Microstructural Finite Element Modeling of Metals

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Front page: Periodic cell generated by the Voronoi algorithm containing 50 polyhedrons.
Preface

When I started as a PhD student in September 1998, I didn’t know much about the Department of Solid Mechanics at KTH. Rumors did however say that Professor Peter Gudmundson was an excellent advisor. Therefore, I immediately accepted the offer to come and work for him. I have had no reason to regret that. Now, I can conclude that Peter is an excellent leader and co-worker that has supported and guided me during the past years.

This work has been financed by the Swedish Foundation for Strategic Research, SSF, through the Brinell Centre at KTH. The Brinell Centre is a multidisciplinary research school where I had the opportunity to meet graduate students from other departments. This has broaden my horizons for research, since I have learnt about research that I would not have seen otherwise. At the Brinell centre, the work has been part of a multidisciplinary project group called Computational Material Science. This project has been performed in collaboration with Dilip Chandrasekaran, at the Department of Materials Science and Engineering at KTH. We have used the same material to model different mechanisms, and we have together performed the experiments reported in the thesis. I really appreciate Dilip’s thorough knowledge of the steels used, and his microscopical skills that have been fruitful in analyzing the microstructures.

During two trips to the United States I had the pleasure to travel together with Dr Adam Wikström. These were great trips where we learned a lot, especially how to get really large rental cars, but also how cooperation can result in papers.

A reliable computer and network is necessary when you do computational work. I am indebted to Per Berg for supplying that, and also his ability to supply me with the best and newest computers over the years.

I also want to thank all my other colleagues at the Department of Solid Mechanics for making the time at work enjoyable, and especially to all of those participating in all kinds of sport events that we do.

Lastly, to my beloved wife Karin whom I met, married and built our house with during the past years. You have given me wonderful life outside work.

Tullinge in February 2003

Mikael Nygård
List of appended papers

- **Paper A:** Micromechanical Modeling of Ferritic/Pearlitic Steels
  Mikael Nygårs and Peter Gudmundson

- **Paper B:** Three-Dimensional Periodic Voronoi Grain Models and Micromechanical FE-Simulations of a Two-Phase Steel
  Mikael Nygårs and Peter Gudmundson,
  *Computational Materials Science, 24*:513-519, 2002

- **Paper C:** Anisotropy and texture in Thin Copper Films - an Elasto-Plastic Analysis
  Adam Wikström and Mikael Nygårs

- **Paper D:** Number of grains necessary to homogenize elastic materials with cubic symmetry
  Mikael Nygårs

- **Paper E:** Comparison of Surface Displacement Measurements in a Ferritic Steel Using AFM and Non-Local Plasticity
  Dilip Chandrasekaran and Mikael Nygårs
  Report 329, Department of Solid Mechanics, KTH, Stockholm, 2003

- **Paper F:** Incorporating Strain Gradients in Micromechanical Modeling of Polycrystalline Aluminum
  Mikael Nygårs
  Report 330, Department of Solid Mechanics, KTH, Stockholm, 2003

- **Paper G:** Numerical Investigation of the Effect of Non-Local Plasticity on Surface Roughening in Metals
  Mikael Nygårs and Peter Gudmundson
  Report 331, Department of Solid Mechanics, KTH, Stockholm, 2003
Abstract

The mechanical properties of metals have been investigated. This has been done by creating micromechanical models based on the microstructural data available for the materials of interest. Thus, models containing a grain structure with appropriate constitutive equations have been created. Periodic cells on the micrometer scale have been shown to be sufficient to represent the materials, when macroscopic properties are evaluated.

Micromechanical modeling by the finite element method can be divided into three different parts: geometry, boundary conditions and constitutive equations. These parts have more or less been illustrated and used in the seven appended papers.

The geometric outlines of the grain structures are represented by the Voronoi algorithm. Hence, polyhedrons are used to represent three-dimensional grain structures, while two-dimensional models are represented by polygons. Two different approaches are used. Either, space is divided into grains by application of the Voronoi algorithm. Thus, grain boundaries are represented by planes or lines. Thereafter, the grains are meshed with an adaptive mesh generator. Alternatively, a mesh is created before the Voronoi algorithm is applied. The grain boundaries will in the latter case be kinky, since the outline of the predefined mesh is followed when grains are formed. The former method results in smaller elements close to grain boundaries. This fact is used to study two-phase ferrite-pearlite steels, since pearlite and the small elements have the same location.

