Stellingen

behorende bij het proefschrift:

“A Micromechanical Approach to Transformation Toughening in Ceramics”

door

Geert Stam

1. Bij het implementeren van hun scheurgroeimodel in een eindige-elementenformulering, wordt door Ortiz en Giannakopoulos verondersteld dat de oppervlakte-integraalterm verwaarloosd mag worden voor kleine scheuruitbreidingen. Dit is onjuist.


2. De eigenschappen van afzonderlijke korrels en hun korrelgrenzen, die de scheurtip omringen, kunnen het scheurgroei proces zeer sterk beïnvloeden. In de meeste scheurgroei analyses wordt een continuumaanpak gebruikt waarbij de spanningen en vervormingen in het continuumelement in wezen gemiddeld zijn over een groot aantal korrels. Echter, omdat de lokale microstructuur het scheurgroei proces sterk beïnvloedt, kunnen er vraagtekens gezet worden wanneer een continuumformulering op die schaal wordt gebruikt voor scheurgroei analyse.

3. De ontwikkeling van snelle computers en de eindige-elementenmethode heeft ertoe geleid dat in een groot deel van het onderzoek van mechanica van materialen voor een micromechanische aanpak gekozen wordt in plaats van een fenomenologische.

4. Sommige onderzoekers hebben de grootte van de transformatiezone voorspeld onder de veronderstelling dat de transformatie superkritisch is en dat de transformatierekken zelf de spanningsverdeling niet beïnvloeden. Hoewel deze analyses het begrip van transformatievevertaaiing vergroot hebben is de kwantitatieve waarde gering, vooral wanneer de transformatie ook geëxpand gaat met transformatie-afschuifrekken.

Proefschrift pag. 75-77

5. Zelfs wanneer de oplossingsstrategie bekend is en er een foutloos computerprogramma geschreven is, kan het probleem nog steeds onopgelost beschouwd worden indien de tijd die nodig is voor het berekenen van de oplossing in de orde van grootte van een gemiddeld mensenleven is.

6. Het creëren van forums of bulletin boards waar lezers (druk)fouten in boeken en artikelen kunnen rapporteren en becommentariseren zou menig onderzoeker veel tijd besparen bij het bestuderen van vakliteratuur.

7. De honger naar kennis en begrip kan niet worden gestild door het doen van een promotieonderzoek. In feite kan het uitvoeren van zo’n project worden vergeleken met het nuttigen van een eetlust-opwekkend voorgerecht.

8. Het toenemend gebruik van keramisch materiaal zal ons naar een nieuw stenen tijdperk voeren, waar de mensheid dit keer het steen zelf produceert.
A MICROMECHANICAL APPROACH TO TRANSFORMATION TOUGHENING IN CERAMICS
A MICROMECHANICAL APPROACH TO TRANSFORMATION TOUGHENING IN CERAMICS

PROEFSCHRIFT

ter verkrijging van de graad van doctor aan de Technische Universiteit Delft, op gezag van de Rector Magnificus, Prof. ir. K. F. Wakker, in het openbaar te verdedigen ten overstaan van een commissie door het College van Dekanen aangewezen, op maandag 12 september 1994 te 16.00 uur door Gerardus Theodorus Maria Stam, civiel ingenieur, geboren te Nieuwkoop.
Dit proefschrift is goedgekeurd door de promotoren:

Prof. dr. ir. E. van der Giessen

en

Prof. dr. ir. P. Meijers

CIP-GEVEVENS KONINKLIJKE BIBLIOTHEEK, DEN HAAG

Stam, Geert

A micromechanical approach to transformation toughening in ceramics / Geert Stam. - Delft : Delft University of Technology, Faculty of Mechanical Engineering and Marine Technology. - 111.
Thesis Technische Universiteit Delft. - With index, ref.
ISBN 90-370-0106-8
Subject headings: crack growth ; zirconia ceramics / toughening mechanisms.
Aan mijn ouders
Acknowledgements

I would like to express my deepest appreciation to my supervisor Erik van der Giessen, who has been my guiding light. No words can describe the importance of that light. Erik, you are a great colleague!

Also I want to thank Professor P. Meijers who always read my manuscripts with great accuracy. His comments helped me to make my texts ordered and readable. I learned a great deal from his experience.

The computer assistance of Jan Booij was vital. Lunch and work with Jan, Fred, Adrie, Arend (matlab is handy), Paul, Gerald, Jaap (2), Marian, Leo, Hanneke, Vladimir, Valerin, Wu, and Patrick has been a pleasure and was gezellig.

At home, my friend Frank supported me in everything. My sister Willemijn showed me the life outside the university and Kim, you dragged me through that final year and improved my English considerably. Thank you for your support, patience and for expanding my horizons.

Finally I want to thank Marc for his discussions about law and life. I really enjoyed sharing the office with you.

The computing time on the Cray-YMP of NCF was greatly acknowledged.
Summary

One of the major goals of the development of new structural ceramics is to improve the toughness. Since the degree of toughness totally depends on the crack behaviour, it is important to know which mechanisms are responsible for the specific crack growth behaviour. Knowledge about the influence of a specific mechanism can be obtained with the help of micromechanical models which describe the overall effect of microfracture. In chapter 2, first a brief introduction to linear elastic fracture mechanics is given, followed by a brief survey of the toughening mechanisms currently used in ceramics. However, in this work we focused on one toughening mechanism called transformation toughening.

This toughening mechanism is based on a stress-induced (martensitic-like) transformation, which can occur in zirconia containing ceramics. In an unconstrained particle, this transformation from the tetragonal structure to the monoclinic structure induces a volume expansion of about 4.5% and a shear strain of about 16%. However, in a constrained particle twinning occurs and the resulting macroscopic shear strain will be much less, since the sense of the different shear bands alternates from one band to the next. Therefore, up till a few years ago, most constitutive models only took into account the dilatant part of the transformation strain. These models have significantly enlarged the understanding of transformation toughening, but there was unsatisfactory quantitative agreement with experiments (e.g. McMeeking and Evans, 1982; Budiansky et al. 1983; Horn and McMeeking, 1990). Recently, a constitutive model has been proposed which does take into account the shear transformation strains (Sun et al., 1991). This material model is presented in chapter 3, in which we also study the deformation response of such materials. In particular the occurrence of localization is looked at, where localization refers to situations in which the inelastic deformation concentrates as an outcome of the constitutive behaviour.

In chapter 4 the crack growth model is presented which is used to predict the fracture behaviour of zirconia containing ceramics. A so-called small scale crack problem is formulated which is solved using a finite element method. The constitutive equations presented in chapter 3 are cast into a form which can be solved numerically. Crack growth occurs when the critical stress intensity at the crack tip is reached, which is be computed using a transformation domain integral to take into account the effect of the transformation strains surrounding the crack tip. Crack growth is simulated using a nodal release technique.

The results of extensive parameter studies to the effect of transformation strains on the crack growth behaviour are presented in chapter 5. It is shown that the toughness increase upon crack growth is much larger than previous predictions, where only the dilatant part was taken into account. The agreement between predicted toughness values and experimentally derived values is improved considerable. The results are presented in the plots of transformation zones and transformation development curves. In Chapter 6 we focus on the effect of reverse transformation upon unloading on the toughness development, whereas in chapter 7 the effect of non-homogeneous distribution of the transformable phase is studied. We found that reversible transformation lowers the toughness, while non-homogeneous transformation may cause an increased toughness. However, in chapter 8 we allow the crack to defect as result of non-homogeneous transformation, and then results for the toughness are not much different from results of homogeneous distributions. For the latter problem the transformation domain integrals as well as the crack criterion had to be reformulated. Crack growth is simulated by an element vanish technique.
Contents

1 General Introduction 1

2 A survey of the various toughening mechanisms 5
  2.1 Introduction to fracture mechanics 5
  2.2 Brief survey of the toughening mechanisms in ceramics 7
    2.2.1 Transformation toughening 9
    2.2.2 Microcrack toughening 13
    2.2.3 Ductile particle toughening 15
    2.2.4 Whisker, fibre and platelet toughening 17
    2.2.5 Combination of toughening mechanisms 18
    2.2.6 Crack deflection and branching 18

3 Constitutive modelling 19
  3.1 Introduction 19
  3.2 Constitutive model for dilatant transformation behaviour 20
    3.2.1 Stress-strain relations during transformation 20
    3.2.2 Transformation criterion and transformed fraction 22
    3.2.3 The governing parameters 23
  3.3 Constitutive model for both shear and dilatant transformation behaviour 23
    3.3.1 Stress-strain relations during transformation 24
    3.3.2 Transformation criterion and transformed fraction 26
    3.3.3 Comparison of the two constitutive models 31
    3.3.4 The governing parameters 33
  3.4 Localization phenomena of both constitutive models 33
    3.4.1 Short review of the derivation of the localization condition 34
    3.4.2 Investigation of the occurrence of localization 36
  3.5 Comparison with experiments 38
    3.5.1 Stress-strain relations 38
    3.5.2 Estimation of the material parameters 39
4 Formulation of the boundary value problem and the various solution techniques

4.1 Introduction
4.2 Formulation of the crack problem
4.3 The characteristic length
4.4 Calculation of the stress intensity factor at the crack tip
   4.4.1 Application of the J-integral concept
   4.4.2 Stress intensity change due to transforming spots
4.5 Numerical approach
   4.5.1 Description of the mesh and boundary conditions
   4.5.2 Implementation of the constitutive model of Budiantsky et al. (1983)
   4.5.3 Implementation of the constitutive model of Sun et al. (1991)
   4.5.4 Discretization of the J-integral and surface integral concept

5 Results for homogeneous materials

5.1 Introduction
5.2 Assignment of the parameter study
5.3 Transformation zones
   5.3.1 Some remarks about the shear component of the transformation
   5.3.2 Some remarks about the contour line representation
   5.3.3 General description of the subcritical transformation zone
   5.3.4 Detailed discussion of the results for the transformation zones
   5.3.5 Possibility of the formation of shear bands
5.4 Toughness development
5.5 Comparison to experiments
5.6 Supercritical transformations
5.7 Conclusions

6 Analysis of the effect of reversible transformation

6.1 Introduction
6.2 Influence on the stress-strain relation
6.3 Assignment of the parameter study
6.4 Transformation zones
6.5 Toughness development during crack growth
6.6 Conclusions

7 Effect of non-homogeneous distribution of transformable phase

7.1 Introduction
7.2 Modelling the heterogeneous distribution
7.3 Assignment of the parameter study
7.4 Transformation zones
7.5 Toughness development
7.6 Conclusions

8 Crack deflection due to transformation strains

8.1 Introduction
8.2 Crack criterion 116
8.3 Direction of crack extension 116
8.4 Boundary conditions 118
8.5 Modification of the transformation domain integral 119
8.6 Crack deflection 121
8.7 Implementation 122
  8.7.1 Discretization of the crack problem 122
  8.7.2 Discretization of the crack growth formulation 123
8.8 Results 126
8.9 Conclusions 127

9 General Conclusions 129

Appendices 131

References 137

Author Index 143

Subject Index 145

Samenvatting 149
CHAPTER 1

General Introduction

The word 'ceramics' stems from the old Greek word 'kerameikos' which was the name of a part of the old city of Athens where pottery was made and sold (Visser, 1993). In principle the word 'ceramic' stands for 'baking pots', but nowadays the term covers a much broader area. Kingery (1960) defines ceramics as the art and science of making and using solid articles which have as their essential component inorganic nonmetallic materials. This definition includes not only materials such as pottery, porcelain, refractories, structural clay products, abrasives, porcelain enamels, cements, and glass, but also nonmetallic magnetic materials, ferroelastics, manufactured single crystals and glass-ceramics.

In the last decade, there has been a renaissance in the science and technology of ceramics. Ceramics are now recognized as having a special set of electromagnetic, thermal, electrical, magnetic and mechanical properties that allows them to be used in many ways. The variety of ceramic materials has increased enormously and a subdivision of all different types of ceramics has been created (see Fig. 1.1). The first subdivision is between traditional and technical ceramics. Traditional ceramics itself can be further subdivided into fine grained ceramics (china, etc.) and coarse grained ceramics (bricks, concrete, etc.). Technical ceramics are usually subdivided into functional ceramics (with good electrical, magnetic, electromagnetical, thermal, chemical, but also optical properties) and structural ceramics, with good mechanical properties.

Here we focus on structural ceramics, which have already established a solid basis among the more traditional engineering materials such as metals and polymers. Their right of existence can be traced back to their excellent material properties such as high hardness, high strength, high wear resistance, high chemical resistance and good temperature resistance. These properties can be of decisive importance for the development of new technology, or for the enhancement of existing technology. A few examples of applications existing today are: valves, cutting bits, pumps or even complete (turbine) engines.

In most current applications, the increase of efficiency and service life justifies the generally higher fabrication costs of ceramics. In a society which is beginning to use more du-
rable products, the number and variety of applications will probably increase rapidly. However, for a product to be successful, the reliability has to be established. Toughness plays a dominant role in the reliability of ceramics, due to their relative brittleness compared to the traditionally used engineering materials. Therefore, there has been a search for ways to increase the toughness of these materials. Numerous products have been developed, but the processing, design and manufacturing has been a problem as the deformation and fracture behaviour of these materials is considerably different. The development of constitutive models with predictive power is necessary for the improved design and development of standard procedures instead of trial-and-error. Advanced design concepts have proven their value in for example the processing and design as well as the behaviour during service of metal components, resulting in highly reliable products. This research project will contribute in the development of constitutive models for ceramics.

The objective of this project is to gain insight into the constitutive behaviour of ceramics which have the capability to undergo stress-induced crystal transformation. In particular, the deformation and fracture behaviour at roomtemperature is of interest. The influence of various microstructural modifications to increase strength and toughness is investigated. Insight into the physical mechanisms in the material is considered to be very important, because from those analyses the influence of each mechanism to the macroscopical behaviour can be determined. Advanced numerical micromechanical models play an important role in this project. During the development of these models the attempt is made to link up to experimental work in the same field.

As stated before, an accurate description of the material behaviour forms the basis for a reliable strength, stiffness and stability analysis of a structure or a component. Currently, the numerical and conceptual tools have been developed sufficiently far so that these aspects can be described accurately if the material behaviour is known sufficiently accurately. The importance of such calculations in structural ceramics seems to be even greater than in traditional engineering materials as their behaviour is very different from that of traditional materials.

This thesis may be of interest to people who work in the synthesis of zirconia containing ceramics, people who study their mechanical behaviour and people who design components with it. People who are working in synthesis of zirconia containing ceramics may be interested to see how the toughness increase in these materials is established, because a
better understanding may lead to an eventual, better structural design of the material. As these people are usually specialized in the field of chemistry, Sec. 2.1 has been submitted to introduce some important terminology used in fracture mechanics. Chapter 4 and the first part of chapter 8 deal with the solution techniques that have been used to study the crack growth behaviour. These chapters may only be interesting for people who study the mechanical behaviour of material.

First, in chapter 2 we give an overview of the various toughening mechanisms in structural ceramics that are currently available. We discuss in which way each mechanism contributes to a toughening effect and we briefly discuss the mechanical models that have been developed to predict the toughness increase. In chapter 3 a continuum model is introduced which is capable of describing the transformation behaviour of zirconia based ceramics. The governing parameters of this model are discussed and the stress-strain relation is compared to an experimental stress-strain curve. This model is used next to predict the crack growth behaviour. Therefore, in chapter 4, a so-called small scale crack problem is formulated which has been used to study the crack problem. Subsequently, the techniques to solve this boundary value problem are presented. The results of a parameter study are presented in chapter 5. An attempt is made to present the results of the study in a form which makes comparison to experimental work relatively easy. In chapter 6 we study the effect of reversible transformation on the toughness and in chapter 7 we study the effect of a heterogeneously distributed transformable phase. Finally in chapter 8, the effect of crack deflection due to the heterogeneous distribution is studied.

In this thesis both dyadic notation and index notation are used, with tensors being denoted with boldface characters (e.g. \( \sigma \) for stress). Cartesian components with indices running from 1 to 3 are indicated with Latin subscripts, while Greek subscripts run from 1 to 2 only. The analysis is limited to small displacements and small strains, all tensors are symmetric.
CHAPTER 2

A survey of the various toughening mechanisms

2.1 Introduction to fracture mechanics

In this section we do not intend to give an introduction to fracture mechanics in general; but, as we consider it to be essential to realize the value of the possibility of stress redistribution for the failure behaviour of a specimen containing a crack, we give a short introduction. For a more thorough treatment we refer to standard works by Broek (1982), Hahn (1976) or Ewalds and Wanhill (1984).

In the field of fracture mechanics one studies the relation between loading of a specimen with an initial crack and the extension of this crack. Fundamentally this is a difficult problem because a crack tip itself is a non-existing point. The crack can be followed up to the scale of the lattice in crystalline materials. Crack extension must then be seen as the separation grains (transgranular) or the separation of the grain boundaries (intergranular). Barenblatt (1962) proposed crack models based on that scale, but in conventional fracture mechanics one avoids such detail and one works with an energy balance. Griffith (1921) first applied such an energy balance on a infinite plate of unit thickness which contains a though-thickness crack of length $2a$, which is subjected to a uniform tensile stress $\sigma$ applied at infinity. When the total potential energy of this plate is given by $\Pi$, then the criterion for the crack to grow is given as

$$\frac{d\Pi}{da_c} \leq 0.$$  \hspace{1cm} (2-1)

When $U_0$ is the elastic energy of the loaded uncracked plate (a constant), $U_a$ is the change in elastic energy caused by introducing the crack in the plate, $U_r$ is the change in surface energy caused by the formation of the crack surfaces and $F$ is the work performed by the external force, then the criterion for crack growth becomes
\[
\frac{d}{da_c} \left( U_0 + U_a + U_\gamma - F \right) = 0 
\]  
\[ (2-2) \]

Griffith used a stress analysis to show that the change in elastic energy caused by introducing the crack in the plate is

\[
U_a = \frac{\pi \sigma^2 a^2}{E}, 
\]  
\[ (2-3) \]

where \( E \) is Young's modulus of the material. The surface energy caused by the formation of the crack surfaces is equal to the product of the specific surface energy of the material \( \gamma \), and the new surface area of the crack

\[
U_\gamma = 4a\gamma 
\]  
\[ (2-4) \]

When we substitute (2-3) and (2-4) into (2-2) and no work is done by the external forces (fixed grip condition), we find that crack growth occurs for

\[
\frac{\pi \sigma^2 a}{E} = 2\gamma 
\]  
\[ (2-5) \]

The left-hand side of (2-5) has been called the energy release rate, \( G \), and represents the elastic energy per unit crack surface area that is available for infinitesimal crack extension.

The solution of the stresses in the vicinity of the crack for an infinite plate with a central crack of length \( 2a \) was calculated by Irwin (1957). He expressed the near tip fields in terms of a stress intensity factor \( K \). The definition of the coordinate system as used is given in Fig. 2.1. For example, in a state of plane strain, the stresses are given by

\[
\begin{align*}
\sigma_{11} &= \frac{K_1}{\sqrt{2\pi r}} \cos \frac{\beta}{2} \left( 1 - \sin \frac{\beta}{2} \sin \frac{3\beta}{2} \right) \\
\sigma_{22} &= \frac{K_1}{\sqrt{2\pi r}} \cos \frac{\beta}{2} \left( 1 + \sin \frac{\beta}{2} \sin \frac{3\beta}{2} \right) \\
\sigma_{12} &= \sigma_{21} = \frac{K_1}{\sqrt{2\pi r}} \sin \frac{\beta}{2} \cos \frac{\beta}{2} \cos \frac{3\beta}{2} \\
\sigma_{33} &= \nu (\sigma_{11} + \sigma_{22})
\end{align*} 
\]  
\[ (2-6) \]

where \( \nu \) is Poisson's ratio and the mode I stress intensity factor \( K_1 = \sigma_0 \sqrt{\pi a} \). Furthermore \( r \) is the distance from the crack tip and \( \beta \) the angle between the axis parallel to the crack and the radius \( r \). Irwin then demonstrated that if a crack is extended by an amount of \( da \), the work done by the stress field is formally equivalent to the change in strain energy \( G da \).
Thus it is equivalent to use a stress intensity criterion to predict crack growth. For tensile loading the relationship between $K^C$ and $G^C$ is

$$G^C = \frac{(K^C)^2}{E'}$$  \hspace{1cm} (2-7)

where $E' = E$ for plane stress and $E' = E/(1 - \nu^2)$ for plane strain.

Here the specimen was loaded in mode I. However, the specimen may be loaded in three modes viz. I: the opening mode, II: the sliding mode and III: the tearing mode, as shown in Fig. 2.2. For each mode, a separate stress intensity factor is defined, respectively $K_I$, $K_{II}$ and $K_{III}$. The strain energy release rate may be expressed as

$$G = \frac{K_I^2}{E'} + \frac{K_{II}^2}{E'} + \frac{K_{III}^2}{E'} (1 + \nu)$$  \hspace{1cm} (2-8)

We shall limit ourselves to analyses modes I and II.

![Fig. 2.2. The three modes of crack loading](image)

Once the mathematical framework had been established, the fracture toughness of a material could be established as a material parameter. Considering the simple Griffith relation

$$K_i^C = \sigma_t \sqrt{\pi a}$$  \hspace{1cm} (2-9)

with $\sigma_t$ being the failure stress, two actions can be taken to increase the strength of the material. One can control the flaws in the material or one can focus on microstructural changes of the material to increase the toughness, or reduce the stresses near the crack tip while the loading remains constant. Both actions have been taken for structural ceramics. Here we focus on the latter: the effect of microstructural changes on the toughness of ceramics.

### 2.2 Brief survey of the toughening mechanisms in ceramics

In ceramics the known toughening mechanisms can be subdivided into two classes: process
zone and bridging zone mechanisms as shown in Fig. 2.3. The former class exhibits a toughening which is based on mechanisms occurring in the surrounding of the crack tip (the process zone). These mechanisms include phase transformation and microcracking and these phenomena are characterized by nonlinearity in the stress-strain relations. The bridging zone mechanisms exhibit toughening based on intact material ligaments along the crack surface, which enforce bridging tractions. Examples are: toughening by fibers, whiskers, ductile particles or platelets. Both classes demonstrate resistance (R) curve behaviour, dominated by crack wake effects, which means that the resistance against crack growth increases when an initial crack propagates. The mechanisms rely on the fact that the microstructure is changed such that the tensile stresses at the crack tip are reduced. In such materials, the tip is shielded from the applied load characterized by the stress intensity factor $K_{\text{APP}}$. The difference between the applied stress intensity factor and the stress intensity factor at the crack tip, $K_{\text{TIP}}$, is the toughness increase,

$$-\Delta K_{\text{TIP}} = K_{\text{APP}} - K_{\text{TIP}} > 0 \quad (2.10)$$

Crack growth will not occur until the stress intensity at the crack tip equals the critical stress intensity, $K_{\text{TIP}} = K^C$. When $K^C$ is the fracture toughness of the untoughened material, then in the case of toughened material the crack will not proceed until

$$K_{\text{TIP}} = K_{\text{APP}} + \Delta K_{\text{TIP}} = K^C \quad (2.11)$$

For all toughening mechanisms one tries to maximize the toughness. For a better understanding, micromechanical models have been developed to link changes in the material on microstructural level, to the fracture toughness of the material. These models significantly enlarged the understanding of the various mechanisms and will be discussed shortly. For a more elaborated review we refer to e.g. Rühl and Evans (1989), Evans (1990) and Stam et al. (1990). Here we aim at giving a short introduction. Thereafter, we will focus on zirconia based ceramics with transformation toughening. For illustrative reasons the highest verifiable toughness, observed so far, for each toughening mechanism is summarized in Table 2.1.
<table>
<thead>
<tr>
<th>Mechanism</th>
<th>Highest Toughness (MPa/m)</th>
<th>Exemplary material</th>
<th>Limitation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Transformation</td>
<td>~ 20</td>
<td>ZrO₂; (MgO); HfO₂</td>
<td>T ≤ 900K</td>
</tr>
<tr>
<td>Microcracking</td>
<td>~ 10</td>
<td>Al₂O₃/ZrO₂; Si₃N₄/SiC</td>
<td>T ≤ 1300K, Strength</td>
</tr>
<tr>
<td>Metal Dispersion</td>
<td>~ 25</td>
<td>Al₂O₃/Al; ZrB₃/Fr</td>
<td>T ≤ 1300K, Oxidation</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Al₂O₃/Ni</td>
<td></td>
</tr>
<tr>
<td>Whiskers</td>
<td>~ 15</td>
<td>Si₃/SiC; Si₃N₄/SiC</td>
<td>T ≤ 1500K, Oxidation Interface</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Al₂O₃/SOC</td>
<td></td>
</tr>
<tr>
<td>Fibers</td>
<td>≥ 30</td>
<td>LAS/SiC; Al₂O₃/SiC</td>
<td>Processing Interface</td>
</tr>
<tr>
<td></td>
<td></td>
<td>SiC/SiC; SiC</td>
<td>Coatings</td>
</tr>
</tbody>
</table>

Table 2.1. Summary of tough ceramics, after Rühle and Evans (1989), LAS: Lithium Aluminium Silicate Glass-Ceramic.

2.2.1 Transformation toughening

Pure zirconia (ZrO₂) exists in three different crystal structures: monoclinic (m), tetragonal (t) and cubic (c). At room temperature pure zirconia has a monoclinic structure; at about 1150°C this structure transforms to the tetragonal structure, which transforms to a cubic structure at about 2350°C. The cubic form is stable to its melting point at about 2650°C. The shape of these unit cells are given in Fig. 2.4, and the lattice parameters are given in Table 2.2. The lattice parameters are extrapolated to room-temperature using thermal expansion data. A full treatment of the crystallography of these phases is found in for example McCullough and Trueblood (1959) and Kriven et al. (1981). Many studies have been performed into this direction, and Green et al. (1989) give a thorough review of this work.

In the mid-seventies Garvie et al. (1975) discovered that the tetragonal crystal structure of zirconia could be stabilized at room temperature, and that this tetragonal (t) phase can transform to the monoclinic (m) crystal structure when a certain stress level is applied. Green et al. (1989) state that the transformation proceeds with the speed of sound. It was discovered that fracture toughness of zirconia (ZrO₂)-containing ceramics could be greatly enhanced by this stress-induced martensitic-type transformation (Gupta et al., 1978; Evans and Heuer, 1980; Lange, 1982; Rose, 1986; Green et al., 1989). The increasing toughness upon crack growth can be explained readily by considering the stress field near a crack tip. As the stresses are raised near the tip, transformation of the material near the tip occurs, and a zone of transformed material around the crack tip develops. The unconstrained transformation yields a volume expansion of about 4.5% and a shear strain of 16%, as may be clear from the difference in lattice parameters given in Table 2.2. The transformation strains caused by the transformation are such that they reduce the tensile stresses near the tip when the crack progresses. One can say that the tip is shielded from the applied load $K_{APP}$. This toughening mechanism has been applied in, for instance, Partially Stabilized Zirconia (PSZ), Tetragonal Zirconia Polycrystal (TZP) and Zirconia Toughened Alumina (ZTA) materials. The latter material has been developed since alumina is much cheaper than zirconia. The microstructures of above mentioned materials are shown in Fig. 2.6.

The early pioneers McMeeking and Evans (1982), and Budiansky and co-workers
Fig. 2.4. Three crystal structures of zirconia; (a) cubic, (b) tetragonal and (c) monoclinic.

Table 2.2. Lattice parameters data at room-temperature in nm, given by Porter et al. (1979) using thermal expansion data.

<table>
<thead>
<tr>
<th></th>
<th>$l_1$</th>
<th>$l_2$</th>
<th>$l_3$</th>
<th>$\beta$</th>
</tr>
</thead>
<tbody>
<tr>
<td>cubic</td>
<td>0.507</td>
<td>0.507</td>
<td>0.507</td>
<td>90°</td>
</tr>
<tr>
<td>tetragonal</td>
<td>0.507</td>
<td>0.507</td>
<td>0.516</td>
<td>90°</td>
</tr>
<tr>
<td>monoclinic</td>
<td>0.515</td>
<td>0.521</td>
<td>0.531</td>
<td>$\sim$81°</td>
</tr>
</tbody>
</table>

(1983) were the first to develop a micromechanical model which describes the transformation toughening mechanism. They did not take into account the transformation-induced shear strains associated with the $t \rightarrow m$ transformation as these shear strains were assumed to remain small because of twinning (the validity of these assumptions is questioned by the present author, and this is further discussed in chapter 3). The effect of twinning on the residual shear is schematically demonstrated in Fig. 2.5. This dilatant model significantly enlarged the understanding of a process zone in general and the understanding of the working of transformation toughening in particular. It were these studies that focused upon the fact that the size of the process zone was important and that resistance-curve effects are inherent to the mechanism.

In this first model the criterion for transformation to be triggered is chosen to be a critical mean stress. In reality, a shear component will play a role too but as a first approximation the mean stress criterion seems to be quite acceptable and makes the analysis relatively simple. Using the mean stress criterion and the near tip stress field corresponding to an applied stress intensity $K^{\text{APP}}$, we can now simply obtain a contour around the tip where the critical mean stress in met. As a first approximation for the boundary of the transformation

Fig. 2.5. Schematic representation of the influence of twinning on the transformation shear, demonstrating that twinning reduces the influence of the macroscopic shear component.
Fig. 2.6. Microstructures of three typical t-zirconia containing ceramics, obtained from Green et al. (1989); (a) Mg-PSZ showing two orthogonal variants of the t-zirconia phase (penny shaped, light contrast) in a cubic matrix. The third variant cannot be seen, but would be in the plane of the micrograph. The micrograph is obtained using a transmission electron microscope (TEM). (b) TZP material showing single phase t-zirconia. The picture is obtained using scanning electron microscopy (SEM). (c) ZTA material showing an alumina matrix (appearing dark) and t-zirconia precipitates. The picture is obtained using SEM.

zone, McMeeking and Evans (1982) use this contour and report that for a stationary crack this boundary is given by

$$ r(\beta) = \frac{2}{9\pi} (1 + \nu)^2 \left( \frac{K^\text{APP}}{\Sigma_m^C} \right)^2 \cos^2 \frac{\beta}{2} , $$

(2-12)

where $\Sigma_m^C$ is the critical mean stress at which transformation occurs. The initial zone is shown in Fig. 2.7a.

Budiansky et al. (1983) use an approach developed by Hutchinson (1974) to determine the influence of this initial transformation zone on the stress intensity at the tip, $\Delta K^\text{TIP}$. In this approach two transformed spots which are symmetrically located with respect to the crack are considered, as shown in Fig. 2.7b. They show that the effective change of the stress intensity factor induced by these two transformed spots is

$$ \Delta K^\text{TIP}_{\text{spots}} = \sqrt{\frac{\pi}{8}} \frac{Eb^2}{3} \frac{1 + \nu}{(1 - \nu^2)} f \Theta \frac{3/2}{3/2} \cos \frac{3}{2} \beta $$

(2-13)

where $b$ is the radius of the spots. It is essential to note that the transformation strains are taken to be purely dilatant; $\varepsilon_{11}^T = \varepsilon_{22}^T = (1 + \nu) f \Theta / 3$ where $f$ represents the fraction of transformable phase in the matrix and $\Theta$ is the volumetric expansion due to transformation.
Fig. 2.7. (a) Shape of the initial transformation zone. (b) Location of spots with initial strains. (c) Steady state transformation zone.

The term \((1 + \nu)\) results from the plane strain assumption. The toughness increase due to the transformation strains can now be found by integrating over the transformed area. The maximum height \(h\) of the transformation zone occurs when \(\beta = \pi/3\) and when it is assumed that under steady state conditions the height of the transformation zone remains constant, the toughness increase is simply found by integrating (2-13) for various lengths of the crack extension \(\Delta a\). The steady state value can be found by considering a semi-infinite crack as shown in Fig. 2.7c. McMeeking and Evans (1982) obtain the asymptotic value

\[
\Delta K^{\text{TIP}} (\Delta a \to \infty) = -0.21 \frac{Ef\theta h^{1/2}}{1 - \nu}.
\]  

(2-14)

This result, however, has very limited application as it assumes that all material in the transformed zone is fully transformed (supercritical transformation condition) and it is based on the approximation that the transformation has a negligible effect on the near-tip stress field so that, knowing the critical stress level, the size and shape of the transformation zone could be found from the elastic solution. However, in the paper of Budiansky et al. (1983) also steady state crack growth analysis in subcritically transforming material is considered. In subcritically transforming material the stress and strain fields are unique and smooth, and a transition zone with partially transformed material exists between fully transformed and untransformed material (see also section 3.4). A finite element approach was used and an iterative solution method in which estimates of the zone shape and the distribution of the transformed material are used to generate improved estimates in the subsequent step. More analytical work on this matter has been done by Amazigo and Budiansky (1988b), Stump

Fig. 2.8. First estimate of the increase in toughness caused by supercritical volumetric transformation.
and Budiansky (1989a and b).

Hom and McMeeking (1990) performed a finite element analysis, not to determine just the steady state toughness increase, but to simulate the complete crack growth process. Their results confirm the increasing resistance upon crack growth predicted by McMeeking and Evans (1982). However, it was found that the maximum toughness is achieved after a finite amount of crack growth. These studies have significantly enlarged the understanding of transformation toughening, but there is unsatisfactory quantitative agreement with experiments. The predicted toughening values are lower than the values found in the experiments, as discussed e.g. by Evans and Cannon (1986). In an attempt to remedy this discrepancy, they propose an approach in which the transformation is activated in shear bands at \( \pi/3 \) to the crack tip. Then the toughening increment, for a similar supercritical approach as presented above, is found to be

\[
\Delta K_{\text{TIP}} (\Delta a \to \infty) = -0.38 \frac{Ef\theta h^{1/2}}{1 - \nu} .
\]  

(2-15)

Further work of Lambropoulos (1986) has revealed that the influence of the transformation shear component on the shape of the transformation zone may be quite substantial. By means of an approximate analysis, he determines a toughening effect which is in better agreement with experiments viz.:

\[
\Delta K_{\text{TIP}} (\Delta a \to \infty) = -0.55 \frac{Ef\theta h^{1/2}}{1 - \nu} ,
\]  

(2-16)

where the transformation is triggered by a critical principal stress and the transformation strains develop in that direction as well. In his continuum model, however, twinning is assumed to relax all shear stresses in the transforming particle, while he further assumes that the phase transition in all particles occurs instantaneously and completely. Furthermore, in the determination of the boundary of the transformation zone, he neglects the coupling between the development of transformation and the disturbance of the crack tip stress fields due to these transformation strains. Despite the approximate nature of this analysis, Lambropoulos’ conclusions have triggered further research into the effect of transformation-induced shear strains (see e.g. Stump, 1991b; Budiansky and Truskinovsky, 1993).

