a function of the initial number of particles.

Also as can be seen the unnatural introduction of the source particles introduces some peaks in the charge density, which are being filtered out while the system is approaching the quasi-equilibrium state, in which the ion and electron densities are in balance, but still increasing exponentially. The speed of the exponential increase also seems to depend on the initial particle density. This has all to do with the mass of the heavy ions. The more ions there are being produced inside the domain, the earlier the first couple of them will reach the anode to emit more electrons.

5.6.2. Producing Paschen's curve

The previously introduced simulations appear to predict breakdown with the given parameters, and thus should be able to reproduce Paschen's curve. At the lower voltages, the number of ions generated from a single avalanche decreases. Therefore the number of required initial particles must be chosen at a higher value to ensure a proper simulation. The process of finding Paschen's curve is very similar to how it would be done in a lab for a real system. First the geometry of the system is determined. In this case the only parameter defining the geometry is the gap spacing d. By increasing the voltage in small increments, once the right conditions are reached, the number of particles will start the exponential increase that we are looking for. The closer the breakdown voltage is approached, the more likely it is that the charge density will hover around a constant value. Again,

due to the stochastic nature, one will need a larger sample size to find the point at which breakdown will occur. In this case the initial density of particles represents the sample size. The higher the initial number of particles, the more likely that the model will predict breakdown. By using an initial number of particles of 100, and executing the simulation four times, the results can be plotted using a boxplot as seen in Figure 5.12
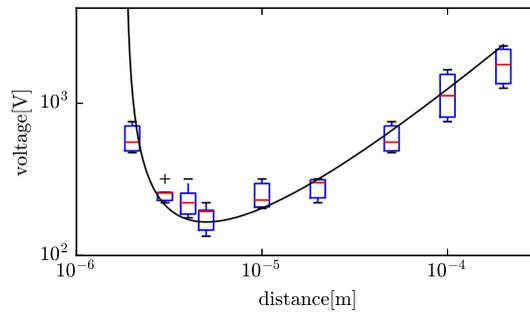
Figure 5.12: Reproduction of Paschen's curve using the developed Particle-in-Cell model.

5.6.3. Including advanced field emission

Sadly time did not allow a full determination of the full curve depicting the breakdown voltage versus the gap distance using one of the more advanced relations for the electron emission coefficient γ. However, using the relation for γ as shown in (2.21) by Radmilovic & Radjenovic, it should be found that the breakdown voltage could easily get below 200 V when the gap distance is small, something that is impossible in the classical theory. By setting the applied voltage to 200 V, the electrode spacing was decreased from 8 μm downwards. From Figure 5.13, the increasing electric field increases the probability of electron emission from the surface. Using the model, the breakdown at a gap spacing of between one and two μm is predicted to occur at around 200 V. This result is very promising, and appears to match the existing theory very well. Also, using this relation, the same asymptotic behaviour towards infinity was found, as compared to the model by Radmilovic & Radjenovic.
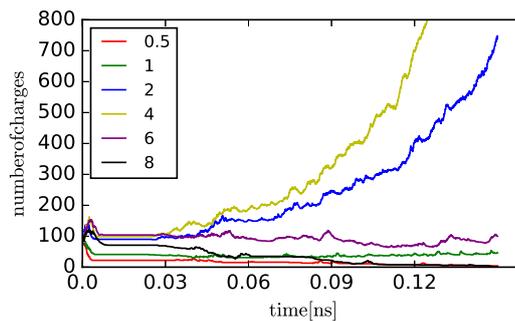
Figure 5.13: Charge density at constant voltage as a function of distance.

6

Discussion and recommendations

6.1. Discussion

Utilizing all that has been treated and discussed, it is now the moment to evaluate and conclude. The topic of electrostatic breakdown has been of particular interest at a very small scale. Micro and Nano electromechanical systems greatly benefit from an *a priori* analysis on the risks of electrostatic breakdown, since it can easily destroy the device. Such an analysis greatly depends on the topology of the system, since the main precursor for breakdown is the electric field, which is greatly influenced by said topology. The well established theory on breakdown, commonly referred to as Townsend breakdown, is built entirely on a one dimensional approach to the problem. Furthermore, large deviations have been observed from this theory at gap distances below $\sim 10\,\mu\text{m}$. Both these complications limit our ability to analyse small scale system on the risk of electrostatic breakdown.

During the literature study, existing publications were investigated that treated small scale breakdown. It has been generally accepted that electron emission from the surface of the electrodes is significantly enhanced by the presence of an electric field, and that this effect can be attributed to the deviations in classical theory. A perfect numerical relation between the emission of electrons and the strength of the local electric field has not yet been agreed upon, but very useful relations have been developed. The problem regarding the one dimensional nature of existing theory is shown to be best approached using a multidimensional numerical method.

A so called Particle-in-Cell method is implemented in Python, to enable the simulation of electrostatic breakdown in multiple dimensions. The computational method involves a framework in which the motion of charged particles (ions and electrons) can be tracked. Extra features of the model that have been added onto the framework are particle collisions and electrode emission. These building blocks can be adapted to include additional effects or improve performance if certain aspects prove to be of no influence. The emission of electrons from the electrode especially can be tuned and modified to incorporate hypotheses from literature.

Using the developed Particle-in-Cell model, breakdown has been effectively simulated. By using the classical theory to incorporate electron emission in the model, Paschen's curve, a well known curve relating the gap distance to the required voltage, has been replicated to show the validity of the model. A more advanced relation for the electron emission coefficient was applied within the model, to verify the lowering of the breakdown potential at small gap distances. A further investigation of the implemented relation will be useful to determine the full breakdown curve with the modified physics.

6.2. Recommendations

Since resources are always limited, there are some recommendations that can be made from this work. As already hinted upon, the developed model has been only utilized far from its full potential.

To start of with one of the main disadvantages of the model: It still requires some fitting parameters, such as the collision probability, which directly relates to the pressure of the neutral gas. Further development could introduce more suitable relations for these parameters to enhance the model. Also many of the parameters such as the cell size, and time steps have been optimized by trial and error, while a thorough analysis could result in a more effective balance between performance and results. The possibility of adapting the model to suit the particular area of interest makes it very versatile. Another major advantage of the model is the implementation of breakdown simulation in multiple dimensions. The effects of geometry can be simulated with this multidimensional model, which is of great interest in practical applications like the design of real world systems. Future expansion of the model would allow new research on the topic without starting from the ground up, because the framework is already present. As seen, there are very promising research directions that tie into the current work, which can be started as a direct follow-up on this work, or derive certain parts and take a new direction.

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