Representative volume elements (RVEs) of the materials are created by considering a sufficient number of grains, and it is shown how this number depends on anisotropy and loading. To avoid edge effects in the models, the volume elements are made periodic and periodic boundary conditions are utilized to constrain the models. In the present implementation of periodic boundary conditions, average stresses and/or average strains are prescribed over the periodic cell.

A non-local crystal plasticity theory that incorporates slip gradients in the hardening has been implemented. It is shown that this concept can be used to account for the effect “smaller is harder”. Furthermore, the effect of non-local plasticity on the deformation of a free surface is investigated in detail. It is shown that the surface roughness decreases as an effect of strain gradients.

Lastly, all numerical work done here aims to mimic experiments that have been performed. This includes microscopic investigations, tensile testing, investigations by atomic force microscopy, but also experimental data from the literature.
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Chapter 1

Introduction to modeling of materials

The fields of solid mechanics and materials science are by tradition old and basic areas of knowledge that are mandatory in several engineering programs. Although, those are cutting edge research areas. Great progress is still made within the respective fields. In this thesis, one branch of solid mechanics research (in the borderland to materials science) is highlighted by modeling materials via microstructure. If one considers solid mechanics as a discipline where the objective is to create models for material and structural behavior, and materials science as a discipline where mechanisms are studied in detail, then the objective has been to combine these two. Modeling is the primary interest, but the models have been formulated by consideration of as much microstructural information as possible. This should be considered as background and motivation for the research presented here.

The arrangement of crystallites and crystal defects are usually referred to as the microstructure of materials. This arrangement is of great importance for the mechanical properties. A good understanding of the role of the microstructure gives great insight into the mechanical behavior of materials.

Generally, it is of interest to characterize materials before they are used. Depending on the use of a material, there are several properties of importance. That can be the material’s mechanical, chemical, physical, biological etc. properties. In this thesis, exclusively metals and their mechanical properties are considered. However, in reality a combination of all environmental aspects should be used in the characterization of a material.

Modeling of materials may be performed at different length scales, depending on the area of interest. Even though there are orders of magnitude between the different scales in modeling of materials, there are still several similarities regarding mechanical properties and modeling approaches.

1.1 Length scales in modeling of materials

Depending on how one looks at a material it can differ considerably. With the bare eye it is difficult to reveal any structure in a piece of steel. A normal person has difficulties in determining the mechanical properties by just looking at the material without
instruments. It is usually necessary to polish and etch the surface to reveal the microstructure. At first (almost visible with the bare eye) a mesostructure is visible. It can be processing parameters that result in a gradient structure, e.g. different grain size through the specimen. This structure influences the properties quite much, but is also difficult to predict since it is a processing effect. Through a microscope it becomes clear that materials have a microstructure. The microstructure of a metal is built by ordered blocks (grains), with a distribution of crystallographic orientations (texture). The process where the material is fabricated determines the microstructure. The polycrystalline structure of grains in metals usually have different size, topology, phase and dispersion. All these parameters affect the mechanical properties of the metal, and materials with very different properties can be created by changing these parameters during processing.

The aim of this thesis is to use the microstructural data to predict the macroscopic behavior of the material. Further studies of the microstructure show that the structure within the grains is not perfectly ordered, it has local disorder (dislocations). Dislocations do to a large extent control the plastic behavior of materials, while the texture control the elastic properties. Lastly, in modeling of materials one can go down to the atomic level, to study atomic configurations and atomic potentials to predict material behavior. Of course, it is possible to go even deeper, but then it is more physics than modeling of materials. When one wants to study materials it is first appropriate to decide what kind of mechanisms that are of interest, and thereafter decide which length scale that is applicable. In Figure 1.1, a schematic representation of the above mentioned scales is shown.

Figure 1.1: Different length scales in materials modeling. Structures - details - mesostructure - microstructures - grains - dislocations - atoms.
1.2 Problem solving strategy

A normal problem solving strategy in micromechanical modeling of materials is shown in Figure 1.2. When a material has been chosen, experiments are performed. In parallel, a numerical model is developed. First, a geometrical model that is representative of the material is made. To solve the problem, constitutive equations for each grain and/or phase are needed. Those relate stresses and strains for the particular problem: elastic, plastic, visco-elastic equations etc., what ever best captures the real material behavior under the given circumstances. To compare the model with experiments, boundary conditions that load the model in the same way as was done in the experiments are needed. The generated boundary value problem is now solved with a numerical method, e.g. the finite element method (FEM). If the agreement between the experiments and the model is not satisfactory, the model generation is iterated to improve the model. If the agreement is acceptable, the model can be used to give insight to the material behavior.