Recently, increasing experimental evidence has been found for the occurrence of significant transformation shear strains. For instance, Chen and Reyes-Morel (1986, 1987) and Reyes-Morel and Chen (1988) presented results of hydraulic compression experiments which showed shear and dilatation effects of comparable magnitude. Based on these and related observations, Sun et al. (1991) developed a new, micromechanics based continuum model to account for both the dilatant and shear transformation effects. In the following chapters of this thesis, we adopt this model, and use it to study the influence on the shape and size of the transformation zone as well as on the toughening during crack growth.

### 2.2.2 Microcrack toughening

This mechanism is based on the formation of microcracks upon loading. The initiation of microcracks can be caused by a number of phenomena, which all have in common that the
Fig. 2.9. Uniaxial tension stress-strain curve for material which exhibits microcracking.

Microcracks are initiated by certain particles which contain very high internal stresses. These high internal stresses may be caused by thermal or elastic anisotropies, second phase particles with different elastic moduli or the stress induced transformation discussed in the previous section. Although quite substantial work has been devoted to this mechanism, it has only been fully validated for a ZTA material reported by Rühle et al. (1987).

A typical uniaxial tension stress-strain curve is shown in Fig. 2.9. We see that initially the material is linearly elastic, and when a certain stress level is reached, microcracks start to develop. The microcracks cause a relieve of the local tensile stresses as the volume of the material increases with the introduction of these small cracks. Furthermore, the microcracks reduce the effective elastic modulus in densely microcracked material. Eventually a saturation stage is reached wherein no further cracking takes place (see also Evans and Faber, 1984; Evans and Fu, 1985 and Ortiz, 1987).

The contribution of microcracking to the toughness increase is calculated similarly to the way in which contribution of the transformation dilatation is determined, which is described in the previous section. Hutchinson (1987) showed that when the microcrack nucleation condition involves a critical mean stress, the steady-state shielding is

$$\Delta K^{\text{TIP}}(\Delta a \to \infty) = -0.32 E \theta_T h^{1/2}$$

(2-17)

where $\theta_T$ represents the microcrack misfit strain, which can be compared to $f\theta$ in (2-14). Typical results for steady-state shielding, in case of a normal critical stress and penny shaped microcracks, are

$$\Delta K^{\text{TIP}}(\Delta a \to \infty) = -1.42 \eta K^C,$$

(2-18)

where $\eta$ is a parameter which depends on the density of microcracks which typically varies between 0 and 0.15. The addition of the dilatational and modulus contribution would indicate the total increase in toughness. Evans and Faber (1984) predict an increasing resistance to fracture upon crack growth similar to the toughness development shown in Fig. 2.8. Furthermore, they conclude that the initial zone, before crack growth, does not yield an appreciable change in toughness. This is due to the countervailing influence of the microcracks.
as they degrade the material. When the degradation of the material is not taken into account, Ortiz (1987) does predict initial toughening values.

Although progress has been substantial in both experimental research and in theoretical modelling, the poor understanding of the influence of degradation and limited knowledge of the interactions between modulus and dilatation contributions to shielding as well as limitations in detectability of microcracks, necessitates further study before authoritative conclusions can be reached (Evans, 1990). It is possible, though, to establish the influence of the grain size of the material on the toughness, given in Fig. 2.10, since the nucleation of microcracks is dependent on the grain size. The stresses necessary to initiate microcracks decreases with increasing grain size. The critical stress will approach small values at grain sizes $l_g$ exceeding the critical size $l_c$. Here, $l_c$ is the grain size at which microcracks are initiated upon cooling, in the absence of an applied stress. These thermally introduced microcracks reduce the initial modulus of the material, diminishing the shielding effect. If the grain sizes become too small no microcracking will occur at all. A peak in crack growth resistance should thus occur when $l = l_c$ (Evans and Faber, 1984).

2.2.3 Ductile particle toughening

Toughening a brittle matrix by adding strong reinforcements is a method which seems to be straightforward. It is a method which is used to reinforce concrete. From this it is known that both the toughness and the stiffness can be influenced. However, the scale of the mechanism in ceramics is much smaller. A ceramic matrix may typically be reinforced by adding 20% of metal particles with sizes in the order of micrometers, see for example Sigl et al. (1988).

The toughening mechanism relies on the traction forces of intact reinforcements in the zone behind the crack tip, as they reduce the crack tip stresses. Budiansky et al. (1988) have analysed the problem in the most fundamental way. They state that the mechanism only works if the ductile particles attract the matrix crack, which can be achieved by applying particles with a lower Young’s modulus then the matrix. In that case, the stresses in the ma-
trix material next to the particles are high, and cracking will occur first in these intermediate segments. Budiansky et al. have modelled the mechanism by a bridging spring model, as shown in Fig. 2.11. The particles are assumed to be homogeneously distributed in the ma-

![Fig. 2.11. The ductile particles are modelled by a set of springs.](image)

trix, so that a continuum approach is valid and the bridging particles can be replaced by a continuous support of springs. The size, shape and volume fraction of ductile particles is incorporated in the spring constant $k$. The springs may be assigned three types of behaviour.

(a) **elastic spring model:** In this model the springs are assumed to be elastic (as given in Fig. 2.12a) and effective over a certain bridge length $L$, shown in Fig. 2.11. The fracture toughness of the matrix material is called $K^C$ and the stress in the springs at a distance $x$ from the tip can be written as $\sigma(x) = kEw(x)/(1 - v^2)$, in terms of the crack-interface displacement $w(x)$ and spring constant $k$. Then, using the $J$-integral of Rice (1968) the critical strain energy release rate $G^C$ of the composite is equal to

$$G^C = \frac{(1 - v^2)(K^C)^2}{E} + \frac{(1 - v^2)[\sigma(L)]^2}{kE}. \quad (2-19)$$

If the peak spring stress $\sigma(L)$, at $x = L$, is equal to the spring rupture stress $\sigma_y$, then the steady state toughening is given by

$$\frac{K^{APP}}{K^C} = \sqrt{1 + \frac{\sigma_y^2}{k(K^C)^2}}, \quad (2-20)$$

and crack propagation is accompanied with simultaneous fracture of the last spring.

(b) **elastoplastic spring model:** In this model the elastic behaviour of a spring changes to perfectly plastic behaviour once the yield stress $\sigma_y$ in that particular spring is reached. The extension of the spring at that time is $w_y$. Failure of the last spring is now assumed to

![Fig. 2.12. Three possible stress-displacement relations of the springs, which model the ductile particles: (a) elastic, (b) elastoplastic and (c) rigid-plastic.](image)
occur when the extension of the spring at \( x = L \) reaches \( w_y \), as shown in Fig. 2.12b. In this case Budiansky et al. (1988) found in a similar way, that

\[
\frac{K_{\text{APP}}}{K^C} = \sqrt{1 + \frac{\sigma_y^2}{k (K^C)^2 \left( 1 + \frac{2 (w_y - w_x)}{w_y} \right)}}
\]  

(2-21)

(c) rigid-plastic spring model: When \( w_y - w_x \) is very large with respect to \( w_y \), the deformation behaviour may be regarded as rigid-plastic, as shown in Fig. 2.12c. Then the toughening ratio is found to be

\[
\frac{K_{\text{APP}}}{K^C} = \sqrt{1 + \frac{2\sigma_y E\nu_t}{(K^C)^2 (1 - \nu^2)}}
\]  

(2-22)

independent of the stiffness of the springs and therefore independent of the particle stiffness.

2.2.4 Whisker, fibre and platelet toughening

In contrast to the application of ductile reinforcements that bridge between the crack surfaces, it is also possible to apply brittle reinforcements. According to Evans (1990), when the bridging material is brittle the occurrence of bridging is more subtle and requires either microstructural residual stresses or weak interfaces or both. Large scale local residual stresses caused by thermal expansion mismatch or anisotropy are capable of suppressing local crack growth propagation and, therefore, may allow intact ligaments to exist behind the crack front. The contribution of weak interfaces to toughness increase may be understood by recognizing that the low fracture energy interfaces can cause the crack to deflect

![Diagram](image-url)

**Fig. 2.13. Schematic indication of various contributions to the steady state toughness.**
along those interfaces, permitting intact ligaments. As the crack extends, further debonding can occur. Eventually, the bridging material fails, either by debonding around the end or by fracture. Frictional sliding may occur along the debonded surface. Another energy dissipative mechanism may be acoustic wave dissipation upon reinforcement failure. The contributions to the toughening have been indicated schematically in Fig. 2.13. Many studies have been devoted to this subject, see for example Marshall et al. (1985), Marshall and Oliver (1987), Thouless and Evans (1988), Budiansky and Amazigo (1989), Evans and Marshall (1989), Evans et al. (1989).

The application of whiskers has recently been limited, since the health hazard due to fine and long whiskers is considered to be far greater than that of asbestos. Claussen (1990) proposed the use of monocristalline platelets as a safe alternative. The study and application of somewhat thicker fibers has also been continued.

2.2.5 Combination of toughening mechanisms

Combination of two or more of the above described toughening mechanisms has also shown to be possible. Quite a few studies have been devoted to the combination of fiber and transformation toughening, e.g. Becher and Tieg (1987), Budiansky and Stump (1990), Cui and Budiansky (1993), and to the combination of particulate and transformation toughening, e.g. Amazigo and Budiansky (1988a) and Stump (1991a). The results are very promising and some authors even report synergism of toughening effects.

2.2.6 Crack deflection and branching

Finally we will introduce briefly a toughening mechanism which neither belongs to the process zone class nor to the bridging zone class, but can occur in both classes: crack deflection and crack branching. Irregularities in the microstructure of ceramics may lead to crack deflection or branching. The general philosophy is that the crack path considerably increases when compared to a straight crack, so that more energy dissipates during crack growth. Branching induced by transformation toughening has been studied by Kirchner et al. (1981). For a theoretical approach to the latter, see for example Andreasen (1992).

![Fig. 2.14. Crack deflection and branching.](image-url)
CHAPTER 3

Constitutive modelling

3.1 Introduction

In this chapter we will discuss two constitutive models of zirconia based ceramics. In contrast to conventional ceramic materials which exhibit linear elastic behaviour up to failure, these materials show a nonlinear stress-strain relation once a certain stress level is reached. It is believed that the occurrence of a crystal transformation (stress-induced) from a tetragonal to a monoclinic ($t \rightarrow m$) structure results in the formation of non-elastic strains. The formation of non-elastic strains allows the material to redistribute stress, which is a very important feature to resist crack growth as demonstrated in Chapter 2.

To reduce the complexity of the transformation we assume that we can identify a material sample which is small compared to all macroscopic dimensions, but which is large enough that statistical averaging over all transformable particles is meaningful. For example, a continuum element for PSZ ceramics may look like the schematic drawing in the left of Fig. 3.1. Such a material sample can then be treated as a continuum element for which all (macroscopic) quantities are averages over the sample. Phenomena on a smaller scale are discarded. This means, for instance, that local stress and strain fields around individual

Fig. 3.1. Schematic representation of the microstructure of PSZ ceramics, with transformed penny-shaped particles.
particles are not considered, but only the macroscopic average of these fields over all particles in the sample.

The difference between the two models discussed in sections 3.2 and 3.3 arises from the assumption of the influence of the shear component of the transformation. The first model is based on the assumption that the shear component may be neglected completely and includes only the dilatant part. The second model, however, includes both the dilatant and the shear transformation strain. In both models, the elastic constants $E$ and $v$ of matrix and inclusions are assumed to be identical. Huang et al. (1993) quantified the effect, which was found to be small for PSZ and TZP materials. However, for ZTA materials the difference may be significant.

As stated in Sec. 2.2.1, the martensitic transformation proceeds with the speed of sound. We neglect any dynamical effects and we therefore may assume that the transformation occurs instantaneously and is time independent.

3.2 Constitutive model for dilatant transformation behaviour

As described in section 2.2.1, the transformation from the tetragonal crystal structure to the monoclinic structure involves both dilatant and shear components. However, the first constitutive model developed by McMeeking and Evans (1982) and Budiansky et al. (1983) neglects the shear component, arguing that when the tetragonal particle is embedded in the surrounding elastic matrix it transforms into a number of bands with the sense of the shear alternating from one band to the next. In this way the average shear component is much less than 16%, and may even play no role at all, while the dilatation remains 4.5%. The effect of twinning on the residual shear is schematically demonstrated in Fig. 2.5. Of course, transformations which produce a single twin variant per particle will also interact with the shear strains, depending on the orientation of the particle. However, this is not considered by the above mentioned assumption of a purely dilatant transformation.

3.2.1 Stress-strain relations during transformation

Assuming that the transformation is purely dilatant, the onset of the transformation occurs at a critical mean stress $\Sigma_m^c$, leading to a stress strain relationship as depicted in Fig. 3.2, where $B$ is the bulk modulus and $G$ is the shear modulus of the matrix as well as the inclusion, all being related in the standard way to Young’s modulus $E$ and Poisson’s ratio $\nu$,

$$G = \frac{E}{2(1 + \nu)} , \quad B = \frac{E}{3(1 - 2\nu)} . \quad (3-1)$$

As long as $\Sigma_m \geq \Sigma_m^c$, the transformation of material occurs until the material is fully transformed. If we define the (maximum) volume fraction of transformable phase by $f^m$ and the $t \rightarrow m$ dilatation by $\theta$, then dilatant transformation strain of $\theta \theta$ develops on the intermediate segment.

During transformation, three types of behaviour may be characterised which are governed by the slope $\bar{B}$, see also Fig. 3.2.
(i) The bulk modulus of the intermediate segment $B < -4G/3$. In this case the transformation occurs spontaneously and immediately to completion, where $G$ is the shear modulus. In fact, the intermediate segment is unstable and the material jumps from an untransformed state to a fully transformed state. This material behaviour is called supercritical.

(ii) The bulk modulus of the intermediate segment $B = -4G/3$. This material behaviour is called critical which is the transition from supercritical material behaviour to subcritical material behaviour.

(iii) The bulk modulus of the intermediate segment $B > -4G/3$. The material behaviour is called subcritical and the material can remain stable in a state in which only part of the particles are transformed. The transformation occurs gradually and without any jumps in stress and strain state.

Budiansky et al. (1983) were the first to make this subdivision when they realised that not only the physical response of the composite is strongly affected, but also the mathematical techniques differ. Namely, if a material is characterised as subcritical, the equations governing the incremental behaviour are elliptic so that the stress strain fields are necessarily smooth and unique. However, for supercritical transformations the incremental equations are hyperbolic and certain discontinuities in stress and strain fields become possible. In general terms this may be called localization, where the term localization refers to situations in which deformation concentrates as an outcome of the constitutive behaviour of the material. For a more extensive treatment of transformation-induced localization phenomena we refer to Sec. 3.4.

The behaviour described above is analogous to that of an elastic-plastic solid. First, the material response is linear elastic, then inelastic transformation strains develop. Contrary to elasto-plastic solids, the behaviour retains its linear elastic behaviour when the transformation is completed ($f = f^0$) but this does not really complicate matters. The incremental stress-strain relations in three dimensions are given by Budiansky et al. (1983) as

![Fig. 3.2. Mean stress vs. dilatant strain response.](image-url)
\[ \dot{E}_{ij} = \frac{1}{2G} \dot{\Sigma}_{ij} + \frac{1}{3B} \dot{\Sigma}_m \delta_{ij} + \frac{1}{3} f \dot{\theta} \delta_{ij} \]  \hspace{1cm} (3-2)

or

\[ \dot{\Sigma}_{ij} = 2G (\dot{E}_{ij} - \frac{1}{3} \dot{E}_{pp} \delta_{ij}) + B (\dot{E}_{pp} - f \dot{\theta}) \delta_{ij} \]  \hspace{1cm} (3-3)

Here \( \dot{\Sigma}_{ij} \) are the stress rates of the continuum element, where \( \dot{\Sigma}_{ij} = \dot{\Sigma}_{ij} - \dot{\Sigma}_m \delta_{ij} \) and \( \dot{\Sigma}_m = \dot{\Sigma}_{pp}/3 \). \( \dot{E}_{ij} \) represents the strain rates. In plane strain, the equations reduce to

\[ \dot{\Sigma}_{\alpha\beta} = 2G (\dot{E}_{\alpha\beta} - \frac{1}{3} \dot{E}_{\mu\mu} \delta_{\alpha\beta}) + B (\dot{E}_{\mu\mu} - f \dot{\theta}) \delta_{\alpha\beta} \]  \hspace{1cm} (3-4)

\[ \dot{\Sigma}_{33} = -\frac{2}{3} G \dot{E}_{\mu\mu} + B (\dot{E}_{\mu\mu} - f \dot{\theta}) \]  \hspace{1cm} (3-5)

\[ \dot{\Sigma}_m = \frac{1 + \nu}{3} \dot{\Sigma}_{\mu\mu} - \frac{E}{9} f \dot{\theta} \]  \hspace{1cm} (3-6)

and

\[ \dot{E}_{\alpha\beta} = \frac{1}{2G} (\dot{\Sigma}_{\alpha\beta} - \nu \dot{\Sigma}_{\mu\mu} \delta_{\alpha\beta}) + \frac{(1 + \nu)}{3} f \dot{\theta} \delta_{\alpha\beta} \]  \hspace{1cm} (3-7)

We recall that Greek indices only take values 1 or 2.

3.2.2 Transformation criterion and transformed fraction.

As already mentioned, we assume that a critical mean stress triggers the transformation, because the change in volume only affects the mean stress component. This simple consideration yields the transformation condition

\[ \Sigma_m = \Sigma_m^C \]  \hspace{1cm} (3-8)

and on the intermediate segment of the curve it follows that

\[ f \dot{\theta} = (1 - \frac{B}{\bar{B}}) \left( E_{pp} - \frac{\Sigma_m^C}{\bar{B}} \right) \]  \hspace{1cm} (3-9)

In the subcritical case, the transformation strain rate \( f \dot{\theta} \) can be calculated by

\[ f \dot{\theta} = \begin{cases} (1 - \frac{B}{\bar{B}}) E_{pp} & \text{when } \frac{\Sigma_m^C}{\bar{B}} + f \dot{\theta} (1 - \frac{B}{\bar{B}})^{-1} \leq E_{pp} \leq \frac{\Sigma_m^C}{\bar{B}} + f^m \theta (1 - \frac{B}{\bar{B}})^{-1} \\ 0 & \text{elsewhere} \end{cases} \]  \hspace{1cm} (3-10)

whereas in the critical and supercritical case, the transformation strain rate is undefined. In this case, the transformation strain is simply given by
\[ f \theta = 0 \quad \text{when} \quad \frac{E_{pp}}{B} < \frac{\Sigma_m^C}{B} \]

\[ f \theta = f^m \theta \quad \text{when} \quad \frac{E_{pp}}{B} > \frac{\Sigma_m^C}{B}. \]  

(3-11)

3.2.3 The governing parameters

In this model, 6 material parameters determine the material behaviour: Poisson’s ratio \( \nu \), Young’s modulus \( E \), the bulk modulus of the intermediate segment \( \bar{B} \), a critical mean stress \( \Sigma_m^C \), the maximum volume fraction \( f^m \) of transformable material and the unconstrained volume dilatation \( \theta \). Dimensional analysis and close examination of the governing equations reveal that the constitutive behaviour can be captured by three dimensionless variables viz.: Poisson’s ratio \( \nu \), the ratio \( \bar{B}/G \) governing the slope of the intermediate stress-strain curve and the ‘strength of the transformation’ \( \omega \), as been defined by Amazigo and Budiansky (1988):

\[ \omega = \frac{E f^m \theta}{\Sigma_m^C} \left[ 1 + \frac{1}{1 - \nu} \right]. \]  

(3-12)

3.3 Constitutive model for both shear and dilatant transformation behaviour

The work of Lambropoulos (1986) has revealed that the influence of the transformation shear component on the shape of the transformation zone may be quite substantial. By means of an approximate analysis, he determines a toughening effect which is in better agreement with experiments. Lambropoulos, assumes that twinning relaxes all shear stresses in the transforming particle, the so-called liquid drop analogy, while he further assumes that the phase transition in all particles occurs instantaneously and completely (supercritical transformation). In his analysis to determine the boundary of the transformation zone, he neglects the coupling between the development of transformation and the disturbance of the crack tip stress fields due to these transformation strains. Despite the very approximate nature of this analysis, Lambropoulos’ conclusions have triggered further research into the effect of transformation-induced shear strains. Recently, increasing experimental evidence has been found for the occurrence of significant transformation shear strains. For instance, Chen and Reyes-Morel (1986, 1987) and Reyes-Morel and Chen (1988) presented results of hydraulic compression experiments which showed shear and dilatation effects of comparable magnitude. Based on these and related observations, Sun et al. (1991) developed a new micromechanics based continuum model to account for both the dilatant and shear transformation effects. In general such models have been called transformation plasticity models to emphasize that the shear component is incorporated in the transformation model, and to indicate that there is some similarity to conventional plasticity theory. Note, however, that the physical mechanism of transformation is completely different from the physical
mechanism of plasticity.

3.3.1 Stress-strain relations during transformation

When deriving the transformation plasticity model, Sun et al. (1991) assume the continuum element to consist of a large number of transformable inclusions (referred to with index I) which are embedded coherently in an elastic matrix (referred to with index M), as shown schematically in Fig. 3.1. Microscopic quantities (in the continuum element) will be referred to with lower case characters. The macroscopic quantities can be found by taking the volume average \( \langle \cdot \rangle \) of the microscopic quantities over the element. For instance, the microscopic stress and strain tensors are indicated by \( \sigma \) and \( \varepsilon \), respectively, and with a given volume fraction of second phase (transformable metastable tetragonal inclusions) \( f^m \), the relation between microscopic and macroscopic stresses is

\[
\Sigma_{ij} = \langle \sigma_{ij} \rangle_V = \frac{1}{V} \int_V \sigma_{ij} dV = f \langle \sigma_{ij} \rangle_{V_i} + (1-f) \langle \sigma_{ij} \rangle_{V_m} \tag{3-13}
\]

where the volume of the element, matrix and inclusions is given by \( V, V_M \) and \( V_I \), respectively and \( f \) is the actual fraction of transformed material which is obviously smaller than or equal to \( f^m \). The macroscopic strains are assumed to be small, and assuming isothermal deformations, they can be decomposed into an elastic part \( E_{ij}^e \) and a ‘plastic’ part \( E_{ij}^p \) due to the \( t \rightarrow m \) transformation in the inclusions,

\[
E_{ij} = E_{ij}^e + E_{ij}^p = M_{ijkl}^0 \Sigma_{kl} + f \langle \varepsilon_{ij}^p \rangle_{V_i} \tag{3-14}
\]

Here \( M_{ijkl}^0 = (L_{ijkl}^0)^{-1} \), with \( L_{ijkl}^0 \) being the elastic moduli of both inclusions and matrix,

\[
L_{ijkl}^0 = \frac{E}{1+v} \left( \frac{1}{2} \delta_{ik} \delta_{jl} + \delta_{jkl} \delta_{il} \right) + \frac{v}{1-2v} \delta_{ij} \delta_{kl} \tag{3-15}
\]

The \( t \rightarrow m \) phase transition involves dilatation and shear strains within the inclusion, thus suggesting a split in the plastic strain into a dilatant part and a deviatoric part, designated with superscripts \( d \) and \( s \) respectively,

\[
E_{ij}^p = E_{ij}^{pd} + E_{ij}^{ps} = f \langle \varepsilon_{ij}^{pd} \rangle_{V_i} + f \langle \varepsilon_{ij}^{ps} \rangle_{V_i} \tag{3-16}
\]

The time rate \( \dot{d} (\cdot) / dt \) is denoted by \( \dot{(\cdot)} \). The rates of plastic strain during progressive transformation, \( \dot{f} > 0 \), can be obtained by the straightforward differentiation of (3-16); but they can also be obtained from the average of the transformation strain \( \varepsilon_{ij}^p \) over the freshly transformed inclusions (per unit time) occupying volume \( dV_i \), i.e.

\[
\dot{E}_{ij}^p = \dot{E}_{ij}^{pd} + \dot{E}_{ij}^{ps} = \dot{f} \langle \varepsilon_{ij}^{pd} \rangle_{V_i} + \dot{f} \langle \varepsilon_{ij}^{ps} \rangle_{V_i} + f \dot{\langle \varepsilon_{ij}^{pd} \rangle}_{V_i} + f \dot{\langle \varepsilon_{ij}^{ps} \rangle}_{V_i} \tag{3-17}
\]

The dilatant part \( \varepsilon_{ij}^{pd} \) within each inclusion can be given in terms of the constant stress-free
lattice volume dilatation $\epsilon^{pd} ( = \theta/3 )$ which typically takes a value of 1.5% at room temperature; hence,

$$\langle \epsilon^{pd}_{ij} \rangle_{dV_i} = \langle \epsilon^{nd}_{ij} \rangle_{V_i} = \epsilon^{pd}_{ij} = \frac{1}{3} \epsilon^{pd}_{pp} \delta_{ij} = \epsilon^{pd} \delta_{ij} \quad (3-18)$$

The deviatoric part $\langle \epsilon^{ps}_{ij} \rangle_{V_i}$ is significantly less than the stress-free lattice shear strain of 16% because of the twinning effect. Based on the earlier work of Reyes-Morel and Chen (1988) and Reyes-Morel et al. (1988), this part is specified through its rate of change $\dot{f} \langle \epsilon^{ps}_{ij} \rangle_{dV_i}$, which is assumed to depend on the average deviatoric stress $s^M_{ij}$ in the matrix according to

$$\langle \epsilon^{ps}_{ij} \rangle_{dV_i} = A \frac{g^M_{ij}}{\sigma^M_e}, \quad \sigma^M_e = \sqrt{\frac{3}{2}} s^M_{ij} s^M_{ij} \quad (3-19)$$

Here, $A$ is a material function, which can be considered as a measure of the constraint of the elastic matrix, and $\sigma^M_e$ is the von Mises stress in the matrix, which will be specified later. When $\sigma^M_e = 0$, $A$ should be put zero because there is no stress bias. However, experimental data of Chen and Reyes-Morel (1986, 1987) and Reyes-Morel and Chen (1988) show that under proportional loading the value of $A$ is almost constant during the whole transformation process. Sun et al. (1991) have emphasized that (3-19) is a macroscopic constitutive relationship that is assumed to apply to the ensemble of transformable particles mentioned in the beginning of the section. The deviatoric transformation strain over individual transformed particles will not depend on the local matrix stresses in such a simple manner. Firstly, twinning in a particle will occur in well-defined directions on specific crystallographic planes. Furthermore, the amount of twinning within particles is dependent on the particle size (e.g. Evans and Cannon, 1986). Although much research has been devoted to nucleation and twinning in a single particle, these are still phenomena which are not well understood and need further attention. However, since in this model many grains with different orientations are considered within $dV_i$, Sun et al. (1991) argue that (3-19) is an acceptable approximation in the average sense. Combining the expressions (3-17) to (3-19), the plastic strain-rate is found as

$$\dot{E}^{ps}_{ij} = \dot{f} ( \epsilon^{pd} \delta_{ij} + \langle \epsilon^{ps}_{ij} \rangle_{dV_i} ) \quad (3-20)$$

When (3-20) is combined with the elastic law $E^{e}_{ij} = M^{0}_{ijkl} \Sigma^{kl}_{ij}$ this yields the total macroscopic strain rate

$$\dot{E}_{ij} = \dot{E}^{e}_{ij} + \dot{E}^{ps}_{ij} = M^{0}_{ijkl} \Sigma^{kl}_{ij} + \dot{f} ( \epsilon^{pd} \delta_{ij} + \langle \epsilon^{ps}_{ij} \rangle_{dV_i} ) \quad (3-21)$$

In inverted form, we have

$$\dot{\Sigma}_{ij} = 2G ( \dot{E}_{ij} - \dot{E}_m \delta_{ij} ) + 3B \dot{E}_m \delta_{ij} - \dot{f} ( 3B \epsilon^{pd} \delta_{ij} + 2G \langle \epsilon^{ps}_{ij} \rangle_{dV_i} ) \quad (3-22)$$

where $\dot{E}_m = \dot{E}_{pp}/3$. For future reference, we note that for plane strain conditions, $E_{33} = E_{13} = E_{23} = 0$, so that (3-14) and (3-22) reduce to

$$\dot{\Sigma}_{\alpha\beta} = \frac{1}{2G} ( \dot{\Sigma}_{\alpha\beta} - \nu \dot{\Sigma}_{\mu\nu} \delta_{\alpha\beta} ) + (1 + \nu) \dot{f} \epsilon^{pd} \delta_{\alpha\beta} + \dot{f} ( \langle \epsilon^{ps}_{\alpha\beta} \rangle_{dV_i} - \nu \langle \epsilon^{ps}_{\mu\nu} \rangle_{dV_i} \delta_{\alpha\beta} ) \quad (3-23)$$
and

\[ \Sigma_{\alpha\beta} = 2G(E_{\alpha\beta} - \frac{1}{3}E_{\mu\nu}\delta_{\alpha\beta}) + B\varepsilon_{\mu\nu}\delta_{\alpha\beta} - \dot{f}(3B\varepsilon^{pd}\delta_{\alpha\beta} + 2G\langle\varepsilon^{ps}\rangle_{d\nu_1}) \] , (3-24)

\[ \Sigma_{23} = -\frac{2}{3}G\varepsilon_{\mu\nu} + B\varepsilon_{\mu\nu} - \dot{f}(3B\varepsilon^{pd} + 2G\langle\varepsilon^{ps}\rangle_{d\nu_1}) \] , (3-25)

\[ \Sigma_m = B(E_{\mu\nu} - 3\dot{f}\varepsilon^{pd}) = \frac{1 + \nu}{3}\Sigma_{\mu\nu} - \frac{E_f}{3}\varepsilon^{pd} + \frac{E_f}{3}\varepsilon_d^{ps}_{\mu\nu} \] . (3-26)

3.3.2 Transformation criterion and transformed fraction

The constitutive equations have to be completed by specifying the transformation condition and the evolution relation in terms of \( \dot{f} \). We will start with a brief derivation of the (forward and reverse) transformation yielding conditions. To that end, some concepts from thermodynamics are used. First, the free energy of the continuum element is determined, which is found by addition of the elastic strain energy, the chemical free energy and the surface energy. Here we will only give the results, for a more detailed treatment we refer to Sun et al. (1991).

The elastic strain energy \( W \) per unit volume of the continuum is given by

\[
W = \frac{1}{2} \Sigma_{ij} M^0_{ijkl} \Sigma_{kl} - \frac{1}{2} \frac{1}{V} \int_{V_1} \sigma_{ij}^T e_{ij}^p dV = \frac{1}{2} \Sigma_{ij} M^0_{ijkl} \Sigma_{kl} - \\
\int_{V_1} \left[ 1 B_1 A^2 + \frac{3}{2} B_2 (e^{pd})^2 \right] + \frac{1}{2} \int_{V_1} \left[ B_1 \langle e_{ij}^{ps} \rangle_{V_1} \langle e_{ij}^{ps} \rangle_{V_1} + 3B_2 (e^{pd})^2 \right]
\] (3-27)

where

\[ \bar{\sigma}_{ij} = \sigma_{ij}^\infty + \langle \sigma_{ij} \rangle_{V_1} = \sigma_{ij}^\infty - \dot{f} \langle \sigma_{ij}^\infty \rangle_{V_1} , \] (3-28)

is the transformation-induced internal stress or eigenstress in the inclusion defined by (Mura 1987), and

\[ \sigma_{ij}^\infty = L_{ijkl}^0 (\Lambda_{klmn} - I_{kmn}) e_{mn}^\infty , \] (3-29)

which is the stress in a spherical inclusion after Eshelby (1957, 1961). The tensor \( \Lambda_{klmn} \) is the so-called Eshelby tensor which for spherical inclusions reads,

\[
\Lambda_{1111} = \Lambda_{2222} = \Lambda_{3333} = \frac{7 - 5\nu}{15 (1 - \nu)}
\]

\[
\Lambda_{1122} = \Lambda_{2233} = \Lambda_{3311} = \Lambda_{1133} = \Lambda_{2211} = \Lambda_{3322} = \frac{5\nu - 1}{15 (1 - \nu)}
\]

\[
\Lambda_{1212} = \Lambda_{2323} = \Lambda_{3131} = \frac{4 - 5\nu}{15 (1 - \nu)} . \] (3-30)
Mura determined the stress field in a composite, resulting from misfitting inclusions, with the help of the work of Eshelby and the averaging method of Mori and Tanaka (1973). For a particle which contains so-called eigenstrains (in this case transformation strains) $\varepsilon_{ij}^p$, embedded in an infinitely extended elastic body, Eshelby has derived the exact solution for the stress field in both the particle and the surrounding matrix. Subsequently, the averaging method of Mori and Tanaka has been used to obtain the general solution for more transforming particles. It must be noted that the shape of the transforming particle influences the stress field; here a spherical shape has been assumed. The stresses in the matrix, decomposed in deviatoric stress components and the mean stress, $s_{ij}^M$ and $\sigma_m^M$ respectively, are found to be

\[
s_{ij}^M = S_{ij} - fB_1 (\varepsilon_{ij}^{ps})_V, \quad \sigma_m^M = \Sigma_m - fB_2 \varepsilon_{pd}, \tag{3-31}
\]

where $S_{ij} = \Sigma_{ij} - \Sigma_m \delta_{ij}$, and $\Sigma_m = \Sigma_{pp}/3$ are the deviatoric part and the mean stress of the macroscopic stress tensor $\Sigma_{ij}$, and where

\[
B_1 = 2G \frac{5v - 7}{15(1-v)} \quad \text{and} \quad B_2 = 2B \frac{2v - 1}{1 - v} \tag{3-32}
\]

are two bulk moduli like parameters which result from the approach of Mura.

The chemical free energy change per unit volume can be derived by subtraction of the chemical free energy in the martensitic phase from the chemical free energy in the tetragonal phase. This temperature ($T$) dependent contribution of the free energy is given by

\[
\Delta G_{chem}(T) = f\Delta G_{t \rightarrow m}(T) \tag{3-33}
\]

For spherical, equal-sized particles, the total change in surface energy per unit volume is

\[
A_{sur} = fA_0 = \frac{6\gamma_p f}{a_0} \tag{3-34}
\]

where $a_0$ is the diameter of the grain and $\gamma_p$ is the surface energy change per unit area during the $t \rightarrow m$ transformation.