Figure 1.2: Flow chart for micromechanical modeling of materials
Chapter 2

Material characterization

In Paper A, Paper B and Paper E, hot rolled HSLA-steels with varying carbon contents are chosen as appropriate model materials. The microstructure of these steels usually consists of several phases with different mechanical properties. This makes them suitable for modeling the effect of different grain structures on the mechanical properties. The general microstructure including specifically the lamellar spacing in the pearlite is investigated. From the mechanical viewpoint, the stress-strain relationship and the hardness of the materials are studied.

2.1 Microstructural aspects

The materials used in this study are four different steels with varying amounts of ferrite and pearlite. The steels, from SSAB Swedish Steel AB, were delivered as sheets in the hot rolled condition, in a thickness range of 3-5 mm. The four steels have different carbon contents ranging from 0.05w% to 0.76w% but otherwise similar composition of other alloying elements, see Table 2.1 for compositions.

<table>
<thead>
<tr>
<th>Element</th>
<th>Material 1</th>
<th>Material 2</th>
<th>Material 3</th>
<th>Material 4</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>0.05</td>
<td>0.19</td>
<td>0.45</td>
<td>0.76</td>
</tr>
<tr>
<td>Mn</td>
<td>0.18</td>
<td>0.52</td>
<td>0.7</td>
<td>0.71</td>
</tr>
<tr>
<td>Si</td>
<td>0</td>
<td>0.19</td>
<td>0.24</td>
<td>0.25</td>
</tr>
<tr>
<td>P</td>
<td>0.011</td>
<td>0.008</td>
<td>0.009</td>
<td>0.01</td>
</tr>
<tr>
<td>S</td>
<td>0.012</td>
<td>0.005</td>
<td>0.002</td>
<td>0.002</td>
</tr>
<tr>
<td>N</td>
<td>0.0032</td>
<td>0.0033</td>
<td>0.0042</td>
<td>0.0032</td>
</tr>
<tr>
<td>Cr</td>
<td>0.03</td>
<td>0.25</td>
<td>0.24</td>
<td>0.24</td>
</tr>
<tr>
<td>Ni</td>
<td>0.04</td>
<td>0.07</td>
<td>0.05</td>
<td>0.08</td>
</tr>
<tr>
<td>Cu</td>
<td>0.01</td>
<td>0.02</td>
<td>0.01</td>
<td>0.01</td>
</tr>
<tr>
<td>Mo</td>
<td>0.01</td>
<td>0.02</td>
<td>0.01</td>
<td>0.02</td>
</tr>
<tr>
<td>Al</td>
<td>0.027</td>
<td>0.01</td>
<td>0.009</td>
<td>0.009</td>
</tr>
<tr>
<td>Nb</td>
<td>0.001</td>
<td>0.002</td>
<td>0.002</td>
<td>0.002</td>
</tr>
<tr>
<td>V</td>
<td>0.004</td>
<td>0.011</td>
<td>0.01</td>
<td>0.023</td>
</tr>
<tr>
<td>Ti</td>
<td>0.001</td>
<td>0.002</td>
<td>0</td>
<td>0.002</td>
</tr>
</tbody>
</table>

The microstructure of the steels consists of ferrite and pearlite, where the volume
fractions depend on the carbon and alloying contents. Pearlite is a lamellar structure consisting of two phases, namely ferrite and cementite. In this work, the steels are characterized with respect to the volume fractions of the two structural constituents, ferrite and pearlite, present. For Material 2, 3 and 4, equilibrium fractions of pearlite were calculated from the iron-carbon phase diagram (Figure 2.1), using the lever rule. The volume fraction pearlite in Material 1 was evaluated from micrographs. The determined volume fractions pearlite are 1%, 25%, 58% and 99%. Eventual deviations from equilibrium values resulting from other alloying elements like Mn and Cr or manufacturing at non-equilibrium conditions are not taken into account. The steels were examined by light optical microscopy (LOM) and by a JEOL 840 scanning electron microscope (SEM), the latter for measuring the lamellar spacing of pearlite. The specimens were polished and etched in a solution of 4% nital prior to microscopic examination. Representative microstructures of the four steels are shown in Figures 2.2.

In Material 1, ferrite is the dominating phase with a sparse distribution of pearlite, especially at grain corners. In Material 2, the ferrite is seen as the white areas with a slightly banded structure and the pearlite as the dark areas quite evenly distributed in between the ferrite. In Materials 3 and 4 with higher carbon contents, pearlite is the dominating structure and the ferrite is seen as white pockets between pearlite colonies (Material 3) or as grain boundary ferrite (Material 4). The nucleation of pearlite is known to take place preferentially on austenite grain boundaries and/or at grain corners.

2.2 Grain size and lamellar spacings

An important objective is to characterize the microstructure in relation to the mechanical properties, i.e. especially identify important microstructural features that can influence the deformation process. Two important parameters are the lamellar spacing,
Figure 2.2: Light optical microscopy pictures of the ferrite/pearlite steel qualities used. (a) Material 1, 1% pearlite; (b) Material 2, 25% pearlite; (c) Material 3, 58% pearlite; (d) Material 4, 99% pearlite.
2.3 Stress-strain relationship

The lamellar spacing of pearlite was measured using SEM. Since the lamellar spacing may vary within the steel specimens it can be difficult to measure. This is partly due to variations in the processing parameters of the steels, partly due to artifacts from the polishing of the specimens. Typical pictures of fine pearlite for the different materials are seen in Figure 2.3. The values presented below in Table 2 should be considered as qualitative measurements taken from a representative part of the sample. Grain sizes, \( d \), were measured using the intercept method and as an average of 25 - 40 lines, this is also presented in the table below. The smaller grain size measured in Material 2 is expected since the pearlite has grown in the material, and thereby decreased the ferrite grains.

Table 2.2: Microstructural data

<table>
<thead>
<tr>
<th>Material</th>
<th>( C_{\text{w}} )%</th>
<th>( V_{\text{pearlite}} )%</th>
<th>( l/\mu m )</th>
<th>( d/\mu m )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Material 1</td>
<td>0.05</td>
<td>1</td>
<td>-</td>
<td>11</td>
</tr>
<tr>
<td>Material 2</td>
<td>0.19</td>
<td>25</td>
<td>0.3</td>
<td>6</td>
</tr>
<tr>
<td>Material 3</td>
<td>0.45</td>
<td>58</td>
<td>0.25</td>
<td>-</td>
</tr>
<tr>
<td>Material 4</td>
<td>0.76</td>
<td>99</td>
<td>0.15</td>
<td>-</td>
</tr>
</tbody>
</table>

The main objective is to compare the four materials with different amounts of ferrite and pearlite. The most important feature namely the amount of pearlite, was approximated from the phase diagram. Other important microstructural features, which influence the mechanical behavior, are the lamellar spacing and the grain size. Measured lamellar spacings indicate that the steels with higher carbon contents show a finer pearlite.
Figure 2.3: Scanning electron microscopy pictures of typical lamellar spacings in the materials. Measured lamellar spacing are: (a) Material 2 0.3 μm, (b) Material 3, 0.25 μm, (c) Material 4 0.15 μm.
2.3. STRESS-STRAIN RELATIONSHIP

Figure 2.4: The tensile test specimen.

Figure 2.5: Stress-strain curves for the four materials as captured by the strain gauges at low strains.
modeling based on microstructural data is possible, in order to predict the deformation behavior. The deformation seems to follow a parabolic hardening which is as expected for these materials. The four steels show a fairly similar hardening behavior, while the difference in yield stress is large. This is mainly due to the increasing amounts of pearlite with increasing alloying contents, but also due to an increase in the yield strength due to alloying elements by solid solution hardening.

## 2.4 Hardness

Vickers hardness was first measured at a fairly high load, $P = 1.000 \, \text{N}$, on the four different materials. At this load, the indentations cover several grains, and both phase constituents. An average hardness is obtained from five indents on each sample. The purpose behind this is to compare the indentation data to the tensile test results by use of the Tabor relationship (Tabor, 1951). Tabor showed that the indentation stress at a plastic strain of 0.08 can be expressed as:

$$\sigma(\varepsilon^p = 0.08) = \frac{1}{28} \frac{P}{A},$$

where $A$ is the projected area of the indent. Comparisons between the hardness measurements and the tensile test results are shown in Table 2.3. The results show a good agreement.