The Helmholtz (or free) energy per unit volume, $\Phi$, can be calculated by addition of the above contributions:

\[
\Phi(E_{ij}, T, f, \langle \varepsilon_{ij}^{ps} \rangle_V) = W + A_{sur} + \Delta G_{chem} \tag{3-35}
\]

The complementary free energy is formulated as

\[
\Psi(\Sigma_{ij}, T, f, \langle \varepsilon_{ij}^{ps} \rangle_V) = -(W + A_{sur} + \Delta G_{chem} - \Sigma_{ij}E_{ij})
\]

\[
= \frac{1}{2} \Sigma_{ij} M_{ijkl} \Sigma_{kl} + f\Sigma_{ij} (\varepsilon_{ij}^{ps} \delta_{ij} + \langle \varepsilon_{ij}^{ps} \rangle_V) + f\left[ \frac{1}{3} B_1 A^2 + \frac{3}{2} B_2 (\varepsilon_{pd}^2)^2 \right] -
\]

\[
\frac{1}{2} f^2 \left[ B_1 \langle \varepsilon_{ij}^{ps} \rangle_V \langle \varepsilon_{ij}^{ps} \rangle_V + 3B_2 (\varepsilon_{pd}^2)^2 \right] - fA_0 - f\Delta G_{t \rightarrow m} \tag{3-36}
\]

It is clear from (3-35) that the thermodynamic state of the continuum element is completely defined by the variables $\Sigma_{ij}$, $T$, $f$ and $\langle \varepsilon_{ij}^{ps} \rangle_V$, in which $f$ and $\langle \varepsilon_{ij}^{ps} \rangle_V$ are the internal vari-
ables describing the microstructural changes of the material during transformation. Denoting the thermodynamic forces conjugate to the internal variables $f$ and $\langle \varepsilon_{ij}^{ps} \rangle_{V_i}$, by $F_f$ and $F_{ij}^{ps}$ respectively, then the second law of thermodynamics requires:

$$
\dot{\Psi}_P = \frac{\partial \Psi}{\partial f} \dot{f} + \frac{\partial \Psi}{\partial \langle \varepsilon_{ij}^{ps} \rangle_{V_i}} \dot{\langle \varepsilon_{ij}^{ps} \rangle_{V_i}} = F_f \dot{f} + F_{ij}^{ps} \langle \varepsilon_{ij}^{ps} \rangle_{V_i} \geq 0
$$

(3-37)

with, according to (3-36)

$$
F_f = \sum_{ij} (\varepsilon^{pd} \delta_{ij} + \langle \varepsilon_{ij}^{ps} \rangle_{V_i}) - \left[ A_0 + \Delta G_{ij} \rightarrow m - \frac{1}{3} B_1 \varepsilon^2 - \frac{3}{2} B_2 (\varepsilon^{pd})^2 \right]
$$

$$
- f \left[ B_1 \langle \varepsilon_{ij}^{ps} \rangle_{V_i} \langle \varepsilon_{ij}^{ps} \rangle_{V_i} + 3 B_2 (\varepsilon^{pd})^2 \right]
$$

(3-38)

and

$$
F_{ij}^{ps} = f (S_{ij} - fB_1 \langle \varepsilon_{ij}^{ps} \rangle_{V_i})
$$

(3-39)

The energy dissipation during transformation is defined as the dissipation during the interface motion. The interface motion is subjected to the resistance of the lattice friction and a finite driving force is needed to meet the resistance. However, note that interface friction is not the only cause of energy dissipation. For example, the transformation may cause stress waves on a micro-scale and the corresponding energy will be dissipated through conversion to heat. The total energy dissipation per unit volume is denoted by

$$
W^d = D_0 f_{cu}
$$

(3-40)

where $D_0$ is a microstructure-dependent material constant and can be determined by either direct measurement or microstructural calculations. The accumulated fraction of the transformation in the whole deformation history is defined as

$$
f_{cu} = \int_{f} f \mathrm{d}f
$$

(3-41)

The energy dissipation rate $\dot{W}^d$ is thus

$$
\dot{W}^d = D_0 \dot{f}_{cu} = \begin{cases} 
D_0 \dot{f} & \text{(forward transformation, } \dot{f} > 0) \\
- D_0 \dot{f} & \text{(reverse transformation, } \dot{f} < 0)
\end{cases}
$$

(3-42)

Since $\dot{\Psi}_P$ must be equal to $\dot{W}^d$, comparing (3-37) with (3-42), for forward transformation we have

$$
F_f \dot{f} + F_{ij}^{ps} \langle \varepsilon_{ij}^{ps} \rangle_{V_i} = D_0 \dot{f}
$$

(3-43)

while for reverse transformation
\[ F^t \dot{f} + F^p_{ij} \langle e^{p^b}_{ij} \rangle_v = -D_0 \dot{\sigma} \]  
\[ (3-44) \]

Substitution of (3-38) and (3-39) into subsequently (3-43) and (3-44) and elimination of \( \dot{f} \) by using (3-17) and (3-19), we have the transformation yield functions \( F^+ \) and \( F^- \) in stress space:

forward transformation  
\[ F^+ (\Sigma_{ij}, f, T, \langle e^{p^b}_{ij} \rangle_v) = \frac{2}{3} A \sigma^M_e + 3 \sigma^M_m e^{p^d} - C_0(T, f) = 0 \]  \[ (3-45) \]

reverse transformation  
\[ F^- (\Sigma_{ij}, f, T, \langle e^{p^b}_{ij} \rangle_v) = \frac{2}{3} A \sigma^M_e + 3 \sigma^M_m e^{p^d} - \tilde{C}_0(T, f) = 0 \]  \[ (3-46) \]

where

\[ C_0(T, f) = D_0 + A_0 + \Delta G_{t \rightarrow m}(T) - \frac{1}{3} B_1 A^2 - \frac{3}{2} B_2 \left( e^{p^d} \right)^2 + \alpha B_0 \left( e^{p^d} \right)^2 f \]  \[ (3-47) \]

and

\[ \tilde{C}_0(T, f) = C_0(T, f) - 2D_0 \]  \[ (3-48) \]

Here the term with \( \alpha \) is introduced to describe a material with a hardening response. Note that this hardening term is due to processes on a microstructural scale, such as

(i) particle size dependence: it takes a higher stress level to transform smaller particles;

(ii) crystallographic orientation: favourably oriented planes transform first, and

(iii) the mutual interference of transformed regions.

As the constitutive model is derived for the macroscopic scale, considering many transformable particles in one constitutive element, the hardening effect does not follow from the derivation itself and Sun et al. (1991) introduced the last term in (3-47) on more phenomenological grounds. Introducing the parameters \( B_0 \) and \( h_0 \) by

\[ B_0 = \frac{4G (1+\nu)}{1-\nu} + \frac{G h_0^2}{5 (1-\nu)} \quad , \quad h_0 = A / (3e^{p^d}) \]  \[ (3-49) \]

if follows that the forward transformation function (3-45) can be written as,

\[ F^+ = \frac{2}{3} A \sigma^M_e + 3 \sigma^M_m e^{p^d} + B_0 (1 - \alpha) f \left( e^{p^d} \right)^2 - C_0(T) \]  \[ (3-50) \]

Thus linear hardening is introduced by submitting an extra term, dependent on \( f \), to the transformation yielding function. The form of this term is identical to the only term in the transformation yielding function dependent on \( f \), before hardening was introduced: \( B_0 f (e^{p^d})^2 \). If \( \alpha = 0 \), the equations describe the supercritical transformation behaviour defined by Budiansky et al. (1983), see also Secs. 3.2 and 3.4.

The condition (3-45) furnishes a 'transformation surface' in stress space (\( \Sigma_{ij} \)) within which transformation is excluded, similar to a yield surface in the usual theory of plasticity. When the transformation proceeds, the transformation surface expands (or contracts) as well as translates in stress space. Borrowing further notions from plasticity theory, the present material with transformation plasticity may be regarded to exhibit mixed hardening; isotropic expansion (or contraction) as a function of \( f \) is governed through \( C_0(T, f) \),
while kinematic hardening originates from the internal stresses appearing in the relations (3-31) between the matrix stresses and the macroscopic stresses.

The incremental stress-strain relations for forward transformation may be obtained by the usual routine of internal variable constitutive theory (Rice, 1971), substituting (3-17) to (3-19)

\[ \dot{E}_{ij} = \dot{E}_{ij}^e + \dot{E}_{ij}^p = M_{ijkl}^0 \dot{\Sigma}_{kl} + \frac{\partial F_f}{\partial \Sigma_{ij}} \dot{f} + \frac{\partial F_{ps}}{\partial \langle \epsilon_{ij}^p \rangle} \langle \epsilon_{ij}^p \rangle_{V_1} \]

\[ = M_{ijkl}^0 \dot{\Sigma}_{kl} + \langle \epsilon_{ij}^p \rangle_{V_1} \dot{f} + \frac{\partial F_{ps}}{\partial \langle \epsilon_{ij}^p \rangle} \langle \epsilon_{ij}^p \rangle_{V_1} \]

\[ = M_{ijkl}^0 \dot{\Sigma}_{kl} + \dot{f} \left( \epsilon_{ij}^{pd} \Sigma_{ij} + \frac{A M_{ij}}{\sigma_e} \right) \tag{3-51} \]

And \( \dot{f} \) can be determined by the consistency condition:

\[ \dot{F}_+ = \frac{\partial F_f}{\partial \Sigma_{ij}} \dot{\Sigma}_{ij} + \frac{\partial F_f}{\partial f} \dot{f} + \frac{\partial F_{ps}}{\partial \langle \epsilon_{ij}^p \rangle} \langle \epsilon_{ij}^p \rangle_{V_1} = 0 \tag{3-52} \]

Solving the above equation, we obtain

\[ \dot{f} = \frac{\sigma_e}{2 B_1 A^2 + (3 B_2 + \alpha B_0) (\epsilon^{pd})^2} \left( \epsilon_{ij}^{pd} \dot{\Sigma}_{ij} + \frac{A}{\sigma_e^M} \dot{\Sigma}_{ij} + 3 \epsilon^{pd} \dot{\Sigma}_{ij} \right) \tag{3-53} \]

Expression (3-53) holds as long as the transformation progresses, i.e., when the current stress state satisfies the transformation condition (3-45) while there is still a transformable fraction left, \( f < f^m \), and no unloading takes place. This is called the loading or transformation branch. When the response is elastic, either because the criterion (3-45) is not satisfied, \( F_+ < 0 \), or because elastic unloading occurs from a plastic state, \( F_+ = 0 \) and \( \dot{f} < 0 \) according to (3-53), we must set \( \dot{f} = 0 \).

In summary

\[ \dot{f} = \begin{cases} \frac{\langle \epsilon_{ij}^p \rangle_{d V_1} \dot{\Sigma}_{ij} + 3 \epsilon^{pd} \dot{\Sigma}_{ij}}{2 B_1 A^2 + (3 B_2 + \alpha B_0) (\epsilon^{pd})^2} & \text{when } (F_+ = 0 \text{ and } \dot{f} > 0) \\ 0 & \text{when } (F_+ < 0) \text{ or } (F_+ = 0 \text{ and } \dot{f} \leq 0) \end{cases} \tag{3-54} \]

Obviously a similar argument holds for reverse transformation, resulting in
\[
f = \begin{cases} 
\frac{\langle e_{ij}^{ps} \rangle_d v_i \dot{\Sigma}_{ij} + 3 e_{ij}^{pd} \dot{\Sigma}_m}{2 B_1 A^2 + (3 B_2 + \alpha B_0) (e_{ij}^{pd})^2} & \text{when } (F_+ = 0 \text{ and } \dot{f} < 0) \\
0 & \text{when } (F_+ < 0) \text{ or } (F_+ = 0 \text{ and } \dot{f} \geq 0)
\end{cases}
\] (3.55)

From Eqs (3.51) and (3.53) we see that
\[
\dot{\varepsilon}_{ij}^0 = \dot{f} \left( e_{ij}^{pd} \delta_{ij} + A \frac{\dot{\Sigma}_m}{e^M} \right) = \frac{\partial F_+}{\partial \Sigma_{ij}} \dot{f},
\] (3.56)
i.e. the inelastic strain rates are normal to the yield surface (3.45) in stress space. The normality rule is naturally satisfied and there is no need to assume normality a priori, as is sometimes done in conventional phenomenological treatments.

Finally, the constitutive equations will be rearranged into a form which is necessary for the subsequent numerical analysis. With the relation (3.22) between strain rates and stress rates, and introducing the following definitions,
\[
T_{ij} = \frac{\partial F_+}{\partial \Sigma_{ij}} = e_{ij}^{pd} \delta_{ij} + A \frac{\dot{\Sigma}_m}{e^M} \quad \text{and} \quad g = \frac{2}{3} B_1 A^2 + 3 B_2 (e_{ij}^{pd})^2 + \alpha B_0 (e_{ij}^{pd})^2,
\] (3.57)
one can derive the following rate equations
\[
\dot{\varepsilon}_{ij} = L_{ijkl} \dot{E}_{kl}
\] (3.58)
where the instantaneous moduli \(L_{ijkl}\) are given by (see Appendix A),
\[
L_{ijkl} = \begin{cases} 
L_{ijkl}^0 - \frac{1}{g} L_{ijmn}^0 T_{mn} T_{pq} L_{pqkl}^0 & \text{when } F_+ = 0 \text{ and } \dot{f} > 0 \\
L_{ijkl}^0 & \text{when } F_+ \neq 0 \text{ or } \dot{f} \leq 0
\end{cases}
\] (3.59)

3.3.3 Comparison of the two constitutive models

It is clear that incorporation of the shear component has led to a far more complex constitutive model than the dilatant model. However, in case the shear component of the transformation is set to zero, the two models should be equal. This is accomplished by choosing \(h_0 = 0\), so that \(e_{ij}^{ps} = 0\). In the model of Budiansky et al. (1983) the volumetric transformation is called \(\theta\). Comparing this to the model of Sun it follows that \(\theta = 3 e_{ij}^{pd}\). It follows from (3.51) that
\[
\dot{E}_{ij} = \frac{1}{2G} \dot{\varepsilon}_{ij} + \frac{1}{3B} \dot{\Sigma}_m \delta_{ij} + f e_{ij}^{pd} \delta_{ij}
\] (3.60)
which corresponds to (3-2), and
\[ \dot{E}_{pp} = \frac{1}{B} \dot{\Sigma}_m + 3 \dot{j} \varepsilon^{pd} \]  

(3-61)

Then from (3-54), with \( \alpha = 0 \), it follows that

\[ \dot{j} = \begin{cases} \frac{\dot{\Sigma}_m}{B_2 \varepsilon^{pd}} & \text{when } F_+ = 0 \text{ and } \dot{j} > 0 \\ 0 & \text{when } F_+ \neq 0 \text{ or } \dot{j} \leq 0 \end{cases} \]  

(3-62)

Thus, using (3-61) and (3-62), on the transformation branch, the volumetric plastic strain rate is given by

\[ 3 \dot{j} \varepsilon^{pd} = \frac{3 \dot{E}_{pp}}{B_2 (\frac{1}{B} + 3)} = \left( 1 + \frac{4}{3} \frac{G}{B} \right) \dot{E}_{pp} \]  

(3-63)

This result can also be obtained by using the model of Budiansky et al. (1983), when we substitute \( B = -4G/3 \) into (3-10), proving the similarity between the two models. When \( \alpha > 0 \) the equations turn to a subcritical formulation and the relationship between \( \alpha \) and \( B \) can be written as,

\[ \alpha = \frac{9BB - 3BB_2 + 3B_2B}{BB_0 - B_0B} \quad \text{or} \quad \frac{1}{B} = \frac{B (B_2 + \frac{1}{3} \alpha B_0)}{B_2 + \frac{1}{3} \alpha B_0 + 3B} \]  

(3-64)

When the transformation yield functions prior to any transformation \( (f = 0) \) are compared, then for the model of Budiansky et al. (1983) we may write

\[ \Sigma_m = \Sigma_m^C \]  

(3-65)

Suggesting a similar approach for the model of Sun, we use (3-45) with \( f = 0 \) and \( \langle \varepsilon^{pl}_i \rangle_{\gamma_1} = 0 \); this leads to the initial yielding condition

\[ F_+ = 2h_0 \varepsilon^{pd} \Sigma_c + 3 \varepsilon^{pd} \Sigma_m - C_0(T, 0) = 0 \]  

(3-66)

where

\[ \Sigma_c = \sqrt{\frac{3}{4}} S_{ij} S_{ij} , \quad S_{ij} = \Sigma_{ij} - \Sigma_m , \quad \Sigma_m = \frac{1}{3} \Sigma_{pp} \]  

(3-67)

\[ C_0(T, 0) = D_0 + A_0 + \Delta G_{1 \rightarrow m}(T) - 3B_1 (h_0 \varepsilon^{pd})^2 - \frac{3}{2} B_2 (\varepsilon^{pd})^2 \]  

(3-68)

The yielding condition is called ‘initial’ to emphasize that it is not affected by the transformation strains itself, as can be the case if the material exhibits a hardening response. Next we define the critical stress

32
\[
\Sigma^C = \frac{C_0(T, 0)}{3\epsilon^{pd}}, \tag{3-69}
\]

and (3-66) can be written in the form

\[
\frac{2}{3} h_0 \Sigma_e + \Sigma_m = \Sigma^C. \tag{3-70}
\]

### 3.3.4 The governing parameters

From the previous sections we may expect that the variables \( E, \nu, D_0, A_0, \Delta G_{t \rightarrow m}(T), f^m, \epsilon^{pd}, h_0 \) and \( \alpha \) determine the material behaviour. Dimensional analysis and close examination of the governing equations reveal that this set can be replaced by a smaller set of five nondimensional parameters:

(i) Poisson's ratio \( \nu; \)

(ii) the strength of the transformation

\[
\omega = \frac{3Ef^m\epsilon^{pd}(1 + \nu)}{\Sigma^C(1 - \nu)}; \tag{3-71}
\]

(iii) the influence of the transformation shear \( h_0; \)

(iv) the hardening parameter \( \alpha; \)

(v) a parameter \( M \) which governs the so-called `shape memory' phenomenon,

\[
M = \frac{\tilde{C}_0(T, 0)}{C_0(T, 0)}. \tag{3-72}
\]

The definition of the parameter \( \omega \) is similar to the one defined in Sec. 3.2. For an overview of the shape memory behaviour we refer to Sun and Hwang (1993).

### 3.4 Localization phenomena of both constitutive models

The hydrostatic stress-mean strain response shown in Fig. 3.2 for purely dilatant behaviour exhibits softening in the intermediate segment where transformation occurs when \( \bar{B} < 0 \). Budiansky et al. (1983) pointed out that when \( \bar{B} < -4G/3 \), the incremental governing equations cease to be elliptic, thus enabling discontinuities in the stress and strain fields. In that case, discontinuities may also occur in the transformation strains \( f^m \) so that if \( \bar{B} \leq -4G/3 \), all particles can transform spontaneously and completely to give the maximum volumetric transformation strain \( f^m = 3f^m\epsilon^{pd} \). Accordingly, they designated materials with \( \bar{B} < -4G/3 \) as supercritically transforming materials, while subcritical materials are characterized by \( \bar{B} > -4G/3 \). In the latter case, the governing equations remain elliptic and the material can exist in stable, partially transformed states, \( f < f^m \).

In this section, we wish to explore these different ranges of material behaviour for the more general model of transforming composite materials discussed in Sec. 3.3. We shall do so by considering the possibility that the associated governing equations lose ellipticity, making use of the observation that, for a class of constitutive equations of the type (3-58)--
(3-59), this coincides with the onset of localization (e.g. Rice, 1976). In contrast to the situation considered by Budiansky et al. (1983), loss of ellipticity is no longer a material characteristic alone, but depends also on the current state. Hence, we will have to adopt the term subcritical in a more narrow sense for materials that, under a given macroscopically homogeneous state of deformation or stress, exclude loss of ellipticity. Nevertheless, it is of importance to know which combination of material parameters may lead to localization during a certain deformation history. We will not analyse the deformation behaviour for materials where localization does occur, since this requires special solution.

3.4.1 Short review of the derivation of the localization condition

After Rice (1976), Ortiz et al. (1986) consider a homogeneous, homogeneously deformed solid subjected to a quasi-static rate of deformation $\dot{\epsilon}$, and attention is confined to infinitesimal deformations and thermally decoupled, rate-independent material behaviour. Whereas the displacement field $u$ remains continuous after the onset of localization, the displacement gradients $\nabla u$ will exhibit a jump, denoted with symbol $[ ]$, across a plane of discontinuity, i.e.,

$$ [u_{i,j}] = u^a_{i,j} - u^b_{i,j} \neq 0 \quad , \quad (3-73) $$

where the superscript 'a' refers to one side of the plane of discontinuity and 'b' to the other side. Maxwell's compatibility conditions necessitate that the jump, described in equation (3-73) is of the form

$$ [u_{i,j}] = g_i n_j \quad (3-74) $$

where the unit vector $n$ is normal to the plane of discontinuity and $g$ is some vector, as shown in Fig. 3.3. In the example the localization is represented as a shear band, with the direction of the deformation entirely in the $x_1$-direction ($n_1 = 0$, $n_2 = 1$). When the vector $g$ is decomposed along the $x_1$ and $x_2$ axis, it is clear that

$$ [u_{i,j}] = \begin{bmatrix} 0 & g_1 \\ 0 & g_2 \end{bmatrix} = \begin{bmatrix} 0 & 2\varepsilon_{12} \\ 0 & 0 \end{bmatrix} \quad , \quad (3-75) $$

where $2\varepsilon_{12}$ is the shear strain discontinuity. Further, a unit vector $m$ is defined along $g$, i.e.,

$$ m_i = g_i / g \quad , \quad g = |g| \quad . \quad (3-76) $$

The corresponding strain jump is given by

$$ [E_{ij}] = \frac{1}{2} (g_i n_j + g_j n_i) \quad . \quad (3-77) $$

Next we investigate under what conditions localization is possible. To this end, let us assume that the solid is at the onset of localization. At this point, the stresses $\Sigma$ and strains $E$ are continuous throughout the body. However, the stress and strain rates $\dot{\Sigma}$ and $\dot{E}$ will exhibit discontinuities across a plane whose orientation is to be determined. Assuming rate-independent material behaviour, the stress-strain rate relations are taken in the form
\[ \dot{\Sigma}_{ij} = L_{ijkl} \dot{E}_{kl} \]  

(3-78)

where \( L \) is the tangent stiffness matrix of the material. Usually, as in classical plasticity \( L \) has two branches, one corresponding to plastic loading, the other to elastic unloading. For elastic-plastic solids, the analysis is carried out using the same branch of the moduli \( L \) across the incipient planes of discontinuity. Hence, taking the jumps in (3-78) leads to

\[ [\dot{\Sigma}_{ij}] = L_{ijkl} [\dot{E}_{kl}] \]  

(3-79)

Equilibrium across the discontinuity planes requires that the tractions \( t \) are continuous, i.e.,

\[ [t_j] = [n_i \dot{\Sigma}_{ij}] = n_i [\dot{\Sigma}_{ij}] = 0 \]  

(3-80)

Combining (3-79) and (3-80), it follows that,

\[ n_i L_{ijkl} [\dot{E}_{kl}] = 0 \]  

(3-81)

Finally, using the kinematic relation (3-77) and the definition (3-76) we obtain

\[ A_{jk} (n) m_k = (n_i L_{ijkl} n_i) m_k = 0 \]  

(3-82)

This equation has to be satisfied by \( m \) and \( n \) for the localized mode to be possible. The onset of the localization occurs at the first point in the deformation history for which a non-trivial solution of (3-82) exists. For localization to occur along the plane normal to \( n \), the localization (or acoustic) matrix \( A(n) \) has to have at least one zero eigenvalue. This in turn necessitates

\[ f(n) = \det\{A(n)\} = 0 \]  

(3-83)

For plane strain the localization matrix \( A(n) \) is a 2 \( \times \) 2 matrix and one readily finds that

\[ \det\{A(n)\} = a_0 n_1^4 + a_1 n_1^3 n_2 + a_2 n_1^2 n_2^2 + a_3 n_1 n_2^3 + a_4 n_2^4 \]  

(3-84)

---

*Fig. 3.3. Example of a localization; a shear band.*
where

\[ a_0 = L_{1111}L_{1212} - L_{1112}L_{1211} \]

\[ a_1 = L_{1111}L_{1222} + L_{1111}L_{2212} - L_{1112}L_{2211} - L_{1122}L_{1211} \]

\[ a_2 = L_{1111}L_{2222} + L_{1112}L_{1222} + L_{1211}L_{2212} - L_{1122}L_{1212} - L_{1122}L_{2211} - L_{1212}L_{2211} \]

\[ a_3 = L_{1112}L_{2222} + L_{1211}L_{2222} - L_{1122}L_{2212} - L_{1222}L_{2211} \]

\[ a_4 = L_{1212}L_{2222} - L_{2212}L_{1212} \]  \hspace{1cm} (3-85)

Setting \( n_1 = \cos \theta \), \( n_2 = \sin \theta \) in (3-84) the localization condition (3-83) becomes

\[ f(x) = a_4x^4 + a_3x^3 + a_2x^2 + a_1x + a_0 = 0 \]  \hspace{1cm} (3-86)

where \( x = \tan \theta \). Prior to localization, the polynomial \( f(x) \) in (3-86) is positive everywhere. Thus the onset of localization can be determined by simply examining the sign of the minima of \( f(x) \). These occur at the roots of the cubic polynomial \( f'(x) \). As long as the minima of \( f(x) \) remain positive, localization does not develop. The onset of localization is signalled by one or more minima of \( f(x) \) crossing the \( x \)-axis.

3.4.2 Investigation of the occurrence of localization

As a check on this procedure, we shall first briefly reconsider the loss of ellipticity for the model with purely dilatant transformation. In this case, the shear part of the macroscopic response is entirely linear elastic. Therefore, to detect localization we need only to consider purely dilatant deformation paths. For various values of \( \overline{B} \), we scan the total mean stress-dilatancy path of Fig. 3.2 by increasing incrementally the dilatancy. For each increment, the current values of the components of \( L \) are used to compute the coefficients \( (a_0, \ldots, a_4) \) to be substituted into the localization condition (3-83). Evidently, in the linear-elastic branches, no localization is found; but, on the intermediate branch where transformation takes place, we find that localization occurs if \( \overline{B} \leq -4G/3 \) (or \( \alpha \leq 0 \)). This agrees completely with the results of Budiansky et al. (1983).

Next the shear effects of the phase transformation will be taken into account as well (\( h_0 \neq 0 \)). To detect the possible occurrence of localization, again we will scan the total stress-strain path for a number of values \( \alpha \) and \( h_0 \), but now we also need to specify the direction of the deformation path in strain-space. Assuming plane strain situations, we will do so by considering proportional incremental deformation paths in \( E_{\alpha \beta} \)-space. To get a reasonably complete picture of the behaviour, we cover a rather wide range of directions by prescribing the various ratios of incremental principal strains. The ratio \( \rho = \Delta E_{22}/\Delta E_{11} \) will be varied within the range \([-1, 1]\).

For chosen values of \( h_0 \) and \( \rho \) (and \( \nu = 0.3 \)), the critical hardening parameter \( \alpha \) at which localization can occur has been determined numerically from (3-83) in a similar fashion as discussed above. In Fig. 3.4 the critical values of \( \alpha \) are plotted as a function of the strain ratio \( \rho \in [-1, 1] \) for various values of \( h_0 \). The curve for each value of \( h_0 \) separates the elliptic region from the non-elliptic region. Above each curve, localization is im-
Fig. 3.4. The critical value of the hardening parameter $\alpha$ for which, with various values of $h_0 \in \{0.001, 0.25, 0.5, 1, 1.5, 2, 3\}$, ellipticity is lost during a proportional deformation path specified by $\rho = \Delta E_{22}/\Delta E_{11}$ under plane strain conditions.

possible and ellipticity of the equations is ensured; for values of $\alpha$ below the curve, localization will develop as soon as the transformation is initiated. Borrowing the Budiansky et al. (1983) terminology, the curves in Fig. 3.4 thus separate the supercritical transformation regimes from the subcritical regimes in which the transformation process develops gradually. It should be remembered, however, that this holds essentially only for the plane strain proportional deformations considered here.

From Fig. 3.4 we see that when $h_0$ is reduced to zero the critical value of $\alpha$ asymptotically reduces to $\alpha = 0$, independent of the strain ratio $\rho$. This confirms the earlier result for the purely dilatant model. If the transformation shear effects are not neglected ($h_0 \neq 0$), it can be seen that for ellipticity to be guaranteed for an increasing influence of the transformation shear effects, i.e. increasing values of $h_0$, the hardening parameter $\alpha$ must be increased. For increasing values of $h_0$, and for negative values of $\rho$, the numerical results show that the critical hardening parameter $\alpha$ tends unity, which can be expected if we look at (3-50).

It should be noted that for increasing values of $h_0$, the model is increasingly sensitive to non-proportional loading histories; but here, no attempt has been made to investigate the influence of non-proportional loading histories. Nevertheless, the results suggest that a value of $\alpha \geq 1$ will probably be large enough to avoid localization. All crack growth results presented later have used values for $\alpha$ in this range. Experimental results described by Sun et al. (1991) indicate values $h_0 = 1.4$, $\alpha = 1.16$ for TZP materials, and $h_0 = 1.3$. 

37
\( \alpha = 1.2 \) for PSZ materials. Clearly, these values fall in the subcritical regimes of Fig. 3.4, ensuring ellipticity of the equations.

3.5 Comparison with experiments

3.5.1 Stress-strain relations

To illustrate the capabilities of the continuum model of Sun et al. (1991), in Fig. 3.5 the predicted stress-strain relations are compared with experimental stress-strain curves for TZP and PSZ materials. The experimental data of TZP and PSZ were obtained under triaxial compression by Reyes-Morel and Chen (1988) and Chen and Reyes-Morel (1986), respectively. The dashed lines show the theoretical response in the axial \( x_1 \) and radial \( x_2 \) and \( x_3 \) directions. The strain in the axial direction is negative and the strains in the radial directions are positive. Obviously, plastic strains of that nature cannot be described by the purely dilatant model, presented in Sec. 3.2.

For the TZP material, the experiments suggest a nearly perfectly-plastic regime just after initiation of transformation which later turns into a region where linear hardening is observed. This bi-linear transformation behaviour in TZP cannot be modelled with the present model of Sun et al. (1991). In the model we use linear hardening immediately after transformation, shown in Fig. 3.5a. In future, one may consider implementation of bi-linear or non-linear hardening in the model. For PSZ we see that in the experiment the transition

![Stress-strain curves for TZP (a) and PSZ (b) obtained by triaxial compression at room temperature. The dashed lines give the response of the constitutive model.](image-url)
from linear elasticity to transformation behaviour occurs more gradually, whereas in the theoretical model the transition is sharp. Note that in the model the response becomes linear elastic again once the transformation is completed, whereas in the experiment the specimens fail before reaching complete transformation.

We may conclude that compared to the capabilities of the dilatant model, the general material behaviour is described much better: in the triaxial compression test, negative transformation strains develop in the axial direction due to the influence of the shear component. The model is capable of following the general trend of the experimentally derived stress-strain relation, more detailed material characteristics however, like the bilinear transformation regime for TZP, are not captured.

3.5.2 Estimation of the material parameters

In case of TZP, the estimation of the material parameters for the constitutive model (ν, ω, \( h_0 \) and \( \alpha \), see Sec. 3.3.4) will be demonstrated, using experimental data. For PSZ material only the results are given.

For the TZP-material described in Reyes-Morel and Chen (1988) the elastic properties are given as \( E = 190 \text{GPa} \) and \( \nu = 0.3 \). Since the body is completely tetragonal, we have \( f^m = 1.0 \), and the constant lattice volume dilatation is always assumed to be \( \epsilon^{pd} = 0.015 \). The remaining parameters \( \Sigma^C \), \( \alpha \) and \( h_0 \) will be estimated from results of a hydraulic compression test performed by Reyes-Morel and Chen (1988). The experimental stress-strain curve for TZP is reproduced in Fig. 3.5a, from which Fig. 3.6 can be derived, showing the shear transformation strains in the \( x_1 \) and \( x_2 \) direction as a function of the transformed fraction. In the experiment, the loading is almost proportional, and as a consequence the shear transformation strains in the continuum model (3-19) are given by

\[
E_{ij}^{ps} = 3fh_0\epsilon^{pd} (S_{ij}/\Sigma_c).
\]  

(3-87)

With this relation the value of \( h_0 \) can be estimated by curve fitting to the experimental curves of Fig. 3.6. The dashed lines show the theoretical response for \( h_0 = 1.4 \) in the axial (\( x_1 \)) and radial (\( x_2 \) and \( x_3 \)) direction. The critical transformation stress \( \Sigma^C \) can be determined using the transformation condition (3-45) prior to any transformation, i.e. (3-70)

\[
F_+(\Sigma_{ij}, \langle \epsilon_{ij}^{ps} \rangle, \nu_{ij}) = \frac{2}{3} h_0 \Sigma_c + \Sigma_m - \Sigma^C = 0
\]  

(3-88)

For a material loaded in compression \( \Sigma_{11} \) with an additional hydrostatic pressure \( P \), it follows from (3-88) that

\[
\Sigma^C = -\frac{(2h_0 - 1)}{3} \Sigma_{11} - P
\]  

(3-89)

so that if we estimate the stress level at which the transformation is initiated as \( \Sigma_{11} = -13 \times 10^5 \text{MPa} \) from Fig. 3.5a and \( P = 125 \text{MPa} \), we find \( \Sigma^C = 660 \text{MPa} \). Finally the value of the hardening parameter \( \alpha \) is found by comparison of the tangent of the predicted inelastic branch of the stress-strain curves of Fig. 3.5 with the experimental curves. Here the value of the hardening parameter \( \alpha \) is estimated to be 1.16. Note that the response
becomes linear elastic again once the transformation is completed, whereas in the experiment the specimen failed. The experimentally observed bilinear regime of the transformation cannot be modelled, as the present model only can take into account a linear hardening, governed by the last term of $C_0(T,f)$ in (3-47): $\alpha B_0 (\varepsilon^{pl})^2 f$.

Summarizing we have $E = 190$ GPa, $\nu = 0.3$, $\varepsilon^{pl} = 0.015$, $f^m = 1$, $\alpha = 1.16$, $h_0 = 1.4$ and $\Sigma^C = 660$ MPa at constant room temperature $T_0$. These parameters are used to determine the nondimensional parameters discussed in Sec. 3.3.4 which are used in the theoretical model. For the TZP material described above it follows that $\nu = 0.3$, $\omega = 24$, $\alpha = 1.16$ and $h_0 = 1.4$.