<table>
<thead>
<tr>
<th>Material</th>
<th>$\sigma_{1.000, \text{N}}$/MPa</th>
<th>$\sigma_{\exp}$/MPa</th>
</tr>
</thead>
<tbody>
<tr>
<td>Material 1</td>
<td>330</td>
<td>350</td>
</tr>
<tr>
<td>Material 2</td>
<td>560</td>
<td>540</td>
</tr>
<tr>
<td>Material 3</td>
<td>750</td>
<td>760</td>
</tr>
<tr>
<td>Material 4</td>
<td>1200</td>
<td>1250</td>
</tr>
</tbody>
</table>
Chapter 3

Experimental findings

Experimental results show that materials with different grain size have different properties; smaller grains are plastically harder. The grain size effect in polycrystals has been known for a long time (Hall, 1951; Petch, 1953). It has also been reported for a variety of materials; Al (Fujita and Tabata, 1973), iron and steel (Bergström and Hallén, 1983), Cu (Thompson and Baskes, 1973) etc. Among the reported stress-strain data two mechanisms can be seen. Firstly, there is a yield point change, which is referred to as the Hall-Petch relation. Secondly, some of the data also exhibit a change in hardening, while the rest are only shifted due to the yield point change. Data for Al and Cu have been plotted in Figure 3.1 to show the change in hardening.

![Figure 3.1: Stress-strain curves for different grain sizes (a) Al (Fujita and Tabata, 1973) and (b) Cu (Thompson and Baskes, 1973).](image)

3.1 The Hall-Petch effect

The Hall-Petch relationship,

\[ \sigma_s = \sigma_0 + \frac{K}{\sqrt{D}}, \]

(3.1)
Figure 3.2: Inverse Hall-Petch behavior in nanocrystalline Cu investigated by hardness testing (Chokshi et al., 1989) \((H - H_0)\) denotes the hardness increment, \(D\) the grain size). The classical behavior breaks down at a grain size of about 50 nm. (From Arzt (1998).)

has long been accepted to relate the yield stress, \(\sigma_y\), and the grain size, \(D\). The increase in yield stress with decreasing grain size is due to the grain boundaries, since they become obstacles for dislocation movement.

The Hall-Petch relationship is widely accepted for materials with normal grain size, but when the grain size gets smaller the yield stress would approach infinity as the grain size decreases. As a consequence, the Hall-Petch relationship is not valid for small grain sizes, however, materials normally obey the relationship over several orders of magnitude (Arzt, 1998). Generally, the Hall-Petch relationship is considered valid as long as one Orowan loop can be fitted within the grain.

Below the Hall-Petch limit, different mechanisms have been suggested (Arzt, 1998). Several investigations have proposed an inverse Hall-Petch relationship, which has been reported for copper. In copper the estimated critical grain size is about 50 nm, which seems to be in agreement by experimental data reported by Chokshi et al. (1989) (Figure 3.2).

3.2 Local behavior

The recent attempts to incorporate non-local effects in continuum based theories aim to generate local strain fields that resemble experimental observations. In the formulation of non-local theories internal length scales must be introduced. In polycrystals, one characteristic length is the grain size. The anisotropic behavior of single crystals in combination with varying crystal orientations between different grains result in strain gradients that scale with the inverse of grain size. So far, many theories have been proposed, but the experimental evidence is not complete. This is mainly due the difficulties associated with the measurement of local strain fields. There are however several techniques available that make it possible to study local deformation fields, e.g., atomic force microscopy (AFM), speckle methods and oriented image microscopy (EBSP). All these methods are however surface techniques, which complicate the interpretation of data, since only plane stress conditions can be observed.
3.2.1 Atomic Force Microscopy (AFM)

AFM offers the opportunity to study surface topology, and thereby deformations already at initiation of plastic deformation. Essentially, two types of deformations at different length scales may be evaluated from the measurements. First, there are discrete steps that form on the surface due to slip bands, which has successfully been studied by the technique in single crystals (Brinck et al., 1998; Coupeau et al., 1999; Stanford and Ferry, 2001). Secondly, deformation bands, consisting of many slip bands, can be studied as they form gradients within grains and closer to boundaries (Tong et al., 1997). The former is of the length of nm, while the latter can be of the length of μm.

3.2.2 Speckle methods

Digital speckle photography is commonly used to map strain fields. A random dotted pattern is applied on the surface, and the displacement field is measured by a comparison of the pattern before and after deformation. Thereafter, in-plane strain components are determined by differentiation of the displacement fields. The method works well for fairly large specimens, where the camera is placed in front of the specimen, e.g. shear testing specimens (Petterson, 2002). The method should also work for microstructures, if the camera is mounted on a microscope (microscopic speckle photography). However, it does not seem to have been applied for measurements of local strain fields in polycrystals.

3.2.3 Electron backscattered diffraction (EBSD)

Plastic deformations generally result in crystal rotations. By the EBSD technique it is possible to study crystal orientation locally. Thereby, maps of local orientation perturbations within grains can be created. The main problem today lies in the interpretation of the results at small deformations. One has to reach deformations of 10-30% to get representative and reproducible results over grain boundaries (Randle et al., 1996; Davies and Randle, 1999, 2000). One possible approach is to use the results and correlate those to the formation of geometrically necessary dislocations (Sun et al., 1998).

3.2.4 Future needs

All methods mentioned above measure surface activity, although different mechanisms. AFM measures out-of-plane deformation. Speckle methods measure in plane deformation, while EBSD measures lattice rotations. Even though different properties are measured there should be a relation between the results. The character of deformation is the same. As a material volume deforms it can be elongated, and at the same time rotate and thus also change its out-of-plane position. A very promising and extremely interesting work in this area is done by Chandrasekaran and Nygård (2003). Quantitative comparisons are made between data from AFM and ESD. Preliminary results indicate a close correlation between the two methods. This opens new possibilities for data evaluation of the two methods.
Chapter 4

Micromechanical modeling

Micromechanical modeling has potential to increase the understanding of material behavior. A representative volume element (RVE), that has the same average behavior as a larger model, is considered. As discussed in the earlier sections, a polycrystalline material consists of grains with different orientations. A micromechanical model of a polycrystalline material should therefore consist of a grain structure. A material can also have different constituents; a two-phase material has two different materials that build up the grain structure. In micromechanical modeling it is important to catch the most important issues in the model formulation. For a two-phase material, the volume fractions of the two phases may be more important to consider, than the directions of the constituents. To create the best model, both issues should however be included. However, at the end of the model generation, it is often necessary to make trade-offs between details and computational efficiency. At that point it is important to remember the importance of different effects. Hence, in generating micromechanical models certain aspects need to be considered. The following issues should be considered in a finite element model:

- Geometry
- Representativity
- Boundary conditions
- Constitutive equations

4.1 Geometrical models

When accurate stress and strain fields are desired within the RVE, the morphology should be as realistic as possible. The microstructure should be represented by a grain structure. Since grain structures are three-dimensional, three-dimensional models should be preferred as was done in Papers B, C, D, E, F and G. However, since these models are computational demanding, two-dimensional approximations can be made in several applications to enlighten certain issues, as was done in Paper A. Below some approaches to generate geometrical models are outlined.
4.1.1 Voronoi models

A random microstructure can be approximated by the so-called Voronoi algorithm. The Voronoi algorithm utilizes a set of randomly distributed points (seeds) to partition space into regions, i.e., Voronoi cells, one per point. In practice, there are two different ways to apply the Voronoi algorithm. First, cells are created by considering each point and its nearest neighbors by application of a Delaunay triangularization algorithm. Thus, space is divided into polygons by using the seeds and dividing the distance between them (as was done in Paper A and B). A two-dimensional example of this procedure is seen in Figure 4.1. When periodic structures are desired the same algorithm can be used. Random points are then distributed within the unit cell, but before the algorithm is applied, the point set is copied to all neighboring cells, i.e. 8 cells in a two-dimensional analysis (illustrated in Figure 4.2) and 26 cells in a three-dimensional analysis. Thus, the Voronoi tessellation creates a structure that in its center is periodic, and a periodic cell with the same size as the original unit cell is chosen. Examples of periodic grain...
structures both in two and three dimensions created by this method can be seen in Figure 4.3. The periodic cells seen in the figures both contain ten grains.

![Figure 4.3: Two and three dimensional periodic cells containing 10 grains (note the periodicity).](image)

The Voronoi algorithm is very old and well known. By now there are several implementations available. A very good one is Qhull (Barber et al., 1996), which creates both two and three-dimensional cells, but also Matlab (1997) has a two-dimensional version. As the grain structure has been generated, the polygons are divided into a mesh. The advantage with this method is that grain boundaries will be respected, and they will thereby be represented by lines or planes. On the other hand, an adaptive mesh generator is needed. When complex geometries are used, this will result in an excessive number of elements.