For PSZ we have $E = 190$ GPa, $\nu = 0.3$, $\varepsilon^{pl} = 0.015$ and $f^m = 0.35$. The remaining parameters can be calculated in a similar way as discussed above and are estimated to be: $\alpha = 1.2$, $h_0 = 1.3$, and $\Sigma^C = 490$ MPa (based on $\Sigma_{11}^i = -11.5 \times 10^5$ MPa and $P = 120$ MPa from Fig. 3.5b). It follows that the four non-dimensional parameters for this particular PSZ material are $\nu = 0.3$, $\omega = 11$, $\alpha = 1.2$ and $h_0 = 1.3$.

![Diagram](image)

Fig. 3.6. Representation of the amount of shear transformation to the transformed fraction for TZP material. The dashed lines show the fitted curve of the constitutive model.
CHAPTER 4

Formulation of the boundary value problem and the various solution techniques

4.1 Introduction

Both models described in chapter 3 are used to predict the failure behaviour of zirconia containing ceramics. To that end, loading experiments on a specimen with a pre-existing crack are simulated using a finite element program to investigate the \( t \rightarrow m \) transformation induced by the high stresses that develop in the neighbourhood of the crack tip. If the crack proceeds, a zone of transformed material is left behind and it is this transformation zone that is responsible for the measured increasing resistance against fracture. First we will specify the boundary value problem that is studied and subsequently we will present the techniques to solve the problem.

4.2 Formulation of the crack problem

As substantiated in the previous chapter, the initiation of the transformation of tetragonal zirconia requires a certain critical stress level, and because of the high stresses that develop in the neighbourhood of the crack tip, the material near the crack tip undergoes such a transformation. Among others, Rühle and Evans (1989) report that the height of the transformation zone \( h \) remains small compared to the length \( a \) of the crack. This is a necessary and sufficient condition to allow for a so-called 'small scale’ treatment, where one assumes that the elastic stress field remote from the tip is not disturbed by the transformation strains, so that the singular terms still dominate, and an asymptotic problem can be formulated for a
semi-infinite crack (see Fig. 4.1). Under remote Mode I loading and plane strain conditions, the stress field outside the transformation zone is given by the well known linear elastic solution

$$
\Sigma_{ij} = \frac{K_{\text{APP}}}{\sqrt{2\pi}r} f_{ij}(\beta) \quad h \ll r \ll a
$$

(4-1)

where $K_{\text{APP}}$ is the elastic stress intensity factor which will be referred to as the applied stress intensity factor, and $f_{ij}(\beta)$ are dimensionless angular functions in terms of polar coordinates $r$ and $\beta$ at the current crack tip, as given in (2-6). Thus, a domain $\Omega$ enclosing the crack tip can be considered where the displacement boundary conditions can be prescribed by using the linear elastic relations (see Fig. 4.1).

As the tip of the crack is approached, the transformation zone is encountered, and the stress field is disturbed by the transformation strains. In the immediate vicinity of the crack tip, a zone of completely transformed material ($f = f_m$) will be present, surrounded by a zone of partially transformed material ($f < f_m$). Inside the fully transformed zone, the incremental response of the material is again linear elastic, so that the stress field has precisely the same form as in (4-2) but characterized by a different intensity factor $K_{\text{TIP}}$, i.e.

$$
\Sigma_{ij} = \frac{K_{\text{TIP}}}{\sqrt{2\pi}r} f_{ij}(\beta) \quad (r \to 0).
$$

(4-2)

We assume that $K_{\text{TIP}}$ governs the fracture process near the tip, so that the crack advances when $K_{\text{TIP}}$ equals the fracture toughness of the composite $K^C$. Due to the transformation, $K_{\text{TIP}}$ and $K_{\text{APP}}$ will differ by an amount $\Delta K_{\text{TIP}}$ defined through

$$
K_{\text{TIP}} = K_{\text{APP}} + \Delta K_{\text{TIP}},
$$

(4-3)

where $\Delta K_{\text{TIP}} < 0$ if shielding occurs due to the transformation strains.

It is the reduction from $K_{\text{APP}}$ to $K_{\text{TIP}}$ that determines the toughness enhancement due to transformation. Obviously, when no transformation occurs $K_{\text{TIP}} = K_{\text{APP}}$. If transformation strains start to develop under monotonically increasing $K_{\text{APP}}$, even when there is no

![Diagram](image-url)

*Fig. 4.1. Small scale transformation problem for a stationary crack.*
crack growth yet, then in general $K_{\text{TIP}} \neq K_{\text{APP}}$. Budiansky et al. (1983) showed, however, that for the purely dilatant model, the conclusion $K_{\text{TIP}} = K_{\text{APP}}$ is retained prior to crack propagation on the basis of the path-independence of the $J$-integral. The proof relies on the observation that the dilation at each point will increase monotonically as $K_{\text{APP}}$ is increased, so that the transformation-induced inelastic behaviour can be approximated by a nonlinear elastic set of constitutive equations, for which the path-independence of the $J$-integral still holds. This conclusion does not apply to the constitutive model of Sun et al. (1991) accounting for shear transformation strains that was discussed in Sec. 3.3. Due to the stress re-distributions in the vicinity of the crack tip that will accompany the phase transformations, the deformation path of a material point does not remain proportional. Hence, even when the unloading response can be disregarded, the actual response cannot be replaced with a nonlinear elastic response as in the purely dilatant case. Therefore it must be concluded that, with the constitutive model of Sun et al. (1991), the initial transformation zone, i.e. the zone prior to crack growth, can already give rise to a toughening effect.

If $K_{\text{TIP}}$ reaches the critical stress intensity $K_C$, the crack propagates and a wake of transformed material is formed. $K_{\text{TIP}}$ decreases relative to $K_{\text{APP}}$, so that in order to maintain crack growth, $K_{\text{APP}}$ must be continually adjusted so that $K_{\text{TIP}}$ remains equal to the critical value $K_C$. Although the intrinsic material toughness does not change, the effective toughness is given by $K_{\text{APP}}$ and will in general be a function of the crack advance $\Delta a$. The relative toughness increase is defined by $\Delta K_{\text{TIP}} / K_C$.

4.3 The characteristic length $L$

The transition of the Mode I experiment to the small scale problem, defined in Sec. 4.2, implies the loss of the crack length $a$ as an explicit length scale, which is then implicitly prescribed in $K_{\text{APP}}$. A certain characteristic length $L$ must be defined to be able to normalize all length scales so that the results of calculations of crack tip problems can be represented in nondimensional form. Following Stump and Budiansky (1989), we choose for a parameter $L$ which represents the distance on the axis in the direction of the crack, from the tip to the boundary of the transformation zone, just before crack growth ($K_{\text{APP}} = K_C$) and when, for the determination of the transformation zone, the transformation strains are assumed to be so small that they do not disturb the elastic stress field. However, they based the size and shape of the transformation zone on the constitutive equations derived by McMeeking and Evans (1982) where only the dilatant part of the martensitic phase transformation was taken into account, see Sec. 3.2. Here we will derive an updated version of $L$, based on the constitutive model of Sun et al. (1991) where also the shear strains of the transformation are taken into account.

This initial transformation zone is readily obtained by substituting the unperturbed elastic stress field into the transformation criterion (3-70). With the elastic stress distribution near the crack tip given in (2-6), it follows that the hydrostatic stress and the von Mises stress are given by

$$
\Sigma_m = \frac{K_1}{\sqrt{2\pi r}} \cos\left(\frac{\beta}{2}\right) \frac{2}{3} (1 + \nu)
$$

and

$$
\Sigma_e = \frac{K_1}{\sqrt{2\pi r}} \cos\left(\frac{\beta}{2}\right) \sqrt{\frac{(1 - 2\nu)^2 + 3\sin^2\beta}{2}}
$$

(4-4)
When we introduce the shorthand notation

\[ P(\beta) = \sqrt{(1 - 2\nu)^2 + 3\sin^2\frac{\beta}{2}} \]  

(4-5)

it follows that \( R(\beta) \), the distance from the crack tip to the point with the critical stress level \( \Sigma^C \), defined in (3-70), for an angle \( \beta \), is given by

\[
R(\beta) = \frac{2}{9\pi} \left[\frac{K_1^{\text{APP}} \cos \left(\frac{\beta}{2}\right) \{ h_0 P(\beta) + (1 + \nu) \}}{\Sigma^C} \right]^2.
\]

(4-6)

Thus, \( R(\beta) \) is the distance from the tip to the boundary of the transformation zone, when it is assumed that the transformation strains are so small that they do not disturb the elastic stress field. This expression emphasizes that the parameter \( h_0 \) governs the influence of the shear transformation strains and, as a result, the shape of the (initial) transformation zone. The approximate initial transformation zones thus found are shown in Fig. 4.2 for various values of \( h_0 \). If \( h_0 = 0 \), then the constitutive model reduces to the dilatant model. For this special case, the shape of the transformation zone was already determined by McMeeking and Evans (1982). If the value of \( h_0 \) is increased the height of the transformation zone is increased, and the shape also changes. The characteristic length \( L \) is then obtained from (4-6) by substituting \( \beta = 0 \) and \( K_1^{\text{APP}} = K^C \). It follows that

\[
L = \frac{2}{9\pi} \left[\frac{K^C \{ h_0 (1 - 2\nu) + (1 + \nu) \}}{\Sigma^C} \right]^2.
\]

(4-7)

![Figure 4.2](image)

*Fig. 4.2. The shape of the transformation zone, normalized by the length parameter \( L \), for various values of \( h_0 \).*
When only the dilatant transformation is taken into account \((h_0 = 0)\), \(L\) reduces to the expression given by Stump and Budiansky (1989). Note that the transformation zones shown in Fig. 4.2 have been normalized by \(L\).

### 4.4 Calculation of the stress intensity factor at the crack tip

In the previous section we assumed that the crack will grow once the critical stress intensity at the crack tip is reached \((K_{\text{tip}} = K^C)\). This leaves us with the problem of how to calculate \(K_{\text{tip}}\). In our analyses we use one of two methods. The first one is via a \(J\)-integral, the second method uses an area integral over the transformed area. In both approaches it is assumed that the crack is parallel to the \(x_1\)-axis. Approaches to analyse stress intensities at crack tips due to initial strains may be found in Bakker (1985) or Stam (1992), but these turned out to be less convenient for the present problem.

#### 4.4.1 Application of the \(J\)-integral concept

In fracture mechanics a common way to calculate \(K\) for complex two-dimensional geometries is to apply the \(J\)-integral concept of Rice (1968). The concept has proved to be very useful and convenient. However, the concept is valid only under the conditions:

1. the material is homogeneous;
2. the deformation behaviour is (non)linear elastic or the deformation theory of plasticity holds. The assumption of nonlinear elasticity remaining compatible with the actual deformation behaviour holds when no unloading occurs in any part of the material and the stresses follow a proportional loading path. Therefore \(J\) is certainly not applicable during crack growth, and finally
3. the problem is two-dimensional. Three-dimensional crack problems demand a somewhat more complex surface integral, developed by Budiansky and Rice (1973).

When all of the conditions are met, the path independent \(J\)-integral may be calculated by

\[
J = \frac{1}{\Gamma} \oint T_i \frac{\partial u_i}{\partial x_1} \, ds
\]  

(4-8)

when the crack is parallel to the \(x_1\)-axis. Here \(W\) is the specific elastic strain energy, \(u_i\) is the displacement field, \(ds\) is an infinitesimal element of the contour \(\Gamma\) (see Fig. 4.3) and \(T\) is the traction vector with components \(T_i = \sigma_{ij} n_j\), with \(n\) the unit outer normal on \(\Gamma\). When the behaviour of the material is purely linear elastic, \(J\) is Griffith’s energy release rate \(G\). The relation between the \(J\)-integral and the stress intensity factor \(K_1\) in that case is

\[
J = \frac{K_1^2}{E'}
\]  

(4-9)

where \(E' = E\) for generalized plane stress and \(E' = E/ (1 - v^2)\) for plane strain. By definition, the infinitesimal strain energy \(dW\) is given by
\[ dW = \Sigma_{11} dE_{11} + \Sigma_{22} dE_{22} + 2 \Sigma_{12} dE_{12} \quad , \]  
(4-10)

hence the first term of (4-8) is

\[
\int W dx_2 = \int \left[ \frac{1}{2E} (\Sigma_{11} + \Sigma_{22} + \Sigma_{33})^2 + \frac{(1 + \nu)}{E} (\Sigma_{12} - \Sigma_{11} \Sigma_{22} - \Sigma_{22} \Sigma_{33} - \Sigma_{11} \Sigma_{33}) \right] dx_2
\]
(4-11)

and the second term is

\[
\int T \frac{\partial u}{\partial x_1} ds = \int (\Sigma_{11} E_{11} dx_2 + \Sigma_{12} E_{12} dx_2 - \Sigma_{12} E_{11} dx_1 - \Sigma_{22} E_{12} dx_1) \quad .
\]
(4-12)

It was shown by Rice (1968) that the \( J \)-integral is indeed path independent. This means any contour \( \Gamma \), like the one in Fig. 4.3, is valid and will give the same result.

When the crack starts to grow, path independency is lost because unloading takes place in the wake of the crack. This is one of the limitations mentioned above. In case of elastic behaviour, however, it is still path independent. When the load is removed, there are no residual strains and thus the new crack can be seen as stationary again. When the boundary values are updated for the new crack length, the original value for \( J \) will be found.

In the situation of dilatant transformation behaviour, the standard path independent \( J \)-integral can still be applied until crack growth occurs. When the boundary values are increased monotonously, that is \( E_{pp} \) increases in every point as the boundary values are increased (Budiansky et al. (1983)), the separate unloading response of the material can be disregarded. Therefore the material can be thought of as a small strain, nonlinear elastic solid with the three-segment dilatation curve shown in Fig. 3.2. Thus, by path independence it follows immediately that \( K_{\text{TIP}} = K \), irrespective of the location of the transformation zone and the distribution of \( \theta \) (see also Turner, 1979). This shows that the initial transformation zone for dilatant transformations does not give any toughening effect (cf. Sec. 4.2). When \( K_{\text{TIP}} \) exceeds \( K^C \), the crack starts growing and unloading in the wake of the crack takes place. Now the \( J \)-integral concept cannot be applied directly, because path independency definitely is lost. In the wake of the crack the material remains transformed, resulting in a (small scale) shielding effect. This means that \( K \), evaluated from a \( J \)-integral along a path outside the transformation zone, will depend only on the boundary values. If \( K \) is evaluated from a \( J \)-integral along a path inside the completely transformed material (where the
behaviour is linear elastic again) it is affected by the transformation as well as by the boundary values. If $K_{\text{tip}}$ is of interest in a material with a transformation zone as shown in Fig. 4.4, then the contour of the integral must be chosen such that all the material inside the contour is completely transformed.

### 4.4.2 Stress intensity change due to transforming spots

Budiansky et al. (1983) describe a method based on the changes in the stress field caused by two circular cylindrical spots. These spots of radius $R$ are located symmetrically with respect to the crack as shown in Fig. 4.4 and have areas $dA$. Hutchinson (1974) analysed this problem with the spots initially strained by in-plane stress-free strains $E_{ij}$. In the analysis the stress functions of Kolosov and Mushkelishvili are used (see also Appendix B). The origin of the coordinate system is positioned at the crack tip, with the $x_1$-axis is parallel to the crack. The coordinates of the centre of the spot in the upper and lower half plane are given by $z_0 = x_1 + ix_2$ and $z_0$, respectively, where the bar denotes the complex conjugate. If $R \to 0$, the last term in (B.18) can be neglected. The general expression for the influence of these two spots on the stress intensity $dK_{\text{tip}}$ at the crack tip ($z = 0$) is given by

$$
dK_{\text{tip}} = -2\sqrt{2\pi}EdA \Re \left[ \frac{1}{z_0^{3/2}} \left( -c_1 + \frac{c_2(-z_0-3\bar{z}_0)}{4z_0} \right) \right] \tag{4-13}
$$

with

$$c_1 = \frac{1}{2\pi} (E_{22}^P - iE_{12}^P) , \quad c_2 = \frac{1}{4\pi} (E_{11}^P - E_{22}^P + 2iE_{12}^P) . \tag{4-14}
$$

Lambropoulos (1986) further rearranged this expression to the form

$$
dK_{\text{tip}} = \frac{1}{\sqrt{8\pi}} \frac{EdA}{(1 - \nu^2)} r^{-3/2} M(E_{ij}^P) \tag{4-15}
$$

where

$$M(E_{ij}^P) = (E_{11}^P + E_{22}^P) \cos \frac{3\beta}{2} + 3E_{12}^P \cos \frac{5\beta}{2} \sin \beta + \frac{3}{2} (E_{22}^P - E_{11}^P) \sin \beta \sin \frac{5\beta}{2} \tag{4-16}
$$

The transformation strains $E_{ij}^P$ to be substituted into (4-16) are the in-plane transformation strains that would occur under plane strain conditions but without in-plane stresses, i.e. $\Sigma_{\alpha\beta} = 0$ with $E_{ij} = 0$. With the general 3-D transformation strain $E^P$ in each spot being given by (3-16), it follows from the plane strain expressions (3-23) that the resulting nonzero strains are given by

$$E_{11}^P = (1 + \nu) f e_{11}^P + f \left( (\epsilon_{11}^{ps})_{ij} - \nu \left( (\epsilon_{11}^{ps})_{ij} + (\epsilon_{22}^{ps})_{ij} \right) \right) ,$$

$$E_{22}^P = (1 + \nu) f e_{22}^P + f \left( (\epsilon_{22}^{ps})_{ij} - \nu \left( (\epsilon_{11}^{ps})_{ij} + (\epsilon_{22}^{ps})_{ij} \right) \right) ,$$

$$E_{12}^P = f (\epsilon_{12}^{ps})_{ij} . \tag{4-17}$$

47
For the case where only dilatant initial strains are taken into account, it is then easily shown that, in plane strain ($E_{11}^p = E_{22}^p = (1 + \nu) \theta / 3$), the change of the near-tip stress intensity factor induced by two symmetrically located dilatant spots each with area $\pi R^2$, is

$$dK^{\text{tip}} = \frac{\pi R^2 E \theta}{3\sqrt{2 \pi (1 - \nu)}} r^{-3/2} \cos \frac{3\beta}{2}$$  \hspace{1cm} (4-18)

where the positions of the spots are drawn in Fig. 4.4.

This can be used to calculate the stress intensity near the crack tip in a material with transformation strains by considering the transformation zone $A$ with its continuous distribution of $\theta$ to be subdivided into infinitesimal spots of area $dA$. When the transformation zone $A$ and the distribution of $\theta$, the summation of all spots must lead to the difference between $K^{\text{APP}}$ and $K^{\text{tip}}$. It follows that

$$\Delta K^{\text{tip}} = \int \int_{\Omega} dK^{\text{tip}}$$  \hspace{1cm} (4-19)

and with (4-3)

$$K^{\text{tip}} = K^{\text{APP}} + \frac{E \theta}{3\sqrt{2 \pi (1 - \nu)}} \int_A r^{-3/2} \cos \frac{3\beta}{2} \, dA$$  \hspace{1cm} (4-20)

which is reported by Budiansky et al. (1983).

\textbf{4.5 Numerical approach}

A displacement-based finite element method is used to solve the boundary value problem described in Sec. 4.2. First the discretization of the boundary problem is elaborated followed by a discussion on the implementation of the constitutive equations. We used quadrilateral elements, each of these elements is built up of four triangular constant strain elements.
4.5.1 Description of the mesh and boundary conditions

The mesh that is used models only the upper half of the small scale domain $\Omega$ since Mode I loading is symmetric. It contains 2770 elements and 2880 nodes. The mesh generator is designed such that the mesh is highly refined near the tip. The layout of a possible mesh has been outlined in Fig. 4.5. Four zones can be distinguished. Zone 1 is a rectangular area of 90 by 5 elements and is the finest part of the mesh. Along the lower bound of this zone, crack growth is simulated by releasing nodes. The second zone forms the first transition from a rectangular to a circular region, far away from the crack tip. In the last two rows of this zone, mesh refinement reduces the number of elements in the zones further out. The number of elements over the height of this zone is 9. The elements in this area cannot be held squared, but we try to keep the height equal to the base by increasing the height and base length by the same ratio. The third zone forms the transition to the circular boundary and the fourth zone just bring the boundary further out, to reach the ‘far-field’. The number of element rows in these two zones are 5 and 30, respectively. The above described mesh is further illustrated in Fig. 4.6. The starting and end position of the crack tip are shown in Fig. 4.6c. Crack growth in this example was permitted over a span of 80 nodes to the right hand side of the mesh.

The boundary values are given by

$$T_1 = T_2 = 0 \quad \text{at} \quad -r(\pi) < x_1 < 0, \quad x_2 = 0$$

$$T_1 = 0, \quad u_2 = 0 \quad \text{at} \quad 0 < x_1 < r(0), \quad x_2 = 0$$

$$u_1 = 2(1 + \nu) \frac{K^{\text{APP}}}{E} \sqrt{\frac{r}{2\pi}} \cos \frac{\beta}{2} (2 - 2\nu - \cos \frac{\beta}{2}) \quad \text{at} \quad x_1 = r(\beta) \cos \beta$$

$$u_2 = 2(1 + \nu) \frac{K^{\text{APP}}}{E} \sqrt{\frac{r}{2\pi}} \sin \frac{\beta}{2} (2 - 2\nu - \cos \frac{\beta}{2}) \quad x_2 = r(\beta) \sin \beta$$

(4-21)

where the prescribed tractions are denoted by $T_\alpha$ and the displacements by $u_\alpha$. The coordinates $r$ and $\beta$ depend on the instantaneous position of the moving crack tip.

![Diagram of the mesh and boundary conditions](image)

*Fig. 4.5. Layout of the mesh and the boundary conditions.*
Fig. 4.6. The finite element mesh used to analyse the small-scale crack growth problem.

4.5.2 Implementation of the constitutive model of Budiansky et al. (1983)

The finite element equations for the displacement rates are solved in a linear incremental manner. For the sake of clarity the increment number \( i \) is annotated and the symbol \( \Leftrightarrow \) is used with meaning: ‘right-hand side is assigned to the left-hand side’.

In terms of a finite element approach the incremental displacement field \( \Delta u^{(i)} \) can now be calculated by solving the equality
\[ K^0 \Delta u^{(i)} = \Delta F^{(i)} - (D^T \Sigma^{(i)} - F^{(i)}) + D^T S^0 \Delta f^{(i)} \theta \]  
(4-22)

where \( K \) is the global stiffness matrix defined by

\[ K^0 = D^T S^0 D \]  
(4-23)

and \( \Delta F^{(i)} \) is the vector of nodal load increments. To maintain equilibrium, the global imbalance forces after the last increment \( (D^T \Sigma^{(i)} - F^{(i)}) \) are taken as a load increment in the following step. Here \( D^T \) is the transpose of the difference matrix \( D \) relating strains and nodal displacements, and \( S^0 \) is the local stiffness matrix determined by the elastic stiffness tensor \( L^0 \). The final term of (4-22) represents the forces introduced by the transformation strains accompanying the loading increment. It is this term which reflects completely the non-linear material behaviour and which is dependent on \( \Delta u^{(i)} \). Therefore, (4-22) is solved iteratively. In the first step of the iteration, the incremental transformation strains are set to zero as an initial guess, whereas in successive iteration steps, \( \Delta f^{(i)} \theta \) is based on the strain distribution in the previous iteration. One iteration step is given in Fig. 4.7. The iteration process continues until adequate convergence is achieved. Convergence is checked by comparing the transformation energy

\[ \Pi^\theta = \int_A \frac{1}{2} B (f^{(i)} \theta + \Delta f^{(i)} \theta)^2 dA \]  
(4-24)

<table>
<thead>
<tr>
<th>( K \Delta u^{(i)} \leftarrow \Delta F^{(i)} - (D^T \Sigma^{(i)} - F^{(i)}) + D^T S \Delta f^{(i)} \theta )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \Delta E^{(i)} \leftarrow D \Delta u^{(i)} )</td>
</tr>
<tr>
<td>( E^{(i)} \leftarrow D u^{(i)} + \Delta E^{(i)} )</td>
</tr>
<tr>
<td>( \Sigma_m \frac{B}{B} + f^{(i)} \theta (1 - \frac{B}{B}) \leq E_{pp}^{(i)} \leq \Sigma_m \frac{B}{B} + f^{m} \theta (1 - \frac{B}{B}) )</td>
</tr>
<tr>
<td>( \Delta f^{(i)} \theta \leftarrow (1 - \frac{B}{B}) \Delta E_{pp}^{(i)} )</td>
</tr>
<tr>
<td>( E^e^{(i)} \leftarrow B^{(i)} - f^{(i)} \theta - \Delta f^{(i)} \theta )</td>
</tr>
<tr>
<td>( \Sigma^{(i)} \leftarrow S E^e^{(i)} )</td>
</tr>
</tbody>
</table>

Fig. 4.7. Scheme 1, one iteration step for the dilatant model of Budiansky et al. (1983).
between two successive iterations. If \( \Pi^0 \) remains within certain limits, convergence is assumed, and a loading increment is applied,

\[
K^{\text{APP}}(i + 1) = K^{\text{APP}}(i) + \Delta K^{\text{APP}}(i)
\]

\[
u^{(i+1)} = u^{(i)} + \Delta u^{(i)}
\]

\[
f^{(i+1)} \theta = f^{(i)} \theta + \Delta f^{(i)} \theta.
\]  

(4-25)

The size of the load steps is determined so that the critical stress intensity is reached in about 100 increments. However, as can be seen from the flowchart in Fig. 4.8, \( K^{\text{TIP}} \) can only be determined after the summation of the increment. So, to prevent \( K^C \) to be exceeded, the size actual of the load steps is determined by

\[
\Delta K^{\text{APP}} = \zeta \left( \frac{K^{\text{TIP}}}{K^C} - 1 \right) K^C
\]  

(4-26)

once this equation gives lower values for \( \Delta K^{\text{APP}} \) than the usual constant load increment.

---

**Fig. 4.8. Flowchart of finite element program ZIRCON.**
The scaling parameter $\zeta$ should be in the range $\{0, 1\}$ and governs how rapidly $K^C$ is approached. Once the critical stress intensity at the tip is reached ($K^{\text{tip}} = K^C$), crack growth is simulated by a nodal release technique comparable to the method used by Hom and McMeeking (1990): The nodal force at the current crack tip node position is stepped down to zero in five increments with $\Delta F^{(i)} = 0$, and the displacement boundaries at the outer radius are adjusted to the new position relative to the moved tip. Subsequently, loading of the crack continues; however, the first loading increment $\Delta F^{(i)} = 0$ to determine $K^{\text{tip}}$ as the criterion $K^{\text{tip}} = K^C$ may already be reached. The finite element program performing the analysis described here is called ZIRCON.

4.5.3 Implementation of the constitutive model of Sun et al. (1991)

Extensive use is made of the fact that the constitutive equations for the Sun et al. (1991) transformation model have been cast in the form of (3-58) and (3-59), i.e. completely similar to the usual time-independent elastoplasticity equations with an associative flow rule. The resulting finite element equations for the displacement rates are then solved in a linear incremental manner. Comparable to the discretization of the dilatant model in the previous section, in each increment $i$, the nodal displacement increments $\Delta u^{(i)}$ are solved from

$$ K^{(i)} \Delta u^{(i)} = \Delta F^{(i)} - (D^T \Sigma^{(i)} - F^{(i)}) $$

with $K^{(i)} = D^T S^{(i)} D$, \hspace{1cm} (4-27)

where $\Delta F^{(i)}$ is the vector of nodal load increments, but the stiffness matrix $S^{(i)}$ is now determined by the instantaneous moduli $L$ appearing in (3-58). The moduli $L$ are determined as shown in Fig. 4.9. The bracket term in the right-hand side of (4-27) is an equilib-

\[
\begin{align*}
F_+ &= \frac{2}{3} A \sigma^M_\varepsilon + 3 \sigma^M_m \varepsilon^{pd} - C_0(\theta, f) \\
F_- &= \frac{2}{3} A \sigma^M_\varepsilon + 3 \sigma^M_m \varepsilon^{pd} - \tilde{C}_0(\theta, f)
\end{align*}
\]

\[
\text{if } (F_+ = 0 \text{ or } F_- = 0) \text{ and } IP = 1 \text{ then}
\]

\[
\begin{align*}
s^{M}_{ij} &= S_{ij} - fB_1 (\varepsilon^{ps})_{Vi} \\
T_{ij} &= \varepsilon^{pd} \delta_{ij} + A \frac{s^{M}_{ij}}{\sigma^M_\varepsilon}
\end{align*}
\]

\[
T_{ijkl} = L_{ijkl}^0 - \frac{1}{h} \left( L^0_{ijmn} T_{mn} + T^0_{pqkl} \right) + \frac{1}{h} T_{ab} T^0_{abcd} T_{cd}
\]

Fig. 4.9. Scheme 2, determination of the instantaneous tensor $L$, which is used for determination of the stiffness matrix $S^{(i)}$. IP is a help variable to prevent the occurrence of reverse transformation when the forward transformation criterion is met or w.w., see also the flowchart given in Fig. 4.10.
Fig. 4.10. Flow chart of one load increment for the model of Sun et al. (1991).

...
reached so that the transformation criterion $F_+ = 0$ is satisfied, the incremental volume fraction of transformed material $\Delta f^{(i)}$ can be found from the incremental version of (3-54). We emphasize that, in contrast to the situation in case of the purely dilatant model of Budiansky et al. (1983), the current transformation strain will have to be determined incrementally as well. The deviatoric part deserves special attention. With $\langle \varepsilon_{ij}^{PS} \rangle_{V_i}$ being determined from the current stresses $s^{M(i)}$ according to (3-19), the incremental change of $E^{PS}$ is obtained from (3-20) as

$$\Delta E^{PS(i)} = \Delta f^{(i)} \langle \varepsilon_{ij}^{PS(i)} \rangle_{V_i}. \quad (4-28)$$

On the other hand, according to (3-16) we also have $E^{PS(i+1)} = f^{(i+1)} \langle \varepsilon_{ij}^{PS(i+1)} \rangle_{V_i}$ from which we can compute the deviatoric components of the particle transformation strain as

$$\langle \varepsilon_{ij}^{PS(i+1)} \rangle_{V_i} = \frac{f^{(i)} \langle \varepsilon_{ij}^{PS(i)} \rangle_{V_i} + \Delta f^{(i)} \langle \varepsilon_{ij}^{PS(i)} \rangle_{V_i}}{f^{(i+1)}}. \quad (4-29)$$

In our analysis about 100 loading increments $\Delta K^{APP}$ are applied to reach the critical value $K^C$ at the crack tip. This turned out to be necessary to describe accurately the development of the initial transformation zone, and in particular to account adequately for the non-proportional stress changes that accompany the resulting stress re-distributions inside and in the vicinity of the expanding transformation zone. Furthermore, on the transformation branch of the constitutive response, 10 subincrements are taken within each increment in order to be able to take relatively large loading increments to save computing time. The incremental loading displacements $\Delta u$, found from (4-27), are simply divided into 10 equally sized subincremental displacements $\Delta u$, which are then used to incrementally calculate the incremental strains and stresses, and also the transformation behaviour, in a similar manner as discussed above. A flow chart of one increment, with its 10 subincrements is given in Fig. 4.10. For clarity some steps concerning the sub-incrementing are left out of the flowchart. These steps are further elaborated below.

First, if the current stress state is not on the transformation branch, so that the material behaviour is linear elastic, no subincrements are taken in order to reduce computation time. If during an increment the material-response changes from linear elastic to a transformation plasticity response, the first subincrement is taken such that the transformation criterion (3-45) is met exactly, and subsequent subincrements are taken to follow the transformation branch. In case the material regains its linear elastic response, because the transformation is exhausted, $f \geq f^m$, the last subincrement on the transformation branch is adjusted such that the updated value of $f$ is exactly equal to the maximum value $f^m$. This can be done simply by scaling back the subincrement as each increment itself is linear. This scaling process is also applied when the material regains its linear elastic response, when the reverse transformation is exhausted, $f = 0$.

As already mentioned, loading increments are applied until the critical stress intensity $K^{TIP} = K^C$ is reached. Here the same loading scheme is used as is drawn in Fig. 4.8, although the steps 'do an iteration step' and 'convergence' are replaced by one step 'do a loading increment as pictured in Fig. 4.10'. The stress intensity at the crack tip $K^{TIP}$ is computed using (4-3) and the integral formulation (4-19). The area integration is carried out numerically over all transformed elements, however analytical integration around the crack tip is performed to take care of the singularity at the tip. This will be elaborated further in
the next section.

In the program ZIRCON, unwanted violation of the crack propagation condition is prevented by the use of (4-26). There the size of the load increments become smaller as the cracking condition is approached. Here, this algorithm has been substituted by an algorithm which is less time consuming. When, after a load increment $\Delta K^\text{APP}$, it is found that the critical stress intensity $K^C$ at the tip is exceeded, then the solution for the displacement is scaled back such that $K^\text{TIP} = K^C$, within a certain tolerance. Crack growth is simulated similar to the description in the previous section. For future reference, the program, containing the above described algorithms for the model of Sun et al. (1991), is called SHP MEM.

4.5.4 Discretization of the J-integral and surface integral concept

As both methods discussed in Secs. 4.4.1 and 4.4.2 are used in the finite element formulation, they are cast into a discrete form. First we will discuss the J-integral concept followed by the surface integral concept.

For the discrete formulation of the J-integral we formulate a discrete contour through the interpolation points of the triangular elements and sum the contributions of the general definition (4-8) for each triangular element on the contour, see also Parks (1974). For evaluation of (4-8) the expressions and (4-12) are used (finally the outcome is doubled as only half of the problem is investigated). To gain accuracy, the integral is applied for different contours and the final solution is determined by averaging. In the finite element code, the position of the contours is related to the coordinates of the crack tip. Thus, if the crack tip moves one node when the crack grows, also the contours are moved. From theoretical analysis we know that before any crack growth, the amount of transformed material behind the crack tip, the so-called 'wake', is limited. If the restriction on the position of the contours

![Fig. 4.11. Example of the contours for the J-integral.](image-url)
enforced in Sec. 4.4.1 must be considered ("the contour of the integral must be chosen such that all the material inside the contour is completely transformed"), then the contours must not end far behind the crack tip. On the other hand, the accuracy of the integral increases if the contours are positioned somewhat further away from the tip as in that case the number of elements per contour increases. These considerations lead to a contour positioning as depicted in Fig. 4.11. If in the analysis one element is found with \( f < f^m \), then the contour which includes that specific element is not used for the final solution. It must be noted that all contours cross the mid-nodes of the square elements so that per square element only 2 of the 4 triangular elements are used in the evaluation of the contour integral.