The other approach is a discrete version of the Voronoi algorithm that utilizes a predefined mesh. Thus, the grain generation can be simplified to an algorithm that is easily implemented. The grain generation of a periodic cell in a two-dimensional case is schematically shown in Figure 4.4. When the cell is made periodic the same technique as shown in Figure 4.2 is used, i.e. before the Voronoi tessellation is used the original seeds are copied to neighboring cells. Each element is assigned to a grain.

![Figure 4.4: Schematic description of the formation of periodic Voronoi cells when a predefined mesh is used, and the resulting cell. Each grain is build up by the elements closer to the grain seed than to any other seed (including seeds copied to neighboring cells). The algorithm works both in two and three dimensions.](image)
depending on the closest seed, which is described in Paper D. The fact that the mesh is predefined makes the latter method very reliable and computational attractive. On the other hand, grain boundaries become very kinky because of the predefined mesh.

4.1.2 Micrograph model

Another approach is to start with an actual photograph of the microstructure, and from there create a mesh. For this purpose, NIST has developed a software called Object-Oriented Finite Element Analysis of Real Material Microstructures (OOF) (Carter et al., 2000). The program takes a scanned picture of the microstructure as input, and creates a mesh. Basically, different phases and/or grains are sorted out because of their color.

4.2 Representativity

One of the purposes of micromechanical modeling is to consider only a small part of a material. This is possible if the model is a representative volume element. The phrase *representative volume* was introduced by Hill (1963).

In model formulation there is a trade-off between representativity and computational effort. As a model is made larger it becomes more representative, but the memory allocation resources also increases. Thus, the RVE size is mostly determined by the computer capacity. Instead, many simulations can be performed, which gives statistical background of the performance of the model. Especially in grain structures, fairly large models are needed to achieve representativity. This issue is discussed in detail in Paper D.

Also the material models affect the representativity. In Paper D, elasticity is considered. Plastic deformations normally make materials more isotropic, since a relative softening occurs. Evaluation of the number of grains necessary in an elastic analysis should therefore be an upper limit when plasticity is considered.

4.3 Periodic Boundary Conditions

Boundary conditions corresponding to an average strain \( \varepsilon_{ij} \) may for a periodic cell be expressed as

\[
\Delta u_i^\alpha - \Delta u_i^\beta = \varepsilon_{ij} (x_j^\beta - x_j^\alpha),
\]

where \( u_i \) denotes the displacement vector and \( x_j \) the position. In Eq. (4.1), \( \alpha \) and \( \beta \) are equivalent boundary points according to the periodicity conditions. In order for a unit cell to be periodic, all outer edges must fulfill a periodicity condition, i.e. every point must have at least one equivalent point. As long as periodicity conditions can be formulated for a given cell, then the same cell can be used to model material with different configurations. In Figure 4.5, two different models of materials are shown. The periodicity is different in the two materials. However the same cell, indicated by the rectangular box, can be used to model both materials. In this specific case there will be different numbers of equivalent edges, as shown in Figure 4.6. The cell (a) has two pairs of equivalent edges, and all corner points are equivalent. Cell (b) on the other hand has three pairs of equivalent edges, and two sets of equivalent points. More details regarding equivalent points and ways to chose the periodic cells can be found in Paper A.
A condition for using Eq. (4.1) in finite element calculations is a periodic mesh, i.e. to every edge node at least one exact equivalent point must exist at another part of the boundary. If that is not the case, the periodic boundary conditions can be formulated in an approximative way. If an equivalent point is missing, the displacement of the exact position can be estimated by the corresponding finite element shape function. Eq. (4.1) may then be reformulated as

$$u_i^\beta - f_i(u_i^{a\alpha}) = \bar{\varepsilon}_{ij}(x_j^\beta - x_j^\alpha),$$  

(4.2)

where $f_i(u_i^{a\alpha})$ denotes the displacement in the periodicity point. It is here expressed in terms of the corresponding finite element shape function ($f_i$) which linearly depend on the neighboring nodal displacements $u_i^{a\alpha}$.