For the discrete formulation of the surface integral, (4.19) is replaced by a summation of the contributions of all transformed triangular elements. However, this leaves us with the problem of the determination of the contribution of each transformed triangular element as this is a surface integral itself. Using (4.13) and (4.19) we find that this contribution is given by

\[
dK_{\text{element}}^{\text{TIP}} = \iint_A -2\sqrt{2\pi E} \text{ Re} \left[ \frac{1}{z_0^{3/2}} \left( -c_1 + \frac{c_2}{z_0} \frac{-z_0 - 3z_0}{z_0} \right) \right] dA , \tag{4-30}\]

if \( A \) is the area of the subelement and \( z_0 = x + iy \) represents the distance to the crack tip. Note that the transformation strain is constant over the triangular element. With the introduction of the variables

\[
V = -\frac{1}{8} (4c_1 + c_2) \quad \text{and} \quad W = -\frac{3}{8} c_2 , \tag{4-31}\]

and when plane strain conditions are enforced, equation (4-30) can be rearranged to

\[
dK_{\text{element}}^{\text{TIP}} = -\frac{2\sqrt{2\pi E}}{1 - \nu^2} \left( \text{Re} \left\{ \iint_A z_0^{-3/2} dA \right\} + \text{Re} \left\{ W \iint_A z_0 z_0^{-5/2} dA \right\} \right) . \tag{4-32}\]

In case only dilatant transformation strains are taken into account, as is in the model of Budiansky et al. (1983), the last term in (4-32) cancels as in that case \( W = 0 \) and the integration becomes trivial. The general approach is given in Appendix C. The stress intensity at the crack tip, \( \Delta K^{\text{TIP}} \), is computed numerically on the basis of the integral formulation (4.19) and (4.30) by a 13-point Gaussian-integration within each element. Near the crack tip (within a radius of 3 elements or so) the integration is carried out analytically to take care of the singularity in (4.32).
CHAPTER 5

Results for homogeneous materials

5.1 Introduction

We investigate the crack growth behaviour for materials with a homogeneous distribution of transformable phase. A parameter study has been carried out to explore the influence of the strength of the transformation, the transformation hardening and, in particular, the contribution of transformation shear strains on the transformation behaviour and on the crack growth development. The results of the computations are presented in terms of predicted transformation zones and crack growth resistance curves. The results according to the adopted constitutive model show that the shear transformation strains have a significant influence on both the transformation zone and the increase in toughness. This chapter is based on Stam et al. (1993b), Stam and Van der Giessen (1994a), and Stam and Van der Giessen (1994b). Finally, results of calculations for supercritically transforming materials are presented. The parameter \( M \) defined in Sec. 3.3.4, has been chosen such that reverse transformation does not occur. The influence of reverse transformation is described separately in chapter 6.

5.2 Assignment of the parameter study

The crack growth problem defined in the previous chapter is characterized by the following parameters: \( K^{\text{APP}} \), \( \Delta a \), \( L \) (small-scale transformation problem), \( v \), \( \omega \), \( \alpha \), \( h_0 \) (deformation response of material) and \( K^C \) (fracture process). The numerical results of the computer program SHPMEM to be presented here will focus on the evolution of transformation zones and the toughness increase \( K^{\text{APP}}(\Delta a)/K^C \) during crack growth. It follows that these results can be expressed in terms of the following subset of these nondimensional parameters:
\[ \frac{K^{\text{APP}} \Delta a}{K^C} = \frac{\nu}{L}, \alpha, \omega, h_0. \]  

(5-1)

Of course, other combinations may be chosen, but this set turns out to be the most convenient. Note that this set of parameters is similar to that considered by Hom and McMeeking (1990) but augmented with the parameter \( h_0 \) relating the shear transformation strain to the constant lattice dilatation \( \varepsilon^{pd} \).

Throughout the analysis we take \( \nu = 0.3 \) in (5-1), but various combinations of the other parameters \( \omega, \alpha \) and \( h_0 \) are considered to study their effect on toughening as well as on the size and shape of the transformation zone. Proceeding from the parameter study by Hom and McMeeking (1990), the strength of the transformation is varied from \( \omega = 5, 10, 15 \) to 20. For each value of \( \omega \), the hardening parameter \( \alpha \) is chosen to be either 1 or 1.25. The smallest value of \( \alpha \) is chosen to be 1 to avoid localization over a wide range of material parameters, as discussed in detail in Sec. 3.4. The value \( \alpha = 1.25 \) has been chosen as a representative value to cover the experimental values of \( \alpha = 1.16 \) and 1.2 for TZP and PSZ, respectively, given by Sun et al. (1991). For each of the four combinations of these parameters, the influence of the transformation shear is varied by taking \( h_0 = 0, 0.5, 1.0, \) or 1.5, which covers the experimental values given by Sun et al. (1991) for various materials and includes the limit of pure dilatant transformations for comparison. For \( \omega = 15 \) and 20 extra computations have been performed with \( h_0 = 1.25 \). It would have been interesting to perform computations for larger values of \( \omega \), but the number of variations was limited due to time considerations: a typical crack growth computation up to a steady state situation required about 100 CPU hours on a SUN Sparc station 1.

\begin{figure}[h]
\centering
\includegraphics[width=0.8\textwidth]{fig5_1.png}
\caption{The composition of the parameter study.}
\end{figure}

The lower bound of \( h_0 = 0 \) corresponds to a situation where twinning completely eliminates the average shear transformation. In this case the transformation is purely dilatant and the results agree well with those of Hom and McMeeking (1990). Noting that these authors used a quite different, iterative rather than an incremental scheme, this agreement gave us confidence in the numerical procedure.

To check the convergence of the solution, some computations with refined meshes have been performed. In this small-scale problem, mesh refinement can be obtained simply by increasing the characteristic length \( L \) with respect to the dimensions of the smallest element, while leaving all other parameters unchanged. In this way the transformation zone will contain more elements and more accurate results should be obtained, as long as the small scale condition is not violated.
5.3 Transformation zones

5.3.1 Some remarks about the shear component of the transformation

First of all, it is instructive to comment on the way in which the intensity of the transformation shear strains is related to the dilatation $\varepsilon^{pd}$. It must be realized that the amount of shear transformation strains is coupled directly to the amount of dilatant transformation. For example, a convenient parameter to characterize the rate of change of the amount of transformation shear strains in the composite material would be

$$
\dot{E}_c^{ps} = \frac{2}{3} \text{tr} \dot{E}_c^{ps} = 2f h_0 \varepsilon^{pd}, \quad (5-2)
$$

where we have substituted the expressions (3-19) and (3-20) to eliminate $\dot{E}_c^{ps}$. This can be integrated immediately during the deformation process to find that

$$
E_c^{ps} = 2f h_0 \varepsilon^{pd}, \quad (5-3)
$$

showing that the intensity of the transformation strain depends only on the volume fraction $f$. For a certain value of $\varepsilon^{pd}$, the factor $2h_0 \varepsilon^{pd}$ is a constant and thus depends only on the choice of $h_0$. The maximum value of $h_0$ should correspond to a material in which no twinning occurs. As already mentioned, the stress-free lattice shear strain in ZrO$_2$ is 16%, so that with $\varepsilon^{pd} = 1.5\%$ and (3-19) it follows that $h_0^{max} = 3.08$.

5.3.2 Some remarks about the contour line representation

Since for all chosen material parameters the material behaviour is subcritical (see Sec. 3.4), the transformation varies continuously around the crack tip. In this case, a convenient way to visualize the transformation zones is to plot the distribution of transformed material by means of contours of constant value of the ratio of the transformed fraction compared to the maximum available transformable fraction, $f/f^m$. No attempt has been made to smooth the contours so that, in particular when the transformation zone grows outside the highly refined zone around the crack path, the contours may come out somewhat irregular. The transformation zones for the eight combinations of \( \alpha \) and \( \omega \) considered are shown in Fig. 5.2 to Fig. 5.9 for various values of $h_0$. In these plots, the elements in which the material is completely transformed ($f/f^m = 1$) are also shown. For the subsequent discussion it is convenient to follow experimental practice and define the height of the transformation zone $h$ as the distance in $x_2$-direction from the crack surface to the point where the fraction of transformed material is 50% ($f/f^m = 0.5$) (see also Fig. 5.2d).

5.3.3 General description of the subcritical transformation zone

In all cases shown in Figs. 5.2 to 5.9, we see that the area around the crack path is fully
transformed. Moving further into the material, perpendicular to the crack surface in the \( x_2 \)-direction, the fully transformed zone is followed by a region of partially transformed material and finally the untransformed material is reached. In general, the zone height increases as the crack grows. From a mechanical point of view, this can be explained by noting that the transformation-plasticity shields the crack tip, so that \( K_{\text{APP}} \) must be increased to maintain the critical stress intensity at the crack tip, as mentioned before. Increasing the value of \( K_{\text{APP}} \) raises the stresses in the elastic field and thus enlarges the region where the critical transformation stress is reached. After some crack growth, however, the initial sharp increase becomes more gradual due to stress re-distributions and the zone height reaches a maximum. In the present analyses the cracks could only grow over a limited distance and in some cases — particularly for larger values of \( h_0 \) — the maximum value has not yet been attained. In all cases where a steady-state is reached, the steady-state zone height is found to be slightly smaller than the maximum height. This agrees with earlier findings by Hom and McMeeking (1990). In Table 5.1, the value of the peak height \( h \) of the transformation zone, together with the value \( \Delta a/L \) when this peak occurs, is given.

### Table 5.1. Peak values of transformation zone height and fracture toughness.

<table>
<thead>
<tr>
<th>( \omega )</th>
<th>( \alpha )</th>
<th>1.00</th>
<th>1.00</th>
<th>1.00</th>
<th>1.00</th>
<th>1.00</th>
<th>1.25</th>
<th>1.25</th>
<th>1.25</th>
<th>1.25</th>
<th>1.25</th>
</tr>
</thead>
<tbody>
<tr>
<td>( h_0 )</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>( \omega = 5 )</td>
<td>peak ( h/L )</td>
<td>0.45</td>
<td>0.78</td>
<td>&gt;0.96</td>
<td>0.79</td>
<td>0.37</td>
<td>&gt;0.64</td>
<td>&gt;0.75</td>
<td>0.70</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>occurring at ( \Delta a/L )</td>
<td>1.15</td>
<td>3.74</td>
<td>&gt;5.81</td>
<td>3.74</td>
<td>1.00</td>
<td>&gt;4.98</td>
<td>&gt;5.81</td>
<td>1.71</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>peak ( K_{\text{APP}}/K_{\text{TIP}} )</td>
<td>1.19</td>
<td>&gt;1.35</td>
<td>&gt;1.46</td>
<td>&gt;1.89</td>
<td>1.18</td>
<td>&gt;1.33</td>
<td>&gt;1.49</td>
<td>1.74</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>occurring at ( \Delta a/L )</td>
<td>2.98</td>
<td>&gt;4.98</td>
<td>&gt;5.81</td>
<td>&gt;6.50</td>
<td>2.84</td>
<td>&gt;4.98</td>
<td>&gt;5.81</td>
<td>3.04</td>
<td></td>
<td></td>
</tr>
<tr>
<td>( \omega = 10 )</td>
<td>peak ( h/L )</td>
<td>0.33</td>
<td>0.69</td>
<td>0.78</td>
<td>1.38</td>
<td>0.23</td>
<td>0.46</td>
<td>0.51</td>
<td>0.34</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>occurring at ( \Delta a/L )</td>
<td>1.00</td>
<td>4.98</td>
<td>&gt;5.81</td>
<td>5.87</td>
<td>0.70</td>
<td>2.99</td>
<td>&gt;5.81</td>
<td>0.57</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>peak ( K_{\text{APP}}/K_{\text{TIP}} )</td>
<td>1.35</td>
<td>&gt;1.63</td>
<td>&gt;1.72</td>
<td>&gt;2.86</td>
<td>1.31</td>
<td>&gt;1.57</td>
<td>1.79</td>
<td>2.12</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>occurring at ( \Delta a/L )</td>
<td>2.75</td>
<td>&gt;4.98</td>
<td>&gt;5.81</td>
<td>&gt;6.50</td>
<td>2.54</td>
<td>&gt;4.98</td>
<td>&gt;5.81</td>
<td>4.63</td>
<td></td>
<td></td>
</tr>
<tr>
<td>( \omega = 15 )</td>
<td>peak ( h/L )</td>
<td>0.32</td>
<td>0.60</td>
<td>0.63</td>
<td>1.03</td>
<td>1.75</td>
<td>0.17</td>
<td>0.38</td>
<td>0.32</td>
<td>0.32</td>
<td>0.17</td>
</tr>
<tr>
<td></td>
<td>occurring at ( \Delta a/L )</td>
<td>0.63</td>
<td>4.2</td>
<td>10.5</td>
<td>8.2</td>
<td>2.63</td>
<td>0.68</td>
<td>2.87</td>
<td>5.11</td>
<td>6.13</td>
<td>2.2</td>
</tr>
<tr>
<td></td>
<td>peak ( K_{\text{APP}}/K_{\text{TIP}} )</td>
<td>1.48</td>
<td>1.87</td>
<td>1.94</td>
<td>2.64</td>
<td>3.88</td>
<td>1.38</td>
<td>1.76</td>
<td>1.95</td>
<td>2.15</td>
<td>2.2</td>
</tr>
<tr>
<td></td>
<td>occurring at ( \Delta a/L )</td>
<td>2.4</td>
<td>7.6</td>
<td>&gt;10.6</td>
<td>&gt;10.6</td>
<td>&gt;10.6</td>
<td>1.83</td>
<td>6.1</td>
<td>&gt;10</td>
<td>&gt;10</td>
<td>6.33</td>
</tr>
<tr>
<td>( \omega = 20 )</td>
<td>peak ( h/L )</td>
<td>0.23</td>
<td>0.52</td>
<td>0.51</td>
<td>0.95</td>
<td>1.79</td>
<td>0.16</td>
<td>0.32</td>
<td>0.29</td>
<td>0.17</td>
<td>0.14</td>
</tr>
<tr>
<td></td>
<td>occurring at ( \Delta a/L )</td>
<td>0.63</td>
<td>4.79</td>
<td>9.11</td>
<td>7.43</td>
<td>2.32</td>
<td>0.56</td>
<td>2.63</td>
<td>8.63</td>
<td>8.0</td>
<td>0.0</td>
</tr>
<tr>
<td></td>
<td>peak ( K_{\text{APP}}/K_{\text{TIP}} )</td>
<td>1.55</td>
<td>2.10</td>
<td>2.03</td>
<td>3.10</td>
<td>3.52</td>
<td>1.38</td>
<td>1.91</td>
<td>2.15</td>
<td>2.22</td>
<td>2.2</td>
</tr>
<tr>
<td></td>
<td>occurring at ( \Delta a/L )</td>
<td>2.7</td>
<td>&gt;10.6</td>
<td>&gt;10.6</td>
<td>&gt;10.6</td>
<td>&gt;10.6</td>
<td>1.76</td>
<td>7.5</td>
<td>&gt;10</td>
<td>&gt;10</td>
<td>5.74</td>
</tr>
</tbody>
</table>

5.3.4 Detailed discussion of the results for the transformation zones

Examination of the results reveals that, in general, the shape and the size of the transformation zones is strongly influenced by whether or not the transformation is near-critical. As
discussed in Sec. 3.4, this depends on the hardening parameter $\alpha$, the influence of the shear transformation $h_0$ and the deformation history. In Fig. 5.2 for instance, where $\omega = 5$ and $\alpha = 1$, we observe that contours of $f/f^m$ approach each other for $h_0 = 0.5$ and for $h_0 = 1.0$, as compared to the dilatant case ($h_0 = 0$). This is indicative of near-critical behaviour, and can be explained to a certain extent by consideration of Fig. 3.4. Knowing from the finite element analyses that in the range $0.5 \leq h_0 \leq 1.0$, the ratio $\rho = \Delta E_{22}/\Delta E_{11}$ of strain increments in the region where transformation takes place is in the interval $[-0.3, 0.3]$, we see that a value $\alpha \geq 1$ is really needed around $h_0 = 1.0$ to prevent localization, and therefore supercritical behaviour. For $h_0 = 1.5$, the situation is less critical since for this case a hardening of $\alpha = 1$ is only needed for values of $\rho < -0.1$, whereas inside the transformation area, the parameter $\rho$ is found to vary between 0 and 0.6. This results in a much more gradual transition from fully transformed to untransformed material for $h_0 = 1.5$.

As for the frontal regions of the transformation zones shown in Figs. 5.2 to 5.9, we see that the zones enlarge in the $x_1$-direction with increasing value of $h_0$, and also that the transformation zone shapes change rather drastically. When the hardening is increased from a value $\alpha = 1$ to $\alpha = 1.25$, as shown in Fig. 5.3, we observe that for all $h_0$, the transition from fully transformed to untransformed material remains smooth, indicating that the transformation behaviour does not approach the critical regime. In this case, increasing the value of $h_0$ results in transformation zones that are more diffuse and that have larger frontal zones. When the strength of the transformation is increased to $\omega = 10$, as shown in Fig. 5.4 and Fig. 5.5, similar trends are observed. In general, however, for increasing values of $\omega$ the transformation behaviour appears to be less critical, which is probably caused by a larger redistribution of stresses due to the transformation.

The influence of $\alpha$ is quite remarkable. For example, for $\alpha = 1$ the transformation zones for $h_0 > 1.0$ tend to be very large. Especially in the case $h_0 = 1.5$ the transformation zones have a quite different shape, as shown Fig. 5.2d, Fig. 5.4d, Fig. 5.6e and Fig. 5.8e. We have tried to verify whether this is caused by numerical inaccuracy or whether this is a real phenomenon of the model. We found that the small scale assumptions were not violated, and neither reducing the step size during loading nor increasing the number of steps for the nodal release technique made any significant change in the results. Using a coarser mesh, the pronounced variation in height of the transformation zones in the early stages of growth was still found, although the waviness at later stages was somewhat diminished. Concerning the mesh we feel that the transition from the very refined area in the mesh to the much less refined area further out might have some influence, but we have not been able to quantify this. The variation in height is likely a real phenomenon of the model.

A second interesting result for $\alpha = 1.25$ is that for increasing influence of the shear component of the transformation ($h_0$), the area which is fully transformed reduces and even vanishes for $\omega > 10$ and $h_0 = 1.5$. In that case, less than 75% of the maximum transformation strain is found immediately next to the crack surface. In these cases the resolution of the mesh was simply too crude; in the material itself the minimum height of a fully transformed area that is physically possible is equal to the size of the transformable grain.

Concerning the possible occurrence of localization we note that in none of the computations any localization phenomena were found. The assumption that $\alpha \geq 1$ would prevent localization proved to be correct. We must note, however, that in our computations $\alpha = 1.0001$ is actually taken to prevent singularity problems in (3.53). The numerical ex-
Fig. 5.2. Transformation zones (a to d) when $\Delta a = 4L, 4.98L, 5.81L$ and $6.50L$ respectively, and the crack growth resistance curve (e) for the case $\omega = 5$ and $\alpha = 1$ with various values of $h_0$. 
Fig. 5.3. Transformation zones (a to d) when Δa = 4L, 4.98L, 5.81L and 6.50L respectively, and the crack growth resistance curve for the case ω = 5 and α = 1.25 with various values of h₀.
Fig. 5.4. Transformation zones (a to d) when Δa = 4L, 4.98L, 5.81L and 6.50L respectively, and the crack growth resistance curve (e) for the case ω = 10 and α = 1 with various values of h₀.
Fig. 5.5. Transformation zones (a to d) when $\Delta a = 4L, 4.98L, 5.81L$ and $6.50L$ respectively, and the crack growth resistance curve (e) for the case $\omega = 10$ and $\alpha = 1.25$ with various values of $h_0$. 


Fig. 5.6. Transformation zones and crack growth resistance curves (f) for $v = 0.3$, $\omega = 15$, $\alpha = 1.00$ and $0.0 \leq h_0 \leq 1.5$. Crack growth was permitted over a distance $\Delta a = 10L$ for $h_0 = 1.5$ and $10.6L$ otherwise.
Fig. 5.7. Transformation zones and crack growth resistance curves (f) for $v = 0.3$, $\omega = 15$, $\alpha = 1.25$ and $0.0 \leq h_0 \leq 1.5$. Crack growth was permitted over a distance $\Delta a = 10L$. 
Fig. 5.8. Transformation zones and crack growth resistance curves (f) for $\nu = 0.3$, $\omega = 20$, $\alpha = 1.00$ and $0.0 \leq h_0 \leq 1.5$. Crack growth was permitted over a distance $\Delta a = 10.6L$ for $h_0 = 0.0, 0.5$ and $1.25$; for $h_0 = 1.0$ and $1.5$, $\Delta a/L = 10L$. 
Fig. 5.9. Transformation zones and crack growth resistance curve (e) for $\nu = 0.3$, $\omega = 20$, $\alpha = 1.25$ and $0.0 \leq h_0 \leq 1.5$. Crack growth was permitted over a distance $\Delta a = 10L$. 

71
Fig. 5.10. Crack tip opening for various amounts of crack growth, $\Delta a = 0, 1.6L, 3.25L, 4.88L$ and $6.50L$. At $\Delta a = 6.50L$ the deformed mesh is drawn and contours for $f/f^m$ are shown. The deformations are scaled by a factor 12.3.

periments closest to supercritical behaviour are those where $\alpha = 1.00$ and $h_0 = 1.0$ in Fig. 5.2. For $\omega = 10, 15$ and $20$ we can see that, especially in the region $0 \leq \Delta a/L \leq 2$, there is a sharp transition from fully transformed to untransformed material. Here at least some partially transformed material is present as ellipticity of the governing equations was not lost. It is remarkable to see that the frontal parts of the transformation zones enlarge in the $x_1$-direction with increasing $h_0$. Especially when we compare the height (in the $x_2$-direction) to the length of the frontal zone, the above mentioned near-critical cases show a very large frontal zone, which is certainly not semi-spherical as most other frontal zones are. It would be interesting to investigate the frontal zone in supercritically transforming materials. Perhaps this could explain the type of behaviour seen in some kinds of TZP material where Yu and Shetty (1990) report shear bands together with very large frontal zones.

As an illustrative example, the crack tip opening at various stages of crack growth is depicted in Fig. 5.10 for the parameters $\omega = 10$, $\alpha = 1$ and $h_0 = 1.5$. For illustrative purposes, the crack opening displacements are reflected (and scaled by a factor 12.3) to show the actual crack shape. In the first stage (I), shown in Fig. 5.10, no crack growth has occurred yet but some crack tip blunting has occurred. We see that as the crack propagates, the crack faces are pushed towards another due to the phase transformation. In the final stage V also the deformed mesh is drawn, along with contours of $f/f^m$.

5.3.5 Possibility of the formation of shear bands

As there is some experimental evidence of shear bands in PSZ and TZP materials (Chen and Reyes-Morel, 1986; Reyes-Morel and Chen, 1988), any information about the
Fig. 5.11. Direction of the maximum transformation shear strains for the case $\omega = 10$ and $\alpha = 1$; (a) $h_0 = 0.5$, $\Delta a = 4.98L$, (b) $h_0 = 1$, $\Delta a = 5.81L$ and (c) $h_0 = 1.5$, $\Delta a = 6.5L$.  

direction in which these bands are most likely to develop is of interest. It should be recalled that we have chosen our material parameters such as to a priori exclude the possibility of localization into, for instance, a shear band with the constitutive model of Sec. 3.3. A study concerning the occurrence of localization, which may appear as shear bands, is dealt with in Sec. 3.4. Here we will try to gain some insight in the directions into which the transformation shear is most pronounced. Therefore, we have computed the directions of the 'octahedral' planes at which the transformation shear strains reach maximum values. For the case $\omega = 10$ and $\alpha = 1.0$, the direction of the transformation shear strain is visualized in Fig. 5.11 by way of the orientation of crosses; the size of the crosses indicates the value of the maximum transformation shear strain. This figure suggests that there is a tendency that increasing the value of $h_0$ causes a change in the shear directions close to the crack surface from $\pm 45^\circ$ towards around $60^\circ/30^\circ$. Moreover, for $h_0 = 1.5$ it is remarkable that initially the transformation shear strains develop in a well-defined direction of $-60^\circ/30^\circ$, while after some crack growth, the value of the maximum shear near the crack surface decreases. For $h_0 = 0.5$ and 1.0, the value of the maximum transformation shear strain remains more or
less constant during crack advance. These analyses have been repeated with $\alpha = 1.25$ and/or $\omega = 5$, but these trends did not change significantly and the results will not be shown here.

5.4 Toughness development

Prior to any crack growth we find that for $h_0 = 0$ the initial toughness is not changed by the transformation strains. This is in agreement with the proof of Budiansky et al. (1983) who stated that prior to any crack growth it is reasonable to assume that no unloading occurs anywhere in the material. All requirements for the $J$-integral to be path independent have been obeyed, which means the initial transformation zone does not influence the toughness at the crack tip (cf. Sec. 4.2). For $h_0 > 0$ the deformation behaviour becomes history dependent, so that if the loading of the material is non-proportional the $J$-integral is no longer path independent and in this case the initial transformation zone may give rise to a toughening increment. From the numerical results for $h_0 > 0$ presented here, it may seem that the initial toughness is increased. However, when the mesh is further refined a decreasing initial toughness value is found, which finally converges to a value of about 80% of the critical toughness of the material when the mesh size is reduced by a factor of about 10.

Thus, prior to any crack growth, embrittling of the material seems to takes place, but after the slightest crack extension the toughness increases drastically and picks up with the values shown in Fig. 5.2 to Fig. 5.9. Similar convergence checks were performed after crack growth had occurred, and showed that the fineness of the mesh could be reduced to the currently used meshes to obtain accurate results for crack growth analysis.

The toughness increase, expressed in terms of $K_{\text{APP}} / K_{\text{TIP}}$, as a function of crack advance $\Delta a/L$ for each of the cases mentioned above is shown in Fig. 5.2e to Fig. 5.5e and Fig. 5.6f to Fig. 5.9f. As already observed for purely dilatant materials by Hom and McMeeking (1990), the crack growth resistance tends to increase during the first stage of crack growth, then reaches a maximum, followed by a slight decrease before it settles down at the stationary value for steady-state growth. From these figures, as well as from Table 5.1, we may note that, similar to the development of the transformation zone height, the maximum value for toughening has not yet been reached in some cases. For these cases further crack growth would be necessary.

Evidently, the effect of transformation-induced shear strains on the crack growth resistance is of central importance. It is clearly seen in Fig. 5.2 to Fig. 5.9 that for all values of $\omega$ and $\alpha$ considered, the toughness is increased significantly with increasing value of $h_0$. Even a relatively small contribution of transformation shear strains, represented by $h_0 = 0.5$, roughly doubles the toughness increase that is obtained when the transformation would be purely dilatant ($h_0 = 0$). Larger values of $h_0$ result in an even higher toughness increase, but the enhancement depends on the values of $\omega$ and $\alpha$. There does not appear to be a clear relationship though between the value of $h_0$ and the crack advances at maximum crack growth resistance. As in the purely dilatant case, the toughness increases with the strength of the transformation as characterized by $\omega$. We can also see that the peak as well as the steady-state values of the toughness generally increase with decreasing value of $\alpha$, irrespective of $h_0$. The lower the hardening parameter $\alpha$, the more material is fully transformed and the higher the toughness increase.
5.5 Comparison to experiments

Several experimental studies of the shape and the size of the transformation zone are available in the literature [see e.g. Marshall et al. (1990), Rühl and Evans (1989), and Yu and Shetty (1990)]. Depending on the material, the results indicate various kinds of transformation zone shapes. The front of the zone found by Marshall et al. (1990), seems to be similar to the rounded shape found for a purely dilatant material, while Rühl and Evans (1989), for ZTA materials, indicate a zone shape that has the same characteristics as found here for sufficiently large values of $h_0$. We emphasize, however, that completely different experimental techniques for visualization of the transformation zone have been used in the above references. Therefore it is not straightforward to relate directly those experimental observations to the transformation zones shown in Figs. 5.2 to 5.9 in terms of transformed volume fraction.

Before any further comparison is made between the transformation zones, we must note that the length scale parameter $L$ depends on the value of $h_0$, so that the crack has actually grown over different distances for the same value of $\Delta a/L$. If we take the material parameters for the TZP material, as discussed in the previous sections, $\nu = 0.3$, $\omega = 23$, $\alpha = 1.16$, $h_0 = 1.4$, and $K^C = 3\text{MPa} \sqrt{\text{m}}$, (from Yu and Shetty, 1990), the reference length is found as $L = 4.8\mu\text{m}$. When extrapolation is used, we may read from Fig. 5.8 that the maximum toughness will be about $12\text{MPa} \sqrt{\text{m}}$ (compared to the experimentally found value of $\sim 14\text{MPa} \sqrt{\text{m}}$), which is achieved after about $10L$. In this case the crack advance would be $48\mu\text{m}$. In the above mentioned papers [by McMeeking and Evans (1989), Hom and McMeeking (1990), Yu and Shetty (1990)] as well as in many other papers, it is found that in the experiment the resistance curve is much less steep than the toughness development curves which have been presented here. For instance, Yu and Shetty (1990) report that the maximum toughness is achieved after about $1\text{mm}$, which points to one order difference. However 80% of the toughness increase is achieved after only $0.1\text{mm}$. Yu et al. mention that a significant amount of toughness increment is associated without a significant increase in the crack length. Any definitive conclusion to the origin of this discrepancy will have to await a more detailed comparison with experiments for specific materials.

5.6 Supercritical transformations

In the previous sections we have considered subcritically transforming composites. In this section we shall derive an expression which can give a first estimate of the steady state toughness increase for supercritically transforming materials, i.e. $\alpha = 0$. Proceeding along similar lines as Budiansky et al. (1983) did for dilatant transformations, the analysis will lead to an asymptotic result for sufficiently small $\varepsilon^d$.

For sufficiently small $\varepsilon^d$, the transformation has a negligible effect on the near-tip stress field so that the size and shape of the transformation zone can be found from the elastic solution. In this case the transformation condition (3-66) can be rewritten as (3-70)

$$\Sigma^C = \frac{2}{3} h_0 \Sigma_e + \Sigma_m$$

(5-4)

and by substituting the solution for the elastic stresses (2-6) into (3-70), it follows that the
radius were the critical stress $\Sigma^C$ is attained, is given by

$$R(\beta) = \frac{2}{9\pi} \left( \frac{K_{\text{app}}}{\Sigma^C} \right)^2 \cos^2 \frac{\beta}{2} \left[ h_0 P(\beta) + (1 + \nu) \right]^2,$$

(5-5)

where

$$P(\beta) = \sqrt{(1 - 2\nu)^2 + 3\sin^2 \frac{\beta}{2}}.$$

(5-6)

This equation gives the shape of the initial transformation zone as shown in Fig. 5.12. The length parameter $L$ introduced in Sec. 4.3 is recognized to be equal to $R(0)$.

Loading occurs in the forward part of the transformation zone. If the crack advances, the material in the wake of the crack unloads, and no further transformation occurs. Therefore, the transformation strains in the wake are independent of $x_1$. The wake boundary $(x_2 = H)$ merges with the leading zone at the point where the maximum height of the initial zone is reached. The angle $\beta_{\text{max}}$ at which the height is maximal can be found from (5-5) by means of a straightforward numerical analysis. This angle has been computed for different values of $\nu$ and $h_0$, and the numerical results can be fitted by the following expression to within an error smaller than 0.2%:

$$\beta_{\text{max}} = \frac{\pi}{3} + (0.206 + 0.381\nu - 0.349\nu^2) \text{atan} \left[ \frac{(1.79 - 1.46\nu + 1.09\nu^2)}{h_0} \right].$$

(5-7)

Thus, the upper half of the transformation zone at steady state conditions can be written as (5-5) when $0 \leq \beta \leq \beta_{\text{max}}$ and as $R(\beta) = H / \sin \beta$ for $\beta_{\text{max}} \leq \beta \leq \pi$, where the zone height is given through $H = R(\beta_{\text{max}}) \sin \beta_{\text{max}}$. Of course, for supercritically transforming material $f = f_{\text{max}}$ everywhere in the loading zone and in the wake. The dilatant transformation strains are immediately found by $E_{ij}^{\text{pd}} = f_{\text{max}}^\nu \epsilon_{ij}^\nu$, but the sense of the transformation shear depends on the current stress distribution. However, recall that for $\epsilon_{ij}^{\text{pd}} \to 0$ the elastic

---

![Fig. 5.12. Steady state transformation zone for $\epsilon_{ij}^{\text{pd}} \to 0$.](image-url)
stress distribution still holds and it follows that the shear transformation strain is given by $E_{ij}^{ps} = \int_{\Sigma_e}^{\text{max}} AS_{ij} \Sigma_e$. For the evaluation of $\Delta K^{\text{TIP}}$, the integral in (4-15) must be taken over the transformation zone as described in section 4.5.2. The integration has been carried out numerically. In computing the contribution of the wake, the transformation shear strains are calculated for $\beta = \beta_{\text{max}}$ since no further transformation occurs in the wake. Curve fitting was used to find the following asymptotic ($\varepsilon^{\text{end}} \rightarrow 0$) expression for the toughness increase (4-19) within an error $< 1\%$:

$$\Delta K^{\text{TIP}} = [-0.214-c_1(v)h_0-c_2(v)h_0^2] \frac{3E^{\text{end}}\varepsilon^{\text{end}}H}{1-v} \sqrt[4]{H}, \quad 0 \leq v < 0.5 \quad (5-8)$$

By eliminating $H$ and substituting the expression for $\omega$ from (3-71), one can also write

$$\frac{K^{\text{TIP}}}{K^{\text{APP}}} = 1 - \omega [0.214 + c_1(v)h_0 + c_2(v)h_0^2] \cos \frac{\beta_{\text{max}}}{2} \left[ \frac{h_0 \beta_{\text{max}}}{1 + \omega} + 1 \right] \frac{2 \sin \beta_{\text{max}}}{9\pi}$$

where

\begin{align*}
    c_1(v) &= 0.537 - 1.12v + 147.8v^{0.94} \\
    c_2(v) &= 0.007 + 0.0261v + 0.0493v^2 - 36.33v^{10.44}
\end{align*}

(5-9)

The two higher order terms in $v$ in (5-9) are necessary to describe the behaviour for $v \geq 0.4$ properly. For $h_0 = 0$, the expression (5-9) reduces to the one derived by Budiansky et al. (1983). We must note that $\omega$ is restricted to small values as it is assumed that $\varepsilon^{\text{end}} \rightarrow 0$. We found that for values of $\omega < 0.1$, the above asymptotic results agree well with the finite element results in which the history and redistribution of stresses is of course taken into account. For values of $\omega > 1$, the asymptotic results disagree considerably. Already prior to crack growth the size and shape of the transformation zones differ and the estimate of the steady state transformation zone and the steady state toughness Eq. (5-9) cannot be applied.

We must conclude that the differences between subcritical and supercritical behaviour in the presence of transformation shear strains are larger than in the case of the dilatant model. Experiments (e.g., Chen and Reyes-Morel, 1986, 1987) show that the material behaviour is clearly subcritical so that, in view of the dramatic differences between subcritical and supercritical results, further theoretical work on supercritically transforming ceramics seems to bear no relevance.

### 5.7 Conclusions

In this chapter, we have presented numerical studies of transient crack growth in ceramic composites exhibiting transformation-plasticity based on the recent model of Sun et al. (1991) that includes the effect of transformation-induced dilatation as well as shear. Our analyses supplement those of Hom and McMeeking (1990) who considered only dilatational transformations. The finite element results obtained here with the Sun et al. (1991) model show a very significant influence of the transformation shear strains on the transformation zone size and shape, as well as on the toughness development during crack growth. An increasing influence of the shear effect, as governed in the model by the parameter $h_0$, roughly speaking, leads to larger and more diffuse transformation zones. The increase of
toughness with increasing value of $h_0$ has been found to be quite substantial as compared with the toughness increase that is obtained by purely dilatational transformation only. For values of $h_0$ between 1 and 1.5, which are representative for $\text{ZrO}_2$ composites, we have found increases in toughness that are 4 to 8 times larger than without transformation-induced shear strains. Since, so far, dilatant transformation-based theory has underestimated the toughness enhancement found in experiments (Evans and Cannon, 1986), the present results with transformation-induced shear effects contribute to explaining this difference. However, any definitive conclusions to that effect will have to await a more detailed comparison with experiments on specific materials.

The predictions presented here have been obtained with values of the hardening parameter $\alpha$ that are representative for the experimental values suggested by Sun et al. (1991). Smaller values of $\alpha$ would probably have given even stronger toughening, with the limit being set by the occurrence of a supercritical response. We emphasize that for the values of $\alpha$ used in the present study, localization analysis has indicated that the behaviour will be subcritical for all deformation paths, and indeed in our crack growth computations we have not experienced any sign of loss of ellipticity.

It is pertinent here to relate the present work to the first analysis of transformation shear effects by Lambropoulos (1986). There are a number of differences with the constitutive model that he applied as well as his analysis of the small-scale transformation problem. Regarding the constitutive model, we have to refer to the original paper of Sun et al. (1991) for details, but we mention two of the most important differences with the model of Sun et al. used here. First and foremost, Lambropoulos assumed that the $t \rightarrow m$ transformation occurs at the same moment for all transformable particles and proceeds to completion at once; this is similar to what Budiansky et al. (1983) called supercritical behaviour. As mentioned before, here we focused primarily on subcritical behaviour as this was suggested by experiments. We have found that with increasing contributions of transformation-induced shear strains, there is a tendency to develop rather large and diffuse transformation zones; clearly, this does not support Lambropoulos’ assumptions. Secondly, in Lambropoulos’ model the particle is assumed to be incapable of supporting any shear load at transformation, whereas here the stresses inside transformed particles are related to the matrix stress state through an Eshelby type of approach, which is likely to give a more accurate representation. Finally, Lambropoulos assumes that the level of transformation within the transformation zone is small enough so that an asymptotic analysis can be used in which the stress state as the boundary of the transformation zone is approached from outside, is approximately the same as the unperturbed elastic solution. Here, on macro scale, full account is given of the effect of transformation-plasticity on the near-field stress fields.

Supplementary to the above described study, Stam and Van der Giessen (1994b) have studied crack growth in materials where the hardening parameter was chosen as $\alpha = 1$ corresponding to (at least near-) supercritical behaviour, and found that only for very low strengths of the transformation, for instance $\omega < 0.1$, an asymptotic analysis gives reasonable agreement with the numerical results. The results of this study have also been presented in Sec. 5.6 of this thesis.

In relating studies like the present one with real polycrystalline ceramic materials, it should be kept in mind that we have applied a continuum mechanics approach here. As put forward by Lambropoulos (1986) and others, the validity of the continuum approach may be questionable in some cases when the transformation zone height only spans a few grains.
According to data given by Budiansky et al. (1983), the height of the transformation zone for a typical PSZ material is 0.6μm. With a typical size of 0.3μm for the transformable penny-shaped particles, it follows that the number of particles over the height is only about two. For a TZP material described by Reyes-Morel and Chen (1988), it was found that the height of the transformation zone varies between 0.1 and 1mm. Thus, with a typical grain size of 2μm it follows that the transformation zone spans many (50 to 500) particles, from which we may conclude that for the latter material the continuum approach may be valid. For PSZ’s, however, further detailed analysis of t → m transformations in individual particles would be necessary to quantify the minimum number of grains over the transformation height for which the continuum model is still valid. Also, we want to emphasize that the results presented here are only valid for small scale transformations, and the model predictions cannot be applied when the transformation zone is spread out widely throughout the test specimen.

In the present work we have limited our parameter study to values of the strength of the transformation up to ω = 20. However, experimental work on TZP materials by e.g. Reyes-Morel et al. (1988) indicates that the values of ω may be somewhat higher.

Further, we have excluded from our analyses the possibility of reverse transformations. However, some authors have reported reversible transformation, e.g. Marshall and James (1986). The constitutive model used here is potentially capable of describing these phenomena, and it is not unlikely that reversible transformation does occur in places where unloading takes place as a result of for instance crack growth. Work in this direction has been performed and is presented in the next chapter.
CHAPTER 6

Analysis of the effect of reversible transformation

6.1 Introduction

In the crack growth computations of chapter 5 we have assumed that the $t \rightarrow m$ transformation was not reversible. Physically, however, there is no reason why transformation from the monoclinic to the tetragonal phase ($m \rightarrow t$) cannot occur. The martensitic transformation behaviour in this ceramic material is very similar to the martensitic transformation in Shape Memory Alloys (SMA). In these metal alloys (e.g. Cu-Zn-Sn or Cu-Zn-Al) the martensitic transformation between the austenite and the martensite allows the produced plastic deformation to be reversibly recovered upon heating. The transformation can be induced by the application of stress as well as by changes in temperature, as the free enthalpy of the matrix and product phase and thus their equilibria depend on both. A very clear description of the thermoelastic, pseudoelastic and shape memory effects associated with the martensitic transformation of these materials is given in the reviews by Delaey et al. (1974), Krishnan et al. (1974) and Warlimont et al. (1974). Current interest in these materials triggered further research on a practical level, see for example Otsuka and Shimizu (1986), but also on a very fundamental level, see Patoor et al. (1987).

Although the $t \rightarrow m$ transformation in ceramics was immediately recognized as being martensitic, it was not until a few years ago that both shear and dilatation transformation strains where measured in PSZ by Chen and Reyes-Morel (1986) and that pseudoelasticity and shape memory effects were determined experimentally in TZP by Reyes-Morel et al. (1988). Since these investigations, the non-linear deformation behaviour of these materials is often called transformation plasticity. Sun et al. (1991) proposed a constitutive model to describe these phenomena taking into account both dilatation and shear effects of the transformation. This model can also be used for shape memory materials. However, then the dilatant component of the transformation is zero, see Sun and Hwang (1993a and b). The
introduction of this model increased the understanding of the transformation behaviour of zirconia and it opened the discussion about reversible transformation, see Marshall and James (1986). Considering the derivation of the model we learn that during the transformation, energy is dissipated due to, among other things, lattice friction. This energy dissipation term \( W_t \) (as defined in (3-40)) is incorporated in the terms \( C_0(T,t) \) and \( \overline{C}_0(T,t) \), and causes the only difference in the conditions for forward and reverse transformation, as may be clear from (3-45). When the contribution of this term is small, reversible transformation upon unloading may occur. In section 3.3.4 we defined a non-dimensional parameter \( M = \overline{C}_0(T)/C_0(T) \) which expresses the amount of energy dissipation and it governs the behaviour upon unloading.

In the present chapter, we use this model to study crack growth in ZrO\(_2\)-containing ceramic materials for various values of \( M \). The results are obtained by a full field finite element analysis of the small scale transformation problem as defined in Sec. 4.2. The first results were presented in Stam and Van der Giessen (1993). In this chapter we present the results of an extensive parameter study in which the influence of reversibility of the transformation on both the size and shape of the transformation zone around the crack tip, as well as the toughness increase during crack growth is investigated. It is shown that in some cases the influence on the transformation zone can significantly reduce the increase in toughness.

6.2 Influence on the stress-strain relation

For four values of \( M \) the macroscopic uniaxial stress-strain relations (\( \Sigma_{11} \leftrightarrow E_{11} \)) are plotted in Fig. 6.1. The curves are obtained using the constitutive equations given by Sun et al. (1991), incrementally prescribing the stress in axial direction \( x_1 \), so that the specimen passes through a cycle of tension, compression and tension. For experimental work on this matter see also Bowman et al. (1987).

In all cases, the material behaviour is similar during the first tensile loading stage. The material behaves linear elastically up to the critical transformation stress \( \Sigma^C \), then the material starts to transform, up to the point where the material is fully transformed \( f = f^m \). After that the response is linear elastic again. When the specimen is unloaded, the differences in response as a result from the different choices of \( M \) arise.

As shown in Fig. 6.1a, for \( M = 1 \) the material will immediately show a reverse transformation response upon unloading when the stress level is reached where the forward transformation was completed. Obviously, reverse transformation is completed when all material is converted to the original crystal structure \( (f = 0) \) and the stress is equal to the critical (forward) transformation stress \( \Sigma_{11} = \Sigma^C \). Then the material response is linear elastic again, crosses the stress free point and is loaded in compression. The material behaviour is linear elastic up to the point where the critical forward transformation stress in the compression regime is reached. Forward transformation occurs up to completion \( f = f^m \), followed by linear elastic behaviour, similar to the behaviour in the tensile regime.

For \( M = 0 \), as can be seen in Fig. 6.1b, no direct reverse transformation upon unloading occurs, but all transformation strains are zero when the material is stress-free. This is true for the tensile regime as well as for the compression regime.

For \( M = -1 \), as can be seen in Fig. 6.1c, reverse transformation does not occur until
Fig. 6.1. Stress-strain relations for a uniaxial tension-compression-tension loading program for $h_0 = 1.0$, $\alpha = 1.25$ and $M = [1, 0, -1, -\infty]$.

the specimen reaches a certain stress level in the compression regime. Theoretically, the reverse transformation is completed when $f = 0$ and $\Sigma_{11} = -\Sigma^{C}$, however, in this uni-axially loading experiment it is not possible to convert all the transformation strain. Before all material has been transformed back, the transformation criterion is no longer met and the material becomes linear elastic again. Linear elasticity is maintained until the stress level for forward transformation in the compression regime is met. There the remaining transformable phase is transformed up to $f = f^{m}$. Upon unloading the transformed phase is partially transformed back again, before the behaviour becomes linear elastic. It may be clear that in this experiment one part of the transformation strain is permanent while the other part is reversible. This effect is caused by the volume change of the transformation, which does not occur for SMA materials. For $M = -\infty$, no reverse transformation occurs, but even for higher values of $M$ reverse transformation may be impossible. The exact value depends on the loading conditions and we will not investigate this further.

6.3 Assignment of the parameter study

To analyse the effect of the reversibility of the transformation on the mode I fracture toughness increase $K_{APP}(\Delta a)/K_{C}$ during crack growth as well as the effect on the size and the shape of the transformation zone, a finite element crack growth analysis, comparable to the one described in chapter 5, is carried out. The set of parameters which governs the crack growth problem is now enlarged by one extra parameter governing the material response: $M$. It follows that the results can be expressed in terms of the following set of nondimen-
sional parameters:

\[
\frac{K^\text{APP}}{K^\text{C}}, \frac{\Delta a}{L}, \nu, \alpha, \omega, h_0, M
\]

(6-1)

where the last five parameters govern the material response.

First the following set of material parameters was chosen to explore all possible effects of reversibility on the same parameter set as used in chapter 5: \( \nu = 0.3, \omega = 5, h_0 = [0, 0.5, 1.0, 1.5] \) \( \alpha = [1.00, 1.25] \) (for \( \alpha = 1 \) there is no hardening, whereas \( \alpha = 1.25 \) gives rise to a more realistic hardening) and \( M = [1, 0.75, 0.50, 0, -1] \). Also, the very limited influence of the transformation (\( \omega = 5 \)) may allow comparison to analysis where the transformation is taken to be supercritical (Sec. 5.4). Next a second set of parameters is taken which is closer to realistic values (see section 3.5.2): \( \nu = 0.3, \omega = [10, 20], \alpha = [1.15], h_0 = [0, 1.25] \) and \( M = [1, 0.75, 0.50, 0, -1] \) (the case \( h_0 = 0 \) corresponding to purely dilatant behaviour is included in order to allow comparison with earlier work; the value of \( h_0 = 1.25 \) reflects more realistic values). The composition of the parameter study is shown in Fig. 6.2.

\[\text{Fig. 6.2. The composition of the parameter study.}\]

The results of the parameter study into the effect of reverse transformation on the crack growth resistance are shown in Figs. 6.3 to 6.14. In these figures both the transformation zones, after a certain amount of crack growth, are given as well as the toughness development as a function of the crack extension. The results for \( M = -\infty \) (no reverse transformation) have been presented in chapter 5. Note that the crack growth resistance curves and transformation zone plots for \( M = -\infty \) differ hardly from the results for \( M = -1 \). The reason is that the unloading in the wake is not strong enough to cause reverse transformation for the case \( M < -1 \). This was already expected from Fig. 6.1, which shows that for this uniaxial loading experiment no reverse transformation occurs until the stresses change sign.

6.4 Transformation zones

Similar to the presentation in Sec. 5.3, we visualize the size and the shape of the distribution
of the transformed material surrounding the crack tip by means of contours of constant ratio of transformed fraction to the maximum available fraction $f/f^m$. Fully transformed material is represented by plotting the boundaries of the elements which contain fully transformed material.

As already explained in section 5.3.3, the stresses near the crack tip are considerably higher compared to the far field stress level. It is therefore that the transformation is first triggered in the crack tip region. As the crack tip is approached from the front side, in general the amount of transformed fraction increases gradually up to the point where the material is fully transformed $f/f^m = 1$. The crack tip is usually surrounded by a fully transformed zone which itself is surrounded by a partially transformed zone, before the untransformed material is reached. Then, as the crack proceeds, the transformed material in the wake of the crack is exposed to unloading. This unloading may cause reverse transformation in this area. If the tendency to reverse transformation is very strong ($M = 1$) then the material in the wake almost always transforms back; the initial transformation zone seems to move along with the crack tip as the crack proceeds.

In general, it is found that the volume of transformed material is always decreasing if reverse transformation occurs. Reverse transformation does not trigger forward transformation anywhere else around the crack tip. In fact, the frontal zone hardly expands upon crack growth, which is usually the case if no reverse transformation occurs. There the size of the frontal zone expands until a certain steady state value is reached. It may be said that for values of $M$ larger than $-1$, reverse transformation occurs and the size of the frontal zone decreases. This may be seen when we look at the variation of parameter $M$, as seen in corresponding plots in Figs. 6.3 to 6.14. This effect may not be so pronounced for small values of $h_0$, see Figs. 6.3, 6.11 and 6.13, is seen very clearly for parameter combinations where the influence of the transformation shear component is larger, see for example Figs. 6.6, 6.10 and 6.14.

The effect of reversible transformation on the shape of the wake of the crack is, however, more pronounced. When $M \geq 0$, the transformation strains in the wake of the crack are diminished rapidly. Two interesting phenomena can be noted when the amount of transformation shear strain $h_0$ is varied. Firstly, for $M = 0$ and for small values of $h_0$, the wake of the crack is characterized by a sharp tail and the material in the wake near to the crack surface is fully untransformed (see the plots b of Figs. 6.3, 6.4, 6.7, 6.11 and 6.13). For larger values of $h_0$ the shape of the transformation zone in the wake is changed completely. In such cases the material near the crack surface remains transformed and the area further out is fully untransformed (see the plots b of Figs. 6.5, 6.6, 6.9, 6.10, 6.12 and 6.13). Secondly, for small values of $h_0$ and $M > 0$, reverse transformation in the wake of the crack occurs, and the shape of the transformation zone is similar to the shape of the transformation zone before the occurrence of crack growth: the so-called initial zone (see plots c, d and e of Figs. 6.3, 6.4, 6.7, 6.8, 6.11 and 6.13). For larger values of $h_0$, however, the shape of the transformation zone in the wake hardly changes. Only the remaining transformed area in the wake, near the crack surface, narrows down for $M$ approaching 1 (see plot c, d and e of Figs. 6.5, 6.6, 6.9, 6.10, 6.12 and 6.13).

First we discuss the results of the parameter study for $\omega = 5$. The results are given in Figs. 6.3 to 6.10. From a comparison of Figs. 6.3 with 6.7, and of Figs. 6.4 with 6.8, we may conclude that hardening parameter $\alpha$ has a negligible influence for small values of $h_0$. However, for larger values of $h_0$ the differences are considerable. Comparing the results
Fig. 6.3. Transformation zones (a to e) when $\Delta a = 5.33L$, and the crack growth resistance curve (f) for the case $\omega = 5$, $\alpha = 1$, $h_0 = 0.0$ and $M = -1$ to 1.
Fig. 6.4. Transformation zones (a to e) when $\Delta a = 5.33L$, and the crack growth resistance curve (f) for the case $\omega = 5$, $\alpha = 1$, $h_0 = 0.5$ and $M = -1$ to 1.
Fig. 6.5. Transformation zones (a to e) when $\Delta a = 5.33L$, and the crack growth resistance curve (f) for the case $\omega = 5$, $\alpha = 1$, $h_0 = 1.0$ and $M = -1$ to 1.
Fig. 6.6. Transformation zones (a to e) when \( \Delta a = 5.33L \), and the crack growth resistance curve (f) for the case \( \psi = 5, \alpha = 1, h_0 = 1.5 \) and \( M = -1 \) to 1.
Fig. 6.7. Transformation zones (a to e) when $\Delta a = 5.33L$, and the crack growth resistance curve (f) for the case $\omega = 5$, $\alpha = 1.25$, $h_0 = 0.0$ and $M = -1$ to 1.
Fig. 6.8. Transformation zones (a to e) when $\Delta a = 5.33L$, and the crack growth resistance curve (f) for the case $\omega = 5$, $\alpha = 1.25$, $h_0 = 0.5$ and $M = -1$ to 1.
Fig. 6.9. Transformation zones (a to e) when $\Delta a = 5.33L$, and the crack growth resistance curve (f) for the case $\omega = 5$, $\alpha = 1.25$, $h_0 = 1.0$ and $M = -1$ to 1.
Fig. 6.10. Transformation zones (a to e) when $\Delta a = 5.33L$, and the crack growth resistance curve (f) for the case $\omega = 5$, $\alpha = 1.25$, $b_0 = 1.5$ and $M = -1$ to 1.
Fig. 6.11. Transformation zones (a to e) when $\Delta a = 5.33L$, and the crack growth resistance curve (f) for the case $\omega = 10$, $\alpha = 1.15$, $h_0 = 0.0$ and $M = -1$ to $1$. 
Fig. 6.12. Transformation zones (a to e) when $\Delta a = 5.33L$, and the crack growth resistance curve (f) for the case $\omega = 10$, $\alpha = 1.15$, $h_0 = 1.25$ and $M = -1$ to 1.
Fig. 6.13. Transformation zones (a to e) when $\Delta a = 5.33L$, and the crack growth resistance curve (f) for the case $\omega = 20$, $\alpha = 1.15$, $h_0 = 0$ and $M = -1$ to 1.
Fig. 6.14. Transformation zones (a to e) when $\Delta a = 5.33L$, and the crack growth resistance curve (f) for the case $\omega = 20$, $\alpha = 1.15$, $h_0 = 1.25$ and $M = -1$ to 1.
for \( \alpha = 1.00 \) to 1.25 we can see that for \( \alpha = 1.00 \) the transition from untransformed to fully transformed material is much sharper. The transformation seems to be very close to supercritical as described in Sec. 5.3. The computations for \( h_0 = 1.0 \) and 1.5 (Fig. 6.6d and e) required a much smaller loading step size and about ten times as many steps to release a node for crack growth, to obtain a stable solution. Further reduction of the step size, enlargement of the number of releasing steps or mesh refinement did not change the results, the irregular shape of transformation zone remained. However, when the hardening is increased, \( \alpha = 1.25 \) (Fig. 6.10d and e), the shape of the transformation zones becomes much smoother.

Next we discuss the second parameter study which treats more realistic values of the strength of the transformation, \( \sigma = 10 \) and 20. The results are shown in Figs. 6.11 to 6.14. The computations are performed for only one hardening parameter, \( \alpha = 1.15 \), but for two values of \( h_0 \) (0 and 1.25). Two pronounced differences with the previous studies can be noted. Firstly, the fully transformed areas are much smaller and secondly, reversible transformation does occur even for \( M = -1 \). Reversible transformation for \( M = -1 \) occurs near the crack surface, where the unloading is most active. Once more it can be seen that the influence of \( M \) is enormous. The transformed material in the wake of the crack completely transforms back for \( h_0 = 0 \) and the transformation zone reduces to a very narrow band of transformed material close to the crack tip for \( h_0 = 1.25 \).

6.5 Toughness development during crack growth

Prior to any crack growth it is reasonable to assume that no unloading occurs anywhere in the material. This was already stated by Budiansky et al. (1983). Therefore there will be no reverse transformation yet and the starting value of the toughness has to be equal to the starting value for materials that do not show reverse transformation (chapter 5). For \( h_0 = 0 \) (only dilatant transformation) the initial toughening due to the transformation strain is zero, but for \( h_0 > 0 \) the initial transformation zone reduces the initial toughness: the transformation strains elevate the stress intensity near the crack tip. Reverse transformation will only occur in the wake of the crack when the crack grows, and the material in the wake unloads. Similar to Sec. 5.4, the toughness is expressed in terms of \( \frac{K_{\text{APP}}}{K_{\text{TIP}}} \), as a function of crack advance \( \Delta a/L \). The results for the parameter variations of Sec. 6.3 are given in the plots of Figs. 6.3 to 6.14. From these plots we can see that the initial toughness is not affected by the choice of \( M \), as was to be expected.

However, upon crack growth the amount of reversible toughness greatly influences the toughness development. The contribution of the transformation zone to the stress intensity at the crack tip may vary in between two extremes, namely

(i) the lower extreme of a vanishing contribution when all material in the wake transforms back,

(ii) when no material transforms back, the upper extreme for a certain parameter combination, can be found in Sec. 5.4. In that case the toughness increase upon crack advance is found to be most pronounced. The toughness increases monotonously until a certain maximum value is reached, after which it decreases somewhat before it settles on a steady state value.

In general we can conclude that if reverse transformation occurs immediately upon un-
loading \((M = 1)\), the toughening effect reduces dramatically, which is most pronounced for smaller values of \(h_0\). When the transformation is purely dilatant \((h_0 = 0)\), no toughness increase is obtained at all. For \(M = 1\), toughening is observed when \(h_0 > 0\), but only for crack extensions \(\Delta a\) up to about 0.4L and the maximum toughness increase is about 30% of the steady state toughness increase found in the absence of reverse transformation \((M = -\infty)\). After this peak value, the effect reduces to a value close to zero. As already discussed in the previous section, for the cases \(h_0 > 0\) it appeared that these computations required more steps to release nodes for the simulation of crack growth, to maintain stability of the numerical calculation. It must be noted that once the maximum toughness is reached further loading does not take place, and only nodes are released to simulate crack growth. Especially for \(\omega = 5\), it must be noted that for the cases \(\alpha = 1.00\) and \(h_0 = [1.0, 1.5]\) the number of unloading steps for the nodal release technique had to be increased 10 times to obtain reliable results. The same problem occurred for \(M = 0.75\). For \(M = 0.5\) and lower no such problems have been encountered.

The effect of \(M\) on the toughness development for \(h_0 = 0\) is quite different from the effect for \(h_0 > 0\), this can be seen in Figs. 6.3, 6.7, 6.11 and 6.13. In this case no peak toughness is reached, but the toughness monotonously increases to the steady state value. The steady state value steadily increases as the amount of reverse transformation decreases, i.e. \(M\) decreases. For \(h_0 = 0\) the toughness development for decreasing values of \(M\) is a transition of the curve for \(M = 1\), with a maximum toughening effect after a crack extension \(\Delta a = 0.4L\), to the curve for \(M = -\infty\), where the maximum in toughness is reached much later and the drop in toughening after this maximum is far less severe. Note that for increasing values of \(\omega\), reverse transformation does occur for \(M = -1\) and the toughening increase is reduced, see for instance Fig. 6.10.

When comparing the results for \(M = 0\) with the case when no reverse transformation occurs \((M = -\infty)\) a reduction of up to 25% is found for \(\alpha = 1.25\) and \(h_0 = 1.5\); on the other hand, for the case \(\alpha = 1.00\) and \(h_0 = 1.0\) the reduction is less then 1%. Examining Figs. 6.4, 6.5, 6.6, 6.8, 6.9 and 6.10 we see that for increasing hardening \((\alpha)\), reverse transformation occurs already for lower values of \(M\). The differences in the curves of \(M = -1\) and 0 increase when \(\alpha\) increases. For \(\alpha = 1.25\) and \(h_0 = 1.5\) reverse transformation occurs even for \(M = -1\).

### 6.6 Conclusions

From this study we may conclude that the toughening during crack growth does depend strongly on the amount of reverse transformation. In all cases considered the toughness increase upon crack growth is lowered if reverse transformation takes place in the wake of the growing crack. The decrease is most dramatic for so-called super or pseudo-elastic materials \((M = 1)\), where reverse transformation immediately follows upon unloading. It may be concluded from the parameter study, that this class of materials exhibits some initial toughening, but after a small amount of crack growth almost no toughness increase is left.

We did not analyse the effect of reverse transformation on supercritical transforming materials as discussed in Sec. 5.6. However, for dilatant transformation the toughening has been determined by Evans and Cannon (1986). They found that if reverse transformation occurs for some critical mean stress \(\Sigma_m^R \geq 0\) the toughening increment is

99
\( \Delta K^{\text{TIP}} = -0.21 \frac{E\theta h^{1/2} (1 - \Sigma^R_m / \Sigma^C_m)}{(1 - \nu)} \) \quad (6-2)

Consequently when the transformation reverses to give zero final stress \( (\Sigma^R_m = 0) \), the toughening value is identical to that for the supercritical, unreversed case (2-14) and is zero when \( \Sigma^R_m = \Sigma^C_m \). In our terminology the latter case would refer to \( M = 1 \), and the zero result for the increase in toughness agrees with the subcritical results presented here for \( h_0 = 0 \). Analysis of the other extreme, when the dilatation is zero, has been analysed by Sun and Xu (1993) but it is only applicable for shape memory materials.

For ceramics containing zirconia there seems to be no direct experimental evidence for reverse transformation at room temperature in simple tensile tests of currently utilized structural ceramics. Thus, those materials seem to be characterized by \( M < 0 \), for which our results show that the reduction in toughness increase is not so dramatic. However, further experimental work is necessary to establish the real value of \( M \) as the influence of this parameter on the toughness development is enormous.
CHAPTER 7

Effect of non-homogeneous distribution of transformable phase

7.1 Introduction

Zirconia Toughened Alumina (ZTA) is a composite material which consists of two ceramic components, namely alumina (Al₂O₃) and zirconia (ZrO₂). The microstructure of this material is shown in Fig. 2.6c. The toughness of alumina is significantly improved by the substitution of the zirconia phase. Two toughening mechanisms are believed to play a role in this material, namely transformation toughening and microcrack toughening, as indicated by, among others, Rühle et al. (1986). The tetragonal zirconia phase can undergo the stress-induced \( t \rightarrow m \) transformation and the residual stresses around already transformed \( m \)-zirconia particles can cause microcracking. Already upon cooling, after the sintering process, the larger zirconia particles in the alumina matrix transform to the monoclinic phase. Based on thermodynamical considerations, Evans et al. (1981) found that the difference in the volume/surface-ratio causes the larger particles to transform before the smaller ones. Therefore, transformation and microcrack toughening may act as complementary processes, as stated by Karihaloo (1990).

Den Exter (1991) studied ZTA materials which were prepared using fine-grained zirconia and alumina powders to obtain ZTA materials with small \( t \)-zirconia grains to improve the mechanical properties, toughness particularly. However, during the development of this composite, before sintering, the fine grained powders tend to agglomerate, which during the sinter process can cause a non-homogeneous distribution of zirconia in the alumina matrix. Much effort has been put into the development of composites with a homogeneous distribution, but the question was raised whether a certain level of heterogeneity would or would not lower the toughness of the material. Here we want to look at this problem from a theo-
retical point of view.

In our analysis, we assume that the transformation toughening mechanism completely dominates any microcrack mechanism, and that the transformable particles are coherently embedded in a linear-elastic matrix. The heterogeneous distribution will be treated in a smeared out sense as will be explained in the following section. The first results, for dilatant transformation behaviour, were published in Stam et al. (1993a).

7.2 Modelling the heterogeneous distribution

With the help of Fig. 7.1 we describe the kind of non-homogeneous distribution that has been analysed here, and the way in which such a distribution is modelled. The figure shows the microstructure of a ZTA material. In fact, the figure is a composition of 6 schematical representations of a micrograph made by Rühle et al. (1984). Here, the zirconia particles appear dark. It is clear that the zirconia particles are not distributed homogeneously and that areas with high and low contents of zirconia can be found. On the right-hand side of the figure, Rühle derived the percentage of transformed zirconia phase. This may be interpreted as the profile of the transformation zone perpendicular to the crack surface. This profile is inserted in this figure to be able to compare the typical length scale of the clusters to the size of the transformation zone. This heterogeneous distribution of zirconia phase is ana-

![Fig. 7.1. Schematical representation of the microstructure of a ZTA material, where the zirconia particles appear dark. The distribution of transformed material perpendicular to the crack surface has been plotted on the right-hand side.](image-url)
lysed using a smeared out approach. We assume that areas with a higher amount of tetragonal phase are followed by areas with a lower amount of transformable phase according to a periodic pattern. Then the non-homogeneous distribution of t-ZrO₂ particles can be modelled by introducing a function $D(x_1, x_2)$, such that the maximum transformable phase $f^m$ is no longer constant over the area, but varies periodically throughout the material:

$$f^m_{D}(x_1, x_2) = D(x_1, x_2)f^m$$

where $D(x_1, x_2)$ is a non-dimensional periodic function defined by

$$D(x_1, x_2) = 1 + a \cos \left( \frac{2\pi x_1}{L_c} \right) \cos \left( \frac{2\pi x_2}{L_c} \right) \quad \text{with} \quad a \in [0, 1] ,$$

where the amplitude $a$ is the relative deviation from the average value $f^m$ and the characteristic length $L_c$ governs the distance between two maxima in either the $x_1$ or $x_2$ direction. The physical meaning of $a$ and $L_c$ are the level of heterogeneity and a characteristic period of the heterogeneity, respectively. In comparing different distributions, the average amount of transformable phase remains constant, so that the value of $\omega$, the strength of the transformation (as defined in (3-71)) is not affected. The two cosine functions at the sides of the micrograph in Fig. 7.1 illustrate what the wavelength of the variations in (7-1) could be. Once the parameters $a$ and $L_c$ are chosen, the distribution of maximum transformable phase $f^m_{D}(x_1, x_2)$ is defined, as illustrated in Fig. 7.2.

Mode I crack growth computations as described in chapter 4 have been performed, and again symmetry considerations allow analysis of half of the small-scale crack problem. This means, however, that the transformable phase needs to be distributed symmetrically with respect to the symmetry axis of the problem ($x_2 = 0$). When the transformable phase is distributed according to the distribution function $D(x_1, x_2)$ as defined in (7-2), three crack paths are possible which maintain symmetry. As indicated in Fig. 7.2, path A is a path which goes through both minima and maxima, and when $D(x_1, x_2)$ is rotated by 45°, paths

![Figure 7.2](image)

*Fig. 7.2. Assumed periodic distribution of transformable phase, were 'min' corresponds with a transformable phase of $(1-a)f^m$ and 'max' to $(1+a)f^m$. Three possible crack paths have been indicated.*
B and C go through the minima and maxima, respectively. Most results which are presented here, crack path A is used. Some computations with crack path B and C are performed to detect a possible influence of the choice of path.

7.3 Assignment of the parameter study

The analysis of the effect of non-homogeneously distributed transformable phase on the toughness development during crack growth is an extension of the previously presented analyses in chapter 4 and 5. Therefore, the same set of non-dimensional parameters is used to characterize the crack growth problem. However, two parameters have to be added to characterize the measure of heterogeneity, namely the amplitude $a$ and the non-dimensional characteristic period of the heterogeneity $\lambda_c = L_c / L$, where $L$ is the characteristic length as defined in (4-7). Thus the complete set of non-dimensional parameters which govern the deformation response is now given by

$$v, \alpha, \omega, h_0, M, a, \lambda_c$$  \hspace{1cm} (7-3)

An analysis is performed with 18 different combinations of these parameters. However, not all parameters of (7-3) are varied. In this study, it is considered sufficient to vary only $\omega$, $h_0$ and $\lambda_c$. The remaining parameters were set to constant value: $v = 0.3$, $\alpha = 1.15$, $M = -\infty$ and $a = 1$, describing a ZTA material with realistic Poisson's ratio and hardening, and with no reversible transformation. The amplitude $a$ is chosen maximal to achieve a maximal effect of the heterogeneous distribution. This choice is rather arbitrary; however, the qualitative influence is clear as a reduction of $a$ simply means that the material becomes less heterogeneous. For decreasing $a$ the results approach the results for homogenous materials. This has been verified by some test computations.