The periodic boundary conditions can be implemented in a finite element analysis, for example in the commercial program ABAQUS (1998, 2001). In ABAQUS, the periodic boundary conditions are implemented by the command EQUATION, where equations are formed to connect equivalent points. To this end, dummy nodes are introduced with degrees of freedom corresponding to the average strains, $\bar{\varepsilon}_{xx}$, $\bar{\varepsilon}_{yy}$, $\bar{\varepsilon}_{zz}$, $\bar{\gamma}_{xy}$, $\bar{\gamma}_{yx}$, and $\bar{\gamma}_{xz}$. The dummy nodes are placed outside the model, and the displacements of those correspond to average strain components. The displacements of the dummy nodes are connected to the displacements of equivalent nodes according to Eq. (4.2). For nodes lying along an equivalent line there will be equations including the two equivalent nodes and three average strain components. At the corners of the periodic cell there are however more than two equivalent points, and all these need special attention. The nodes need to be connected to each other and still obey the periodicity conditions.
4.4 Crystal plasticity

Deformation of metals occurs on well-defined slip planes. In Figure 4.7, a picture of a deformed stainless steel surface illustrates this feature. The sample has been loaded in uniaxial tension. As the specimen deforms, slip occurs on slip planes where the resolved shear stress is high. At larger deformations, several slip systems can be activated, due to hardening on activated planes and lattice rotations. A general continuum framework to account for deformations on slip planes has been presented by Rice (1971). Below, a small deformation theory of single crystal plasticity is presented, essentially following the formulation by Hutchinson (1970).

In the following equations the tensorial summation convention is employed, where the Latin letters ($i, j$) take values 1, 2, 3. Greek letters ($\alpha, \beta$), on the other hand, are related to slip systems and take values between 1 and the total number of active slip systems, e.g., the greek letters take values between 1 and 12 when fcc-metals are simulated, since there are 12 possible slip systems. The summation convention is applied only to tensorial indices, which always appear as subscripts.

Single crystals are treated as elastic continua, where plastic deformation is evaluated from predefined slip planes. The normal of slip plane $\alpha$ is denoted by $n^\alpha_j$, and $m^\alpha_j$ denotes its slip direction. If the tensor of elastic compliance for the single crystal is
\( M_{ijkl} \) and \( \sigma_{kl} \) denotes the stress tensor, the total strain rate can be expressed as,

\[
\dot{\varepsilon}_{ij} = M_{ijkl} \dot{\sigma}_{kl} + \frac{1}{2} \sum_{\alpha} \dot{\gamma}^\alpha (m_{i}^{\alpha} n_{j}^{\alpha} + m_{j}^{\alpha} n_{i}^{\alpha}),
\]

where \( \dot{\gamma}^\alpha \) is slip on slip system \( \alpha \).

The resolved shear stress, \( \tau^\alpha \), on each slip plane can be evaluated as,

\[
\tau^\alpha = \frac{1}{2} \sigma_{ij} (m_{i}^{\alpha} n_{j}^{\alpha} + m_{j}^{\alpha} n_{i}^{\alpha}).
\]

(4.4)

On each slip plane there is a critical resolved shear stress, \( \tau^\alpha_{cr} \). As deformation progresses hardening occurs. According to Hill (1965) the rate of change in yield stresses are assumed to be related to the slip rates of all active slip planes \( \beta \). Thus, the critical resolved shear stress on slip plane \( \alpha \) changes,

\[
\dot{\tau}^\alpha_{cr} = \sum_{\beta} h_{\alpha\beta} \dot{\gamma}^\beta_{\beta},
\]

(4.5)

where \( h_{\alpha\beta} \) are the instantaneous hardening coefficients, which in general depend on the deformation history. As the constitutive framework is used to model materials, there is a great variety of functions that can be used to represent different materials. Generally, the coefficients \( h_{\alpha\beta} \) are determined from comparisons to experiments.

In the crystal plasticity implementation used here (Huang, 1991) a visco-plastic formulation is used. Then, the flow rule is formulated as

\[
\dot{\gamma}^\alpha = \dot{\gamma}^\alpha_{0} \left( \frac{\tau^\alpha}{\tau^\alpha_{cr}} \right)^{n-1},
\]

(4.6)

where \( \dot{\gamma}^\alpha_{0} \) and \( n \) are a material constants that need to be defined. If a large power-law coefficient \( n \) is chosen, \( n > 30 \), the formulation is essentially rate independent. In the visco-plastic formulation all slip planes are potentially active.

### 4.4.1 Gradient dependent plasticity

A non-local theory has been developed by Acharya and Bassani (1996, 2000) by introducing strain gradients in the hardening moduli, \( h_{\alpha\beta} \). The hardening moduli are made non-local by incorporating Nye’s (Nye, 1953) tensor \( \alpha_{ij} \) as a gradient measure, accordingly