In conformity with the range of variation in previous studies the value of the strength of the transformation $\omega$ has been set to 5, 10 and 20. The amount of transformation shear strain has been set to the realistic value $h_0 = 1.25$, but has also been set to zero to simulate purely dilatant transformation behaviour. Finally, the most interesting parameter in this context $\lambda_c$, the relative period of the heterogeneities, has been set to 2, 4 and 16. As mentioned before, the plot at the right-hand side of Fig. 7.1 gives a cross-section of the transformation zone perpendicular to the crack, as measured by Rühle et al. (1984), from which we could conclude that the period of the heterogeneities is in the order of the height of the transformation zone. For all computations we have chosen for the following set of parameters: $v = 0.3$, $\alpha = 1.15$, $a = 1$ and we varied $\omega = [5, 10, 20]$, $h_0 = [0.0, 1.25]$ and $L_c$ for which three different values where chosen, namely $2L$, $4L$, $16L$. For an over-

\[\begin{array}{ccc}
\omega = 5 & h_0 = 0.0 & \lambda_c = 2 \\
10 & 1.25 & 4 \\
20 & & 16
\end{array}\]

\[\text{Fig. 7.3. The composition of the parameter study.}\]
view of the sets of parameters which have been taken for the parameter study we refer to Fig. 7.3. In Figs. 7.5 to 7.10 the results are compared to results for computations for homogeneous distributions of transformable phase. Similar to the previous chapters, the results of the computations are presented in terms of predicted transformation zones and crack growth resistance curves.

7.4 Transformation zones

Similar to chapters 4 and 5, a contour line representation is used to visualize the transformation zones surrounding the crack. In the previous chapters the contours are lines of constant value of the ratio transformed fraction to maximum available transformed fraction $f/f^m$ and if we use the same ratio for the heterogeneous distributed materials, $f/f^m_D(x_1, x_2)$, we find plots like Fig. 7.4a. This may be a convenient way of representing the numerical results, but the primary goal of these plots, to visualize the state of transformation in such a way that it is easy to compare to experimental results, is not satisfied. In reality the maximum available phase is not distributed according some known periodical function and therefore it seems more applicable to scale the results with 'the maximum transformable fraction', $(1 + a)f^m$. As in all our computations $a = 1$, the newly defined ratio is $f/ (2f^m)$ and in that case we find contour line plots like the one shown in Fig. 7.4b. A disadvantage may be that it is no longer clear that the material next to the crack is fully transformed. Nevertheless, this definition for the contours is used in the Figs. 7.5 to 7.10. For comparison, the plots a in these figures show the results of the transformation zone for homogeneously distributed transformable phase. The length scale parameter $L$ has been used to make the coordinates non-dimensional.

If we consider $f^m_D(x_1, x_2)$ as defined in (7-2), then we see that the minima have a value of $(1 - a)f^m$ and are located at the non-dimensional coordinates

$$x_1/L = \frac{(1 + j) + 2i}{2}\lambda_c, \quad x_2/L = \frac{j}{2}\lambda_c \quad (7-4)$$

for $i$ and $j$ being integers. This pattern of minima is clearly traceable in the contour line plots, if minima are surrounded by transformed material. Then the contour

![Contour line representation of the transformed material surrounding the crack tip](image)

Fig. 7.4. Two contour line representations of the transformed material surrounding the crack tip when $\Delta a = 5.33L$ for the case $\omega = 5$, $h_0 = 0.0$ and $\lambda_c = 2$. 

105
Fig. 7.5. Transformation zones (a to d) when $\Delta a = 5.33L$, and the crack growth resistance curve (e) for the cases $\omega = 5$, $\alpha = 1.15$, $h_0 = 0.0$ and $\lambda_c = 0$ to 16.
Fig. 7.6. Transformation zones (a to d) when $\Delta \alpha = 5.33L$, and the crack growth resistance curve (e) for the cases $\omega = 5$, $\alpha = 1.15$, $h_0 = 1.25$ and $\lambda_c = 0$ to 16.
Fig. 7.7. Transformation zones (a to d) when $\Delta a = 5.33L$, and the crack growth resistance curve (e) for the cases $\omega = 10$, $\alpha = 1.15$, $h_0 = 0.0$ and $\lambda_c = 0$ to 16.
Fig. 7.8. Transformation zones (a to d) when Δa = 5.33L, and the crack growth resistance curve (e) for the cases ω = 10, α = 1.15, h₀ = 1.25 and λₑ = 0 to 16.
Fig. 7.9. Transformation zones (a to d) when $\Delta a = 5.33L$, and the crack growth resistance curve (e) for the cases $\omega = 20$, $\alpha = 1.15$, $h_0 = 0.0$ and $\lambda_c = 0$ to 16.
Fig. 7.10. Transformation zones (a to d) when $\Delta a = 5.33L$, and the crack growth resistance curve (e) for the cases $\omega = 20$, $\alpha = 1.15$, $h_0 = 1.25$ and $\lambda_c = 0$ to 16.
\( f/(2f^m) = 0.05 \) encircles such minima. A remarkable example of such a pattern can be seen in plot b of Fig. 7.6. It is obvious from (7-4) that the distance between the minima increases when \( \lambda_c \) increases, which is demonstrated in plot c and d of Fig. 7.6.

The effect of variation of \( \lambda_c \) on the shape and size of the transformation zone is found to be rather predictable. From the results of the parameter study we may conclude that the size of the transformed zone is hardly affected by the choice of \( \lambda_c \). However, the shape of the transformation zone is changed considerably. The change in shape is most pronounced near the crack surface. There the limit of 'maximum transformed fraction' \( f^m_D(x_1, x_2) \) is often reached, while further away from the crack surface the transformed fraction is so low that the maximum limit is not reached. In that area, only the absolute minima, as defined in (7-4) may affect the shape, as clearly shown in the plots b of Figs. 7.6, 7.8 and 7.10. However, also in plots c and d of the same figures, and in plot b of Fig. 7.7, the effect can be noted.

Note, that if one wants to compare the plots of the homogeneous distributions (plots a of Figs. 7.5 to 7.10) with the plots for the heterogeneous distributions (plots b, c and d of the same figure range), that in the latter case the maximum transformable phase is twice as large.

### 7.5 Toughness development

The toughness development during crack growth is presented in the plots e of Figs. 7.5 to 7.10. In each of these plots the results for 4 numerical crack growth simulations have been plotted, to investigate the influence \( \lambda_c \), for increasing \( \omega \) and for \( h_0 = 0 \) and 1.25. On the horizontal axis, crack growth \( \Delta a \), the difference in start position and current position of the crack, has been made non-dimensional by \( L \), as usual. While on the vertical axis the applied stress intensity as function of crack growth \( K^{APP}(\Delta a) \) is scaled by \( K^C \), the critical stress intensity. Crack growth occurs if the stress intensity at the crack tip reaches the critical stress intensity, \( K^{TIP} = K^C \). When the applied stress intensity, \( K^{APP} \), has to be larger than the critical stress intensity to force crack growth, we must conclude that the transformation strains shield the crack tip and the apparent toughness has been increased.

Similar to the simulations for homogeneous materials we find that, prior to crack growth, the transformation strains hardly influence the stress intensity at the tip. Upon crack growth, however, we find that \( K^{APP} \) needs to be increased considerably, before the critical stress intensity at the tip is reached and crack growth proceeds. Moreover, we can conclude that the development of the toughness during crack growth is strongly affected by the introduction of heterogeneity. In all the results presented here, the initial position of the crack tip is situated in the centre of a rich area, where the amount of transformable strain is twice the average value. Therefore, the increase in toughness develops more rapidly than for a homogeneous material. However, the tip grows into an area where the distribution function \( D \) reaches a minimum, so that the maximum available transformable phase is small and we find that the toughness reaches a local maximum and upon further crack growth, the shielding effect of the transformation strains is reduced. In our analysis, we prescribe the displacements at the boundary of the small scale problem (see section. 4.5.1), which are not changed during crack growth. Thus when the shielding effect reduces, at the tip a stress intensity is found which is larger than the critical stress intensity. Without further loading,
more nodes are released as long as $K_{\text{tip}}^{\text{app}} > K_{\text{c}}^{\text{C}}$, until the shielding effect returns to the value of the local maximum. In fact the ratio $K_{\text{tip}}^{\text{app}} / K_{\text{tip}}^{\text{C}}$, which has been dotted, oscillates during crack growth in order to keep $K_{\text{tip}}^{\text{app}} = K_{\text{c}}^{\text{C}}$. The period of the oscillations if found to vary proportionally with the value of $\lambda_{c}$. Physically, however, once $K_{\text{tip}}^{\text{app}} / K_{\text{tip}}^{\text{C}}$ reaches a maximum, unstable crack growth occurs, and the crack will grow dynamically to the transformation rich area. In the simulation, dynamic crack growth effects have not been taken into account, and the horizontal parts in the resistance curves must be seen as unstable. The maximum toughness, however, is the value which is of interest. It is this value which determines the stress intensity at which unstable crack growth starts. When the starting position of the crack tip is situated in the centre of an area with a low amount of transformable phase, the increase in toughness develops more slowly compared to the results for homogeneous materials. But, apart from the somewhat slower start, the toughness development results curves are similar to those for which the start position is situated in a rich area and are not presented here.

The results, plotted in Figs. 7.5 to 7.10, suggest a general increase of the maximum toughness, compared to results for homogeneous materials. However, the improvement of this maximum value depends on $\omega$. When $\omega$ increases, the improvement decreases. For example, for $\omega = 5$ in Fig. 7.5e, we see that the increase for $\lambda_{c} = 2$ is more than 60%, while for $\omega = 20$, in Fig. 7.9e, the increase is hardly 25%. Furthermore, the results suggest that for decreasing $\lambda_{c}$, the maximal toughness value increases. It must be noted, however, that only a limited amount of crack growth has been performed and that the probability increases that the maximum value for the toughness has not been reached yet for the larger values of $\lambda_{c}$. However, more crack growth requires a larger mesh and the computations would become too time-consuming.

When crack growth was forced to follow the diagonal path B or C (Fig. 7.2), surprisingly we found that the results for the maximum achieved toughness during crack growth are only a little lower, respectively about 5 and 2.5%.

7.6 Conclusions

From these numerical crack growth simulations, we can conclude that a heterogeneous distribution of transformable phase may give rise to an increase in toughness, compared to materials with a perfectly homogeneous distribution of ZrO$_{2}$. Although the effect is tempered for larger values of $\omega$ it certainly seems to be an improvement for the toughness of the material. This might explain the development of duplex materials where relatively large (100 - 50 $\mu$m) spherical $t$-ZrO$_{2}$ zones are dispersed in a ceramic matrix, as discussed by Lutz and Claussen (1991a and b). They found that the toughness was increased, but the strength of the material was decreased, compared to conventional ZTA materials.

In the derivation of the continuum model (see chapter 3), it is assumed that a continuum element contains many grains. However, especially in ZTA materials the transformation zone only spans a few grains, so that the validity of the continuum approach may be questionable in some cases. This also limits our approach to the investigation of the influence of areas with varying transformable phase and excludes the study to the influence of very large particles or flaws on the deformation behaviour. Once more we want to stress that we assumed that microcracks do not exist before crack growth, and do not develop during the
crack growth simulation. Instead, the transformable particles remain coherently embedded in the matrix.

Finally we want to mention that in our analysis crack growth was permitted only over a fixed distance. It may well be that the maximum reported toughness is not the maximal achievable toughness: a larger value for \( K^{\text{APP}}/K^C \) may be found upon further crack growth. It appeared, however, that the computer time and memory, required for such computations is still too much. Another limitation in the current analysis is the required symmetry of the problem and thus the required symmetry for the heterogeneous distribution. Non-symmetry may lead to a reduction of the toughness values. This conjecture is supported by the results for crack growth along paths B and C, as shown in Fig. 7.2, for which lower values for the toughness are found, although the reduction is limited to about 5%. However, the analysis of non-symmetric distribution of transformable phase may also result in a deflection of the crack. This problem is studied in chapter 8.
CHAPTER 8

Crack deflection due to transformation strains

8.1 Introduction

In most crack growth studies the crack is not allowed to deflect from the direction of its original crack path. This simplification is based on two considerations, namely: (i) crack deflection introduces considerable mathematical problems and (ii) the crack will only deflect if the crack problem is non-symmetric to the direction of the original crack path ($x_2 = 0$) which is not often the case. Here, however, we study the crack growth behaviour of a material with a heterogeneous distribution of transformable phase which is not symmetric with respect to line $x_2 = 0$. It is expected that in this case the crack deflects from its initial direction. This may affect the crack growth behaviour as the crack may now find a path which is energetically more favourable.

Similar to (7-1) the transformable phase is distributed using a periodic distribution function $D$, but now the distribution does not need to be symmetric with respect to the initial crack path. In fact we will shift the distribution over a non-dimensional distance $\lambda_{x_2}$ in the $x_2$ direction,

$$f^m_D(x_1, x_2, \lambda_{x_2}) = D(x_1, x_2, \lambda_{x_2})f^m$$  \hspace{1cm} (8-1)

where $D(x_1, x_2, \lambda_{x_2})$ is a non-dimensional doubly periodic function defined by

$$D(x_1, x_2, \lambda_{x_2}) = 1 + a \cos \left( \frac{2\pi x_1}{L_c} \right) \cos \left( \frac{2\pi (x_2 + \lambda_{x_2} L)}{L_c} \right) \hspace{1cm} \text{with} \hspace{1cm} a \in [0, 1]$$  \hspace{1cm} (8-2)

where again $a$ is the amplitude of the variations in $f^m$ and the characteristic length $L_c$ governs the distance between two maxima in either the $x_1$ or $x_2$ direction, similar to Sec. 7.2. Initially the crack is taken to be straight, but due to the inhomogeneous distribution of trans-
formable phase, the crack may deflect. The effect of crack deflection on the toughness during crack growth is investigated as well as the effect on the size and shape of the transformation zone.

The introduction of a nonsymmetric distribution causes some extra computational complications. First, the loss of symmetry requires that the whole domain $\Omega$ (see Fig. 8.1) has to be accounted for in the analysis, and second, the inhomogeneity may cause a mode II loading component at the crack tip which cause the crack to deflect and to proceed under a certain angle with respect to the initial direction. This requires a new formulation of the crack growth criterion on the basis of both mode I (tensile mode) and mode II (sliding mode), and an expression for the direction in which the crack proceeds (see Cotterell and Rice, 1980). Moreover, it necessitates a reformulation of the area integral discussed in sections 4.4.2 and 4.5.4, to be able to determine the effect of a single transformed particle on the mode I and mode II stress intensity components. The implementation of these new formulations opens at the same time the way to analyse mode II loading. Only the boundary condition has to be updated to be able to prescribe mode II (or mixed I, II mode) loading conditions.

8.2 Crack criterion

One of the most widely used crack criteria is the energy release rate criterion, where it is assumed that fracture occurs when the energy required per unit length of crack growth can be delivered by elastic energy that is released. The total energy release rate in mixed mode cracking $G$ can be related to the stress intensity factors by using the general expression

$$G = \frac{1 - \nu^2}{E} \left( K_1^2 + K_II^2 + \frac{K_{III}^2}{1 - \nu} \right).$$

(8-3)

In the present considerations, the mode III stress intensity $K_{III}$ is always zero as we assumed plane strain conditions. We now introduce

$$K_{\text{ref}} = \sqrt{K_1^2 + K_{II}^2}, \quad \text{so that} \quad G = \frac{1 - \nu^2}{E} K_{\text{ref}}^2,$$

(8-4)

and crack growth is assumed to occur when $K_{\text{ref}}$, the reference stress intensity, reaches the critical stress intensity of the material $K^C$. The practical validity of this fracture criterion may, however, be questionable as it predicts that $K_1^C = K_{II}^C$, and the locus for combined mode cracking is a circle with radius $K_1^C$. In practice $K_1^C \neq K_{II}^C$, but nevertheless we will use (8-4) to predict crack growth.

8.3 Direction of crack extension

Broek (1982) states two criteria for mixed mode loading that allow crack growth under an angle: (i) the maximum principal stress criterion postulates that crack growth occurs in a direction perpendicular to the maximum principal stress, or (ii) the strain energy density
criterion states that crack growth takes place in the direction of minimum strain energy density. As the difference in predicted angle between the two criteria is rather small, we made an arbitrary choice and use the maximum principal stress criterion. It is therefore convenient to express the stresses around the crack tip in polar coordinates. Using the stresses $\sigma_{ij}$ given in (2-6), we obtain for the stress components $\sigma_{rr}$, $\sigma_{\beta\beta}$ and $\tau_{r\beta}$,

$$
\sigma_{rr} = \frac{K_1}{\sqrt{2\pi r}} \cos \frac{\beta}{2} (1 + \sin^2 \frac{\beta}{2})
$$

$$
\sigma_{\beta\beta} = \frac{K_1}{\sqrt{2\pi r}} \cos \frac{\beta}{2} (1 - \sin^2 \frac{\beta}{2}) \quad \text{and} \quad \tau_{r\beta} = \frac{K_1}{\sqrt{2\pi r}} \sin \frac{\beta}{2} \cos \frac{\beta}{2}. \quad (8-5)
$$

Similar equations can be derived for mode II (Broek, 1982):

$$
\sigma_{rr} = \frac{K_{II}}{\sqrt{2\pi r}} (-\frac{5}{4} \sin \frac{\beta}{2} + \frac{3}{4} \sin \frac{3\beta}{2})
$$

$$
\sigma_{\beta\beta} = \frac{K_{II}}{\sqrt{2\pi r}} (-\frac{3}{4} \sin \frac{\beta}{2} - \frac{3}{4} \sin \frac{3\beta}{2}) \quad \text{and} \quad \tau_{r\beta} = \frac{K_{II}}{\sqrt{2\pi r}} (\frac{1}{4} \cos \frac{\beta}{2} + \frac{3}{4} \cos \frac{3\beta}{2}) \quad (8-6)
$$

Thus the stresses due to combined mode I and mode II loading can be derived by adding the contribution of mode I and mode II. The result for $\sigma_{\beta\beta}$ and $\tau_{r\beta}$ is as follows:

$$
\sigma_{\beta\beta} = \frac{1}{\sqrt{2\pi r}} \left[ a_{11}(\beta)K_1 + a_{12}(\beta)K_{II} \right]
$$

$$
\tau_{r\beta} = \frac{1}{\sqrt{2\pi r}} \left[ a_{21}(\beta)K_1 + a_{22}(\beta)K_{II} \right] \quad (8-7)
$$

where

$$
a_{11}(\beta) = \frac{1}{4} \left[ 3 \cos \frac{\beta}{2} + \cos \frac{3\beta}{2} \right] \quad a_{12}(\beta) = -\frac{3}{4} \left[ \sin \frac{\beta}{2} + \sin \frac{3\beta}{2} \right]
$$

$$
a_{21}(\beta) = \frac{1}{4} \left[ \sin \frac{\beta}{2} + \sin \frac{3\beta}{2} \right] \quad a_{22}(\beta) = \frac{1}{4} \left[ \cos \frac{\beta}{2} + 3 \cos \frac{3\beta}{2} \right]. \quad (8-8)
$$

Now the angle $\beta_m$, under which the crack will grow — the direction perpendicular to the maximum principal stress — is found by equating the shear stress $\tau_{r\beta}$ of (8-7) to zero. We find

$$
K_1 \sin \beta_m + K_{II} (3 \cos \beta_m - 1) = 0, \quad (8-9)
$$

and it finally follows that

$$
(\tan \frac{\beta_m}{2})_{1,2} = \frac{1}{4K_{II}} \pm \sqrt{\left(\frac{K_1}{K_{II}}\right)^2 + 8}. \quad (8-10)
$$
8.4 Boundary conditions

Again we adopt a small scale transformation formulation, as discussed in chapter 4, but now the symmetry is lost and a full circular region must be analysed. The crack tip is positioned in the centre of this circular region, as shown in Fig. 8.1, where the displacement boundary values are given by a combination of mode I and mode II terms. If we define a ratio

\[ \rho^M = \frac{K_{\text{II}}^{\text{APP}}}{K_{\text{I}}^{\text{APP}}}, \]  

(8-11)

representing the two different modes in the applied loading and we use the relation (8-4), then for an applied reference stress intensity \( K_{\text{ref}}^{\text{APP}} \) it follows that

\[ K_{\text{I}}^{\text{APP}} = \frac{(K_{\text{ref}}^{\text{APP}})^2}{1 + (\rho^M)^2} \quad \text{and} \quad K_{\text{II}}^{\text{APP}} = \rho^M K_{\text{I}}^{\text{APP}} \]  

(8-12)

and the boundary values for \(-\pi < x_1 < 0, \; x_2 = 0\) are given by

\[ T_1 = T_2 = 0. \]  

(8-13)

For \( x_1 = r(\beta) \cos \beta \) and \( x_2 = r(\beta) \sin \beta \) we obtain

\[ u_1 = \frac{K_{\text{I}}^{\text{APP}}}{G} \sqrt{\frac{r}{2\pi}} \left[ \frac{\cos \beta}{2} \left( 2 - 2v - \cos^2 \frac{\beta}{2} \right) + \rho^M \sin \frac{\beta}{2} \left( 2 - 2v + \cos^2 \frac{\beta}{2} \right) \right] \]

\[ u_2 = \frac{K_{\text{I}}^{\text{APP}}}{G} \sqrt{\frac{r}{2\pi}} \left[ \frac{\sin \beta}{2} \left( 2 - 2v - \cos^2 \frac{\beta}{2} \right) + \rho^M \cos \frac{\beta}{2} \left( 1 - 2v + \sin^2 \frac{\beta}{2} \right) \right]. \]  

(8-14)

In contrary to the previous analyses, the change in distance from the crack tip to each individual boundary value during crack growth is assumed to be negligible as the distance from the crack tip to the boundary is much larger than the growth of the crack.

Fig. 8.1. Small scale transformation problem for a stationary crack.
8.5 Modification of the transformation domain integral

The influence of the transformation strains on the stress intensity at the crack tip, which is discussed in sections 4.4.2 and 4.5.4, has been derived by Hutchinson (1974) for two transforming spots which are placed symmetrically on either side of the crack. This makes the method not directly applicable to nonsymmetric transformation zones, as we expect here. Gao (1989), however, derived a solution for the interaction between the crack tip and a single source of internal strain. The analysis is based on investigations of Rice (1985), using three-dimensional "weight functions"-theory, and on Bueckner’s (1987) solution for the complete set of weight functions for a half infinite crack. The derivation is rather extensive and we shall confine ourselves to the results for two-dimensional weight functions and transformation strains.

First we define $K_{\alpha}^{\text{APP}}$, which is the stress intensity that would be introduced at the crack tip by an applied loading in the absence of transformation strains, with mode $\alpha$. Thereupon, the influence of the transformation strains on the stress intensity at the crack tip is obtained by Gao (1989) as,

$$dK_{\alpha}^{\text{TIP}} = 2G \int \bar{U}_{ij}^{\alpha}(x_1, x_2) e_p(x_1, x_2)dx_1dx_2$$

(8-15)

where $G$ is the shear modulus, the components $e_p$ represent the transformation strains and the components $\bar{U}_{ij}^{\alpha}$ are defined by

Mode I:

$$\bar{U}_{11}^{I} = \frac{C}{8r^{3/2}} \left[ \cos \frac{3\beta}{2} + 3 \cos \frac{7\beta}{2} \right]$$

$$\bar{U}_{33}^{I} = \nu C \frac{1}{r^{3/2}} \cos \frac{3\beta}{2}$$

$$\bar{U}_{22}^{I} = \frac{C}{8r^{3/2}} \left[ 7 \cos \frac{3\beta}{2} - 3 \cos \frac{7\beta}{2} \right]$$

$$\bar{U}_{12}^{I} = \frac{3C}{8r^{3/2}} \left[ - \sin \frac{3\beta}{2} + \sin \frac{7\beta}{2} \right]$$

(8-16)

$$\bar{U}_{ij}^{I} = (1+\nu) C \frac{1}{r^{3/2}} \cos \frac{3\beta}{2}$$

Mode II:

$$\bar{U}_{11}^{II} = -\frac{C}{8r^{3/2}} \left[ 5 \sin \frac{3\beta}{2} + 3 \sin \frac{7\beta}{2} \right]$$

$$\bar{U}_{33}^{II} = -\nu C \frac{1}{r^{3/2}} \sin \frac{3\beta}{2}$$

$$\bar{U}_{22}^{II} = \bar{U}_{12}^{I}$$

$$\bar{U}_{12}^{II} = \bar{U}_{11}^{I}$$

(8-17)

$$\bar{U}_{ij}^{II} = - (1-\nu) C \frac{1}{r^{3/2}} \sin \frac{3\beta}{2}$$

Mode III:

$$\bar{U}_{23}^{III} = \frac{(1-\nu) C}{2} \frac{1}{r^{3/2}} \cos \frac{3\beta}{2}$$

$$\bar{U}_{13}^{III} = \frac{(1-\nu) C}{2} \frac{1}{r^{3/2}} \sin \frac{3\beta}{2}$$

(8-18)

In (8-16) to (8-18), $\bar{U}_{ij}^{\alpha}$ and the rest of the components $\bar{U}_{ij}^{\alpha}$ are zero. The constant $C$
is defined as

$$C = \frac{1}{2(1 - \nu) \sqrt{2\pi}}.$$  \hspace{1cm} (8-19)

Using (8-15) and (8-16) the influence of the transformation strains on the Mode I stress intensity at the crack tip is given by

$$dK_1^{\text{TIP}} = G \frac{C}{4} \int_{A_{x_1,x_2}} \left( \frac{1}{r^{3/2}} \left[ \cos \frac{3\beta}{2} + 3 \cos \frac{7\beta}{2} \right] \varepsilon_{11}^p + \frac{1}{r^{3/2}} \left[ 7 \cos \frac{3\beta}{2} - 3 \cos \frac{7\beta}{2} \right] \varepsilon_{22}^p + \right.$$

$$\left. \frac{6}{r^{3/2}} \left[ - \sin \frac{3\beta}{2} + \sin \frac{7\beta}{2} \right] \varepsilon_{12}^p \right) dx_1 dx_2,$$

\hspace{1cm} (8-20)

which can be rewritten as

$$dK_1^{\text{TIP}} = G \frac{C}{4} \int_{A_{x_1,x_2}} \text{Re} \left[ \frac{1}{r^{3/2}} \left\{ \varepsilon_{11}^p + 7\varepsilon_{22}^p - 6i\varepsilon_{12}^p \right\} \left\{ \cos \frac{3\beta}{2} - i \sin \frac{3\beta}{2} \right\} + \right.$$

$$\left. \frac{3}{r^{3/2}} \left\{ \varepsilon_{11}^p - \varepsilon_{22}^p + 2i\varepsilon_{12}^p \right\} \left\{ \cos \frac{7\beta}{2} - i \sin \frac{7\beta}{2} \right\} \right] dx_1 dx_2.$$  \hspace{1cm} (8-21)

Defining a complex variable $z = x_1 + ix_2$, with $x_1 = r \cos \beta$ and $x_2 = r \sin \beta$, it is clear that

$$\frac{1}{r^{3/2}} (\cos \frac{3\beta}{2} - i \sin \frac{3\beta}{2}) = \frac{1}{z^{3/2}} \quad \text{and} \quad \frac{1}{r^{3/2}} (\cos \frac{7\beta}{2} - i \sin \frac{7\beta}{2}) = \frac{\bar{z}}{z^{5/2}},$$  \hspace{1cm} (8-22)

where $\bar{z}$ denotes the complex conjugate of $z$, so that (8-21) can be rewritten as

$$dK_1^{\text{TIP}} =$$

$$G \frac{C}{4} \int_{A_{x_1,x_2}} \text{Re} \left[ \frac{1}{z^{3/2}} \left\{ \varepsilon_{11}^p + 7\varepsilon_{22}^p - 6i\varepsilon_{12}^p \right\} + \frac{3\bar{z}}{z^{5/2}} \left\{ \varepsilon_{11}^p - \varepsilon_{22}^p + 2i\varepsilon_{12}^p \right\} \right] dx_1 dx_2$$

\hspace{1cm} (8-23)

which, in the symmetric case, can be rearranged to (4-13). For the influence on the mode II stress intensity at the crack tip the solution can be obtained along similar lines. It finally follows that

$$dK_2^{\text{TIP}} =$$

$$G \frac{C}{4} \int_{A_{x_1,x_2}} \text{Im} \left[ \frac{1}{z^{3/2}} \left\{ 5\varepsilon_{11}^p + 3\varepsilon_{22}^p + 2i\varepsilon_{12}^p \right\} + \frac{3\bar{z}}{z^{5/2}} \left\{ \varepsilon_{11}^p - \varepsilon_{22}^p + 2i\varepsilon_{12}^p \right\} \right] dx_1 dx_2.$$  \hspace{1cm} (8-24)

To find the total effect of the transformation strains on the stress intensities, the expressions (8-23) and (8-24) have to be integrated over $\Omega$,

$$\Delta K_\alpha^{\text{TIP}} = \int_{\Omega} dK_\alpha^{\text{TIP}}.$$  \hspace{1cm} (8-25)
8.6 Crack deflection

For linear elastic material behaviour, Suresh and Shih (1986) give a review concerning the nominal stress intensity factors \( K_I \) and \( K_{II} \) (based on the projected length \( c \)) and the crack tip intensity factors \( k_I \) and \( k_{II} \), when an idealized crack contains a kink of length \( b \) inclined at an angle \( \beta_1 \) from the main crack plane. All quantities are indicated in Fig. 8.2. They then suggest that a first approximation of the stress intensity factors at the tip of the kinked crack can be calculated from the stresses that exist in the line of the propagating crack. When \( K_I \) and \( K_{II} \) denote the stress intensity factors of the main crack in the absence of the kink, then the local stress intensity factors \( k_I \) and \( k_{II} \), for the infinitesimal kink \((b/a \rightarrow 0)\) can be expressed in the form

\[
\begin{align*}
    k_I &= \lim_{r \to 0^+} \sqrt{(2\pi r)} \sigma_0(r, \beta_1) \\
    k_{II} &= \lim_{r \to 0^+} \sqrt{(2\pi r)} \tau_0(r, \beta_1)
\end{align*}
\]

and with (8-7) we find the stress intensity factors in the local reference system to be

\[
\begin{align*}
    k_I &= a_{11}(\beta_1)K_I + a_{12}(\beta_1)K_{II} \\
    k_{II} &= a_{21}(\beta_1)K_I + a_{22}(\beta_1)K_{II}
\end{align*}
\]

(8-26)

In our small scale analysis we implicitly assume that the length of the initial crack \( c \) is large compared to the permitted growth of the crack, so that in this situation the kink is to be considered as infinitesimal. Thus, if an initially straight crack is loaded by far field stress intensities \( K^\text{APP} \), and the crack is kinked, then the local stress intensity factors \( k_\alpha \) can be calculated using (8-27) and (8-8).

For the contribution of the transformation strains in the kinked configuration, the domain integrals (8-23) and (8-24) over the transformation zone should be determined in the local coordinate system, which has been rotated by an angle \( \beta_1 \), as shown in Fig. 8.2. Therefore, the coordinates of a transforming spot to the crack tip must be expressed in the local coordinate system, and also the transformation strains must be transformed to the local coordinate system. For the latter case the rotation matrix

![Fig. 8.2. Schematic showing a kinked crack](image)
\[ R_{ij} = \begin{bmatrix} \cos \beta_l & \sin \beta_l \\ -\sin \beta_l & \cos \beta_l \end{bmatrix} \quad (8-28) \]

must be used, in the rotation relation which is given by

\[ \varepsilon_{ij,\text{local}}^p = R_{ik} \varepsilon_{kl}^p R_{jl} \quad (8-29) \]

The influence on the stress intensities in this local coordinate system will be called \( \Delta k_T^{\text{TIP}} \). Then the stress intensities at the crack tip, in the local coordinate system, are defined by

\[ k_{\alpha}^{\text{TIP}} = k_{\alpha} + \Delta k_{\alpha}^{\text{TIP}} \quad (8-30) \]

The criterion for crack growth (8-4) [cf. Eqs. (4-19) and (4-20)] reads

\[ K_{\text{ref}} = K_C \quad (8-31) \]

where

\[ K_{\text{ref}} = \sqrt{ \left( k_1^{\text{TIP}} \right)^2 + \left( k_2^{\text{TIP}} \right)^2 } \quad (8-32) \]

The direction in which the crack will propagate (8-10), related to the local coordinate system, is defined by

\[ \left( \frac{\tan \frac{\beta_m}{2}}{2} \right)_{1,2} = \frac{1}{4} k_1^{\text{TIP}} \pm \sqrt{ \left( \frac{k_1^{\text{TIP}}}{k_2^{\text{TIP}}} \right)^2 + 8 } \quad (8-33) \]

again taking the angle belonging to the largest principal stress. In the global coordinate system the propagation direction would then be

\[ \beta_g = \beta_1 + \beta_m \quad (8-34) \]

### 8.7 Implementation

First we discuss the discretization of the boundary value problem as described in Sec. 8.4. Then the implementation of the new crack criterion is described.

#### 8.7.1 Discretization of the crack problem

The mesh is very similar to the mesh used before, see Figs. 4.5 and 4.6. The difference is that now the mesh covers the entire domain \( \Omega \), as defined in Fig. 8.1, and it is therefore twice as large. The lower half of the new mesh is obtained by reflection of the upper half, which is the original mesh. Where the material is not cracked, the two halves are connected with an extra row of elements. The crack is modelled by simply leaving out elements, as can be seen in Fig. 8.4(b) and (c). Again four zones can be distinguished. Zone 1 is a rec-
tangular shaped area which is the finest part of the mesh. This zone contains 92 by 6 square elements. The second zone forms the first transition from a rectangular to a circular region, far away from the crack tip. In the last two rows of this zone mesh adaptation reduces the number of elements in the zones further out. The number of elements over the height of this zone is 9. The third zone has a circular outer boundary and the fourth zone just brings the boundary further out, to reach the ‘far-field’ boundary. The number of rows in these two zones are respectively 5 and 30. The mesh is further illustrated in Fig. 8.4. It can be seen in Fig. 8.4c that, at the start, the crack tip is placed at three elements to the right of the left hand side of the rectangular region (zone 1) of the mesh.

8.7.2 Discretization of the crack growth formulation

From Fig. 8.4(c) and Fig. 8.5, where a close-up of the near tip region is shown, it may be clear that the crack is now modelled by a missing row of elements and thus has the same width as an element. The crack is no longer sharp but has a notch-like geometry. In general, if the length of the crack is large compared to the height, the notch-like geometry asymptotically approaches to the geometry of a sharp crack. However, in our small scale approach the length of the crack is not defined, and the so-called characteristic length \( L \) (as defined in Sec. 4.3) governs the scaling of the crack problem, and in particular it governs the size of the transformation zone. By an increasing value of \( L \), the number of elements over the height of the transformation zone increases and the relative width of the crack decreases. Thus, for large values of the characteristic length (\( L \to \infty \)), the notch geometry approaches a sharp crack. This is a preferable situation if we want to compare the results to our previous
Fig. 8.4. The finite element mesh used to analyse the small-scale crack growth problem.

analyses, where the crack was sharp. Test computations for increasing values of $L$ showed convergence to results for a sharp crack. Also, computations were performed with a special mesh, where the height of the middle row of elements was reduced to simulate a sharp crack.

The initial position of the crack tip is marked in Fig. 8.5 and if the critical stress intensity at the crack tip is reached, $k_{TIP} = K_C$, crack advance is performed. If the failure criterion (8-32) is met, crack growth is simulated by an element vanishing technique, as employed by Tvergaard (1982). The stiffness and the stresses of that particular element are linearly reduced to zero in $n$ steps.

Once the direction in which the crack wants to propagate, $\beta_m$, is determined, using (8-33), the new position of the crack tip is calculated by drawing a straight line from the pre-
Fig. 8.5. Position of the crack tip before crack growth

previous position under an angle $\beta_m$. Thus, the crack tip is now defined at the border of an adjacent element. The stiffness of the element through which the crack just propagated is linearly reduced to zero in $n$ steps. Next, the stress intensity at the tip can be determined and the load can be increased again to reach the critical stress intensity. In this way the crack can proceed through the mesh as shown by the enlarged crack tip area in Fig. 8.6. The shaded elements represent the elements which have vanished during the loading process. The crack path as obtained with the above procedure is marked, and the positions of the crack tips during the discrete crack growth process are indicated by small circles.

The transformation domain integral expressions are not available for non-straight cracks at the moment. Therefore we choose to approximate the crack path by a straight line over a certain length $L_{\text{ref}}$. Since the transformed material around the current crack tip will give the largest contribution to the integral, the straightened-out part of the crack is used to set the local coordinate system at the angle $\beta_1$. The angle $\beta_1$ is defined by fitting a linear

Fig. 8.6. Example of a possible crack path. Elements with zero stiffness appear shaded. The crack path is sketched, with current and previous crack tip positions marked by small circles.
function through the last part of the crack path using the method of least squares. The length over which this function is fitted, is defined by

$$ L_{\text{ref}} = R_{\text{ref}} L $$

(8-35)

where $L$ is the characteristic length of the problem and $R_{\text{ref}}$ is an input variable. The influence of the choice of $R_{\text{ref}}$ on the final results will have to be determined.

### 8.8 Results

The crack growth simulations have been performed over distances somewhat larger than $2L$, with material parameters $\nu = 0.3, \alpha = 1.15, \omega = 5, h_0 = 1.25, M = -\infty, a = 1, \lambda_c = 2$. The distribution of transformable material as defined in (8-1) has been shifted relative to the initial crack tip position over various distances by choosing $\lambda_{x2}$ in (8-2) as

$$ \lambda_{x2} \in [0, 0.125, 0.25, 0.375, 0.5] $$

(8-36)

For $\lambda_{x2} = 0$ and 0.5, the transformable phase is distributed symmetrically with respect to the $x_1$-axis and the crack does not deflect, as expected. For the remaining values of $\lambda_{x2}$, the distribution is not positioned symmetrically and the crack does deflect as shown in Fig. 8.7. The deviation from the initial path is strongest for $\lambda_{x2} = 0.25$. It can be seen that first the crack is attracted to the area with less transformable phase, as crack growth in this area costs less energy. Then the crack starts to feel the influence of the large amount of transformable phase ahead, and at the same time the crack seems to be attracted towards the area with little transformable phase below. Thus after a crack growth of about $L/3$ the sign of the angle between the $x_1$-axis and the tangent of the crack path is altered from positive to negative. The crack crosses the $x_1$-axis and reaches a local minimum for $\Delta a = 4L/3$. The next area with large amount of transformable material is approached and the crack smoothly deflects and grows towards the subsequent area of reduced transformable phase. The amplitudes of the deviations from the original crack path will probably depend on $\omega$. The paths for $\lambda_{x2} = 0.125$ and $0.375$ show a similar crack meandering behaviour. Note that the mode I load tends to direct the crack towards the $x_1$-axis. Computations for $\lambda_{x2}$ close to 0 or 0.5 showed that the crack did not deflect and continued growing along the $x_1$-axis.

The toughness development during crack growth is affected considerably by the value of $\lambda_{x2}$. In chapter 7 it was found that the periodically varying transformable phase caused oscillations in the toughness during crack growth. The results suggested that the maxima of the toughness curves always exceed the toughness curve for homogeneous materials. In the descending parts of the toughness curves, crack growth is unstable. The crack grows dynamically to the following region of high fraction of transformable material. In the simulation, however, dynamic crack growth effects have not been taken into account. In Fig. 8.8 it can be seen that the oscillating behaviour of the toughness is reduced. The curves for the two symmetric cases, $\lambda_{x2} = 0$ and 0.5, are the outer boundaries for fluctuations, and the curves tend to the solution for homogeneous materials, the dashed curve ($a = 0$). Especially for $\lambda_{x2} = 0.25$ the oscillations are very limited and the curve almost coincides with the curve for the homogeneous case.
Fig. 8.7. The results for three crack paths derived from crack growth simulations over \( \Delta a = 2L \), with material parameters \( v = 0.3, \alpha = 1.15, \omega = 5, h_0 = 1.25, M = -\infty, a = 1, \lambda_c = 2 \) and for \( \lambda_{x_2} = [0.125, 0.25, 3.75] \).

Fig. 8.8. Toughness development curves for crack growth over \( \Delta a = 2L \), with material parameters \( v = 0.3, \alpha = 1.15, \omega = 5, h_0 = 1.25, M = -\infty, a = 1, \lambda_c = 2 \) and for \( \lambda_{x_2} = [0, 0.125, 0.25, 3.75, 0.50] \) compared to the crack growth resistance curve of a homogeneous material \( (a = 0) \).

8.9 Conclusions

The current analysis shows that the direction of the crack can be influenced by the transformation strains. A non-symmetric distribution of the transformed zone, with respect to the \( x_1 \)-axis can cause a mode II stress intensity factor component, symmetrical distributions
show no crack deflection. The results show that the toughness development curves have the tendency to approach the curve for the homogeneous material. Thus reducing the positive effect which was predicted in chapter 7. The results presented here, however, must be seen as preliminary and more computations have to be performed before definite conclusions can be made. We feel that computations for different values of \( \omega, h_0 \) and \( \lambda_c \) are necessary. Moreover, crack growth has to be performed over a much larger area, until a certain steady state is reached. Finally, it is necessary to study the effect of different distribution functions, \( D \), for instance the effects of increasing the wave length in \( D \) for only one direction.
CHAPTER 9

General Conclusions

In this thesis, we have presented numerical studies of transient crack growth in ceramic composites exhibiting transformation-plasticity based on the recent model of Sun et al. (1991) that includes the effect of transformation-induced dilatation as well as shear. Our analyses supplement those of Hom and McMeeking (1990) who considered only dilatational transformations. The finite element results obtained here with the Sun et al. (1991) model show a very significant influence of the transformation shear strains on the transformation zone size and shape, as well as on the toughness development during crack growth. An increasing influence of the shear effect, as governed in the model by the parameter $h_0$, roughly speaking, leads to larger and more diffuse transformation zones. The increase of toughness with increasing value of $h_0$ has been found to be quite substantial as compared with the toughness increase that is obtained by purely dilatational transformation only. For values of $h_0$ between 1 and 1.5, which are representative for ZrO$_2$ composites, we have found increases in toughness that are 4 to 8 times larger than without transformation-induced shear strains. Since, so far, dilatant transformation-based theory has underestimated the toughness enhancement found in experiments (Evans and Cannon, 1986), the present results with transformation-induced shear effects contribute to explaining this difference.

Reverse transformation may occur, but will only occur in the wake of the crack when the crack growths, and the material in the wake unloads. From the present study in chapter 6 we may conclude that the toughening during crack growth does depend strongly on the amount of reverse transformation. In all cases considered the toughness increase upon crack growth is lowered if reverse transformation takes place in the wake of the growing crack. The decrease is most dramatic for so-called super or pseudo-elastic materials ($M = 1$), where reverse transformation immediately follows upon unloading. It may be concluded from the parameter study, that this class of materials exhibits some initial toughening, but after a small amount of crack growth almost no toughness increase is left.

In chapter 7 we study materials in which the transformable phase is non-homogeneously distributed. From this study we can conclude that a heterogeneous distribution of transformable phase may give rise to an increase in toughness, compared to materials with a
perfectly homogeneous distribution of ZrO₂. Although the effect is tempered for larger values of \( \omega \) it certainly seems to be an improvement for the toughness of the material. However, in chapter 8 we see that the direction of the crack can be influenced by the transformation strains. A non-symmetric distribution of the transformed zone, with respect to the \( x_1 \)-axis can cause a mode II stress intensity factor component, symmetrical distributions show no crack deflection. The results show that the toughness development curves have the tendency to approach the curves for homogeneous materials.
Appendices

Appendix A

Here the tensor of instantaneous moduli, $L_{ijkl}$, which takes into account the transformation plasticity is derived cf. (3-54). The strain rates are given by

$$\dot{E}_{ij} = M_{ijkl}^{0}\dot{\Sigma}_{kl} + \dot{E}^{p}_{ij}$$  \hspace{1cm} \text{(A.1)}$$

where

$$L_{ijkl}^{0} = \frac{1}{1+\nu} \left[ \frac{1}{2} (\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) + \frac{\nu}{1-2\nu}\delta_{ij}\delta_{kl} \right]$$ \hspace{1cm} \text{(A.2)}$$

With the help of

$$\dot{E}^{p}_{ij} = \frac{\partial F_{+}}{\partial \Sigma_{ij}} \dot{f} = \frac{1}{g} \frac{\partial F_{+}}{\partial \Sigma_{ij}} \dot{\Sigma}_{ij}, \hspace{0.5cm} g = \frac{2}{3}B_{1}A^{2} + 3B_{2}(\varepsilon^{pd})^{2} + \alpha B_{0}(\varepsilon^{pd})^{2}$$ \hspace{1cm} \text{(A.3)}$$

it follows that

$$\dot{E}_{ij} = M_{ijkl}\dot{\Sigma}_{kl} + \frac{1}{g}T_{ij}T_{kl}\dot{\Sigma}_{kl}$$ \hspace{1cm} \text{(A.4)}$$

where

$$T_{ij} = \frac{\partial F_{+}}{\partial \Sigma_{ij}} = \varepsilon^{pd}\delta_{ij} + A\frac{s_{ij}^{M}}{\sigma_{e}^{M}}, \hspace{0.5cm} s_{ij}^{M} = S_{ij} - fB_{1}(\varepsilon_{ij}^{ps})\nu_{i}$$ \hspace{1cm} \text{(A.5)}$$

When we multiply Equation (A.4) with $L_{klij}^{0}$ it follows that

$$L_{klij}^{0}\dot{E}_{ij} = \dot{\Sigma}_{kl} + \frac{1}{g}L_{klij}^{0}T_{ij}T_{mn}\dot{\Sigma}_{mn}$$ \hspace{1cm} \text{(A.6)}$$
and after multiplying by $T_{kl}$ we have

$$T_{kl}L_{kl}^0 \dot{E}_{ij} = \left(1 + \frac{1}{g} T_{ab} L_{abcd}^0 T_{cd} \right) \left(T_{mn} \dot{\Sigma}_{mn} \right). \quad (A.7)$$

Hence,

$$T_{mn} \dot{\Sigma}_{mn} = \left(1 + \frac{1}{g} T_{ab} L_{abcd}^0 T_{cd} \right)^{-1} T_{mn} L_{mnij}^0 \dot{E}_{ij}. \quad (A.8)$$

This equation can be used to eliminate $T_{kl} \dot{\Sigma}_{kl}$ from Equation (A.6) resulting in

$$\dot{\Sigma}_{kl} = \left\{ L_{kl}^0 - \frac{1}{g} L_{klpq}^0 T_{pq} T_{mn} L_{mnij}^0 \right\} \dot{E}_{ij}. \quad (A.9)$$

Thus the rate constitutive equations can be summarized as

$$\dot{\Sigma}_{ij} = L_{ijkl} \dot{E}_{kl} \quad (A.10)$$

where

$$L_{ijkl} = \begin{cases} 
L_{ijmn}^0 T_{mn} T_{pq} L_{pqkl}^0 & \text{when } F_+ = 0 \text{ and } \dot{f} > 0 \\
\frac{1}{g} + \frac{1}{g} T_{ab} L_{abcd}^0 T_{cd} & \text{when } F_+ \neq 0 \text{ or } \dot{f} \leq 0 
\end{cases} \quad (A.11)$$

**Appendix B**

In terms of the stress functions of Kolosov and Muskhelishvili (see Muskhelishvili, 1953) the governing equations for isotropic plane elasticity are

$$\sigma_{11} + \sigma_{22} = 2 \left[ \ddot{\phi}(z) + \phi'(z) \right] \quad (B.1)$$

$$\sigma_{22} - \sigma_{11} + 2i\sigma_{12} = 2 \left[ \ddot{\psi}(z) + \psi'(z) \right] \quad (B.2)$$

$$u_1 + iu_2 = \frac{1 + \nu}{E} \left[ \kappa \phi(z) - z \ddot{\phi}(z) - \ddot{\psi}(z) \right] \quad (B.3)$$

where $\kappa = (3 - \nu) / (1 + \nu)$ for plane stress and $\kappa = (3 - 4\nu)$ for plane strain. The bar denotes the complex conjugate. The solution for the elastic stress field due to two initially strained circular plastic spots with initial strains $\varepsilon_{111}, \varepsilon_{12},$ and $\varepsilon_{12} = \varepsilon_{21},$ which are symmetrically placed on either side of the crack (see also Hutchinson, 1974), is given by

$$\phi(z) = \phi_0(z) + \ddot{\phi}_0(z) + \phi_1(z) + \ddot{\phi}_1(z) \quad (B.4)$$

$$\psi(z) = \psi_0(z) + \ddot{\psi}_0(z) + \psi_1(z) + \ddot{\psi}_1(z) \quad (B.5)$$

132
The functions \( \phi_0(z) \), \( \psi_0(z) \), \( \phi'_1(z) \) and \( \psi'_1(z) \) are

\[
\phi_0(z) = \frac{1}{2} EA c_2 (z - z_0)^{-1}, \quad \psi_0(z) = EA \left[ -(c_1 + c_2) (z - z_0)^{-1} + \frac{1}{2} c_2 z_0 (z - z_0)^{-2} + \frac{1}{2} c_2 R^2 (z - z_0)^{-3} \right],
\]

(\ref{eq:phi_0}) \hspace{1cm} (\ref{eq:psi_0})

\[
\phi'_1(z) = -\frac{1}{2} \left[ 2\phi_0(z) + z\phi''_0(z) + \psi_0(z) \right] - \frac{1}{2} E A f(z) \sqrt{z}, \quad \psi'_1(z) = -z\phi''_1(z),
\]

(\ref{eq:phi_prime_1}) \hspace{1cm} (\ref{eq:psi_prime_1})

and

\[
A = \pi R^2, \quad c_1 = \frac{1}{2\pi} \left( \varepsilon_{22}^p - i \varepsilon_{12}^p \right), \quad c_2 = \frac{1}{4\pi} \left( \varepsilon_{11}^p - \varepsilon_{22}^p + 2i \varepsilon_{12}^p \right),
\]

(\ref{eq:c_1_c_2})

\[
f(z) = \frac{\sqrt{z_0}}{2z_0 (z - z_0)^2} \left\{ -c_1 (z + z_0) + \frac{c_2 (-z_0^2 + 6z_0^2 + 3z_0^2 - 3z_0^2 z_0 - 6z_0 z_0 + z_0^2)}{4z_0 (z_0 - z)} \right. \\
\left. - \frac{3c_2 R^2 (-5z_0^2 + 15z_0^2 z + 5z_0 z_0^2 - z_0^2)}{16(z_0 - z)^2} \right\}.
\]

(\ref{eq:f(z)})

Here the spots have radius \( R \), area \( A \), modulus of elasticity \( E \) and \( z = x_1 + ix_2 \) is the complex variable denoting a point at \( (x_1, x_2) \). Furthermore \( z_0 = x_1^0 + ix_2^0 \) is the point at the centre of the circular spot located above the \( x_1 \)-axis. In the situation of two spots which have dilatant initial strain \( 3\varepsilon_{ii}^{pd} \) and plane strain \( (\varepsilon_{i3} = 0) \) deformation, the nonzero initial strains are \( \varepsilon_{11}^{i} = \varepsilon_{22}^{i} = (1 + v) \varepsilon_{12}^{pd} \). These strains are used to calculate the values \( c_1 \) and \( c_2 \) in (\ref{eq:c_1_c_2}). In this case (\ref{eq:phi_0}) and (\ref{eq:phi_prime_1}) reduce to

\[
\phi_0 = 0,
\]

(\ref{eq:phi_0_zero})

\[
\phi'_1(z) = -\frac{1}{2} EA (1 + v) \frac{\theta}{3} \frac{1}{2\pi} \frac{1}{(z - z_0)^2} + \frac{1}{4} EA (1 + v) \frac{\theta}{3} \frac{1}{2\pi} \frac{1}{z_0} \sqrt{z_0} \frac{(z + z_0)}{(z - z_0)^2}.
\]

(\ref{eq:phi_prime_1_zero})

When we assume plane strain this leads to

\[
\sigma_{11} + \sigma_{22} = \frac{2E\theta R^2}{3(1-v)} \text{Re} \left\{ g(z, z_0) + g^*(z, z_0) \right\},
\]

(\ref{eq:stress})

where
\[ g(z, z_0) = -\frac{1}{2} \frac{1}{(z-z_0)^2} + \frac{1}{4} \frac{\sqrt{z_0}}{z} \frac{(z+z_0)}{(z-z_0)^2} \]  

(B.15)

and \( g^*(z, z_0) \equiv \overline{g(z, z_0)} \). The mean stress at any point \( z \) outside the two spots is given by

\[ \sigma_m = \frac{2}{9} \frac{(1+v)}{1-v} \frac{E\theta R^2}{\text{Re}} \{ g(z, z_0) + g^*(z, z_0) \} \]  

(B.16)

which can be written as

\[ \sigma_m = \frac{E\theta R^2}{18} \frac{(1+v)}{1-v} \frac{1}{\sqrt{(zz_0)} \left[ \sqrt{z} + \sqrt{z_0} \right]^2} + \frac{1}{\sqrt{(zz_0)} \left[ \sqrt{z} + \sqrt{z_0} \right]^2} \]  

(B.17)

The effect on the stress intensity factor \( K_1 \) can be calculated using the standard definition of \( K_1 \). One finds

\[ K_1 = \lim_{x_1 \to 0^+} \sqrt{(2\pi x_1)} \sigma_{22}(x_1, 0) = -2\sqrt{2\pi} E\theta R \text{Re}[f(0)]. \]  

(B.18)

or in the case of the two spots with dilatant initial strains it follows that

\[ K_1 = \frac{E\theta R \exp(d)}{2\sqrt{2\pi} (1-v)} [z_0^{-3/2} + \bar{z}_0^{-3/2}] \]  

(B.19)

Appendix C

The procedure for calculating the term

\[ \text{Re} \int \int_A z_0^{-3/2} dA \]  

(C.1)

appearing in (4-32) is demonstrated for a triangular region \( A \). Suppose the sides of the triangle are defined by one side parallel to the \( x_2 \)-axis and the other two by \( ax + b \) and \( cx + d \), respectively, as shown in Fig. 1.9. When \( z_0 = x_1 + ix_2 \), then we carry out the surface integral by first integrating over \( x_1 \) and then over \( x_2 \). When the coordinates of node \( i \) are defined by \( (x_1^i, x_2^i) \), it follows that the integral can be written as,

\[
\int \int \text{Re} \left[ (x_1 + ix_2)^{-3/2} \right] dx_2 dx_1 = \\
\int \int_1^{x_1} \text{Re} \left\{ \left( \frac{4i}{1+ic} (x + i(cx + d)) \right)^{1/2} - \frac{4i}{1+ia} (x + i(ax + b)) \right\} \]  

\[ x_1^2 \]

(C.2)

Now the boundaries of the integral over \( x_1 \); \( x_2^1 \) and \( x_1^1 \) in (C.2) can be substituted and, for example, evaluation of the first term of (C.2) leads to
Fig. 1.9. Definition of the boundaries of a triangle.

\[
\left[ \text{Re} \left\{ \left( \frac{4i}{1+ic} (x + i(cx + d))^{1/2} \right) \right\} \right] = \frac{4c}{1 + c^2 f_2^{1/2}} \left[ \cos \left( \frac{1}{2} \varphi_2 \right) - \frac{1}{c} \sin \left( \frac{1}{2} \varphi_2 \right) \right]
\]

when \( \cos \varphi_2 = \frac{x_2}{\sqrt{[(x_2)^2 + (cx_2 + d)^2]}} \) and \( r_2 = \sqrt{[(x_2)^2 + (cx_2 + d)^2]} \). All other terms can be calculated along the same lines.

Currently it is also possible to use symbolic algebra programs for such problems. In this case, the full analytical solution of (4-32) was obtained using MAPLE:

Inputfile for Symbolic Algebra Program MAPLE on 22 January 1992
The FORTRAN subroutine will be written by MAPLE and represents the encoded symbolic integration of:

\[
V W (x - i y)
\]

\[
e := \frac{3/2}{5/2} + \frac{(x + i y) (x + i y)}{(x + i y) (x + i y)}
\]

The commands that have been used are:

\[
e := V^*(x+I*y)^(-3/2); \\
f := \text{int}(e, y = a*x+b..c*x+d); \\
g := \text{int}(f, x = x2..x3); \\
\text{fortran}(g, \text{filename}=\text{foo}, \text{optimized});
\]
\[
f := W^*(x+I*y)^(-5/2)*(x-I*y); \\
f := \text{int}(f, y = a*x+b..c*x+d); \\
g := \text{int}(f, x = x2..x3); \\
\text{fortran}(g, \text{filename}=\text{foo}, \text{optimized});
\]
References


Chen, I. W. and Reyes-Morel, P. E. (1986), Implications of Transformation Plasticity in Zirconia-Containing...
Ewalds, H. L. and Wanhill, R. J. H. (1986) Fracture Mechanics, Edward Arnold (Australia) and Delftse Uitgevers Maatschappij, Delft, the Netherlands.
Hahn, H. G. (1976), Bruchmechanik, Teubner Studienbücher Mechanik, Stuttgart, Germany. (In German)

Karihaloo, B. (1990), Contribution of the $t \to m$ Phase Transformation to the Toughness of ZTA. In: *Structural Ceramics Processing, Microstructure and Properties* (Ed. by Bentzen, J. J. and co-workers), pp. 359-364, Riso, Denmark.


pp. 648-657.
Transformable Reinforcement. Submitted to *Mechanics of Materials*.
Visser, A. de (1993), *Hardop kijken; een inleiding tot kunstbeschouwing*, Sun, Nijmegen, the Netherlands. (in Dutch)
Author Index

A-C
Amazigo 12, 18
Andreasen 18
Bakker 45
Barenblatt 5
Becher 18
Bowman 82
Broek 5, 116
Budiansky 9, 11, 12, 13, 15, 16, 17, 18, 20,
21, 29, 31, 32, 33, 34, 36, 43, 45, 46, 48,
51, 55, 57, 74, 75, 77, 78, 79, 98
Bueckner 119
Cannon 13, 78, 99, 129
Chen 13, 23, 25, 38, 39, 72, 77, 79, 81
Claussen 18, 113
Cotterel 116
Cui 18

D-F
Delaey 81
Den Exter 101
Eshelby 26
Evans 8, 9, 12, 13, 14, 15, 17, 18, 25, 41, 43,
44, 75, 78, 99, 101, 129
Ewalds 5
Faber 14, 15
Fu 14

G-I
Gao 119
Garvie 9
Green 9, 11
Griffith 5
Gupta 9

Hahn 5
Heuer 9
Hom 13, 53, 60, 62, 74, 75, 77, 129
Hutchinson 11, 14, 47, 119
Hwang 33, 81
Irwin 6

J-L
James 79, 82
Karihaloo 101
Kingery 1
Kirchner 18
Kolosov 47
Krishnan 81
Kriven 9
Lambropoulos 13, 23, 78
Lange 9
Lutz 113

M-O
Marshall 18, 75, 79, 82
McCullough 9
McMeeking 9, 11, 12, 13, 20, 43, 44, 53, 60,
62, 74, 75, 77, 129
Mori 27
Mura 26
Mushkelishvili 47
Oliver 18
Ortiz 14, 15, 34
Otsuka 81

P-R
Parks 56
Patoot 81
Porter 10
Reyes-Morel 13, 23, 25, 38, 39, 72, 77, 79,
81
Rice 16, 30, 34, 45, 46, 116, 119
Rose 9
Rühle 8, 9, 14, 41, 75, 101, 102, 104
S-U
Shetty 72, 75
Shih 121
Shimizu 81
Sigl 15
Stam 8, 45, 59, 78, 82, 102
Stump 12, 13, 18, 43, 45
Sun 13, 23, 24, 25, 26, 29, 33, 37, 38, 43,
53, 54, 56, 60, 77, 78, 81, 82, 100, 129
Suresh 121
Tanaka 27
Thouless 18
Tiegs 18
Trueblood 9
Truskinovsky 13
Turner 46
Tvergaard 124

V-Z
Van der Giessen 59, 78, 82
Visser 1
Wanhill 5
Wartimont 81
Xu 100
Yu 72, 75
Subject Index

A
agglomeration of powders 101
alumina 9
averaging method 27

B
boundary conditions 118
boundary values 49
bulk moduli like parameters 27
bulk modulus 20

cubic 9
debonded 18
deflection 18
degradation 15
deviatoric components 55
dilatant 11, 20
model 53
dilatation 13, 24
discretization 53, 122
discussion 62
ductile
particles 8
directional 8

E
eigenstrains 27
eigenstress 26
elastic moduli 24
element vanishing technique 124
elements 48
quadrilateral 48
equilibrium 19
energy
chemical free 27
complementary free 27
dissipation 28
elastic strain 26
Helmholtz (or free) 27
potential 5
release rate 6, 7, 45, 116
surface 27

145
Eshelby tensor 26
estimation of the material parameters 39
experimental
  stress-strain curves 38

F
fibre 8, 17
finite element method 48
flowchart 52
forward 26
fracture
  mechanics 5
  toughness 8, 42
fracture toughness 62
friction 28

G
Gaussian-integration 57
grain
  size 15
Griffith relation 7

H
hardening 29, 37

I
inclusions 24
  spherical 26
increment 50
  loading 52
incremental
  stress-strain relations 21
instantaneous moduli 131
integral
  transformation domain 119
integration
  Gaussian 57
intermediate segment 20
internal variable 28
  constitutive theory 30
iteration 52

J
J-integral 43, 56
  concept 45

K
kinking of the crack 121

L
lattice
  parameters 9
liquid drop analogy 23
local 121
local reference system 121
localization 21, 34
  (or acoustic) matrix 35
  condition 36
  shear bands 73

M
macroscopic 19, 24
  quantities 24
  stress tensor 27
martensitic 9
material parameters 39
matrix 24
mesh 49, 50, 123
micromechanical
  models 2, 8
micromechanics 13
microscopic 24
  quantities 24
microstructural
  changes 7
microstructure
  non-homogenous distribution 102
microstructures 11
modes of crack loading 7
moduli
  instantaneous 31
  monoclinic 9

N
nodal release technique 53
nucleation 15
numerical approach 48

O
objective 2

P
parameter study 59
  reversible transformation 83
parameters
  governing 23, 33
  nondimensional 33, 59
nondimensional, reversible transformation 84
non-homogeneous distribution 104
Partially Stabilized Zirconia 9
particles
metal 15
path independent 45
path-independence 43
peak values 62
periodic function 103, 115
plane strain 12
platelet 8
toughening 17
proportional 43
pseudoelasticity 81
PSZ 9, 40

R
rate equations 31
reinforcements 15
relations
incremental stress-strain 30
result
crack deflection 126
results 62
homogeneously 59
non-homogeneous distribution of
transformable phase 101
supercritical 75
reverse 26
rotation matrix 121

S
Shape Memory Alloys
SMA 81
shear 13, 20, 24
band 34
component 61
maximum amount 61
strain 9
shear bands 72
shear modulus 20
shielding 42
steady-state 14
SHPMEM 56
slope of the intermediate stress-strain
curve 23
small scale 41
spots
circular cylindrical 47
transforming 11, 47
spring model 16
elastic 16
elastoplastic 16
rigid-plastic 17
steady state
value 12
strain rate 25
macroscopic 25
plastic 25
transformation 22
strength of the transformation 23
stress 6
critical mean 11, 14, 20
critical principal 13
deviatoric 25
deviatoric components 27
-induced 9
mean 27
mean criterion 10
normal critical 14
von Mises 25
stress intensity factor 7
applied 8
at crack tip 45
stress-strain
reversible transformation 82
stress-strain relations 38
subcritical 12, 21, 33, 37
sub-incrementing 55
supercritical 12, 21, 29, 33
surface integral 57
synergism 18

T
temperature 27
test
triaxial compression 39
tetragonal 9
Tetragonal Zirconia Polycrystal 9
thermodynamic
second law of 28
state 27
toughening
ductile particle 15
microcrack 13
transformation 9
toughness 74
development 74
development for heterogenous distributions 112
development, reversible transformation 98
enhancement 42
relative increase 43
supercritical 77
transformation 9, 61
criterion 22, 26
energy 51
forward 28
fraction 22, 26
martensitic 20
plasticity 23
reverse 28
reversible 81
strains 9
yield functions 29
transformation domain
weight functions 119
transformation zone 12, 44, 61, 62
height of the 41, 61
initial 12
supercritical 76
transformation zones
heterogeneous distributions 105
reversible transformation 84
twinning 10, 25
TZP 9, 40

U
unloading 46

V
variables
dimensionless 23
volume
average 24
expansion 9
fraction 20

W
whiskers 8, 18

Y
yielding conditions 26

Z
ZIRCON 53
zirconia 9
based ceramics 19
Zirconia Toughened Alumina 9
ZTA 101
zone
bridging 8
initial 11
process 7
transformation 61
ZTA 9
Samenvatting

Een van de hoofddoelen in de ontwikkeling van structurele keramieken is het verbeteren van de taaiheid. Omdat de mate van taaiheid volledig afhankt van het scheurgedrag, is het van belang om te weten welke mechanismen verantwoordelijk zijn voor het specifieke scheurgroeigedrag. Kennis omtrent de invloed van een specifieke mechanisme kan worden verkregen met behulp van micromechanische modellen die het alles omvattend effect van microbreuk beschrijven. In hoofdstuk 2 is een korte introductie in de lineaire breukmechanica gegeven, gevolgd door een kort overzicht van de hedendaagse taaiheidsmechanismen. Echter, in de rest van ons werk hebben we ons gericht op een vertaaisingsmechanisme dat transformatievertaaiing genoemd wordt.

Dit vertaaisingsmechanisme is gebaseerd op een spanningsgeinduceerde (martensitisch-achtige) transformatie, die op kan treden in zirconia bevattende keramieken. In een deeltje dat onbelemmerd vervormen kan, veroorzaakt de transformatie van de tetragonale structuur naar de monoclinc structuur een volume vergroting van 4.5% en een afschui vervorming van 16%. Echter, in een ingeklemd deeltje treedt tweekleuringen op en de resulterende macroscopische afschuifrek in een ingeklemd deeltje zal veel kleiner zijn omdat de richting van de verschillende afschuiifbanden wisselt van band tot band. Het was daarom dat, tot een paar jaar geleden, de meeste materiaalmodellen alleen de volume vergroting in rekening brachten. Deze modellen hebben een grote betekenis gehad bij het begrijpen van transformatievertaaiing, maar de kwantitatieve overeenkomst met experimentele gegevens was onbevredigend (zie McMeeking en Evans, 1982; Budiansky et al. 1983; Hom en McMeeking, 1990). Recent is er een materiaalmodel voorgesteld dat ook de transformatie afschuifrek in rekening brengt (Sun et al., 1991). Dit materiaalmodel is beschreven in hoofdstuk 3, waarin we ook het vervormingsgedrag van zulke materialen bestuderen. In het bijzonder is er gekeken naar eventueel optreden van lokalisatie. Hier doelen wij met lokalisatie op situaties waarin inelastische vervorming zich concentreert als een gevolg van het materiaalgedrag.

In hoofdstuk 4 is het scheurgroei model behandeld dat is gebruikt bij het voorspellen van het breukgedrag van zirconia bevattende keramieken. Er is een zogenaamd small scale scheur probleem geformuleerd dat wordt opgelost met behulp van een eindige elementen methode. De materiaalvergelijkingen, die in hoofdstuk 3 zijn gepresenteerd, zijn in een zodanige vorm gegeten dat die op een numerieke manier kunnen worden opgelost. Scheurgroei treedt op als de kritische spanningsintensiteit aan de scheurtop bereikt wordt, die berekend wordt met behulp van een transformatie domein integraal om het effect van de transformatierekken rondom de scheurtip in rekening te brengen. Scheurgroei wordt gesisimuleerd met een nodal release methode.

De resultaten van uitgebreide parameter studies naar het effect van transformatie rekken op het scheurgroeigedrag zijn gepresenteerd in hoofdstuk 5. We laten zien dat de taaiheidstoename tijdens scheurgroei veel groter is dan de vorige voorspellingen, waar alleen de volume vergroting was meegenomen. De overeenstemming tussen de voorspelde taaiheids waarden en de experimenteel bepaalde waarden is aanzienlijk verbeterd. De resultaten zijn weergegeven met behulp van afbeeldingen van de transformatie zones en grafieken van de taaiheidsontwikkeling gedurende scheurgroei. In hoofdstuk 6 onderzoeken we het effect van reversibele transformatie, daar waar onlasten optreedt, op de taaiheidsontwikkeling, en in hoofdstuk 7 onderzoeken we het effect van een niet-homogeen verdeelde
transformeerbare fase. Uit de resultaten beschreven in hoofdstuk 6 kunnen we concluderen dat reversibele transformatie altijd resulteert in een gereduceerde taaiheid ten opzichte van irreversible transformatie. Uit hoofdstuk 7 kunnen we concluderen dat een niet homogeen verdeelde transformeerbare fase resulteert in een toenemende taaiheid. Echter, in hoofdstuk 8 staan we de scheur toe om af te buigen als gevolg van de transformatie rekken van de niet homogene doorsnede. Dan blijkt dat de taaiheid voor deze materialen nauwelijks afwijkt van de taaiheid van homogene materialen. Voor dit laatste probleem moesten zowel de transformatie domein integralen worden geherformuleerd als ook het breukcriterium. Scheurgroei wordt nu gesimuleerd door een zogenaamde element vanish techniek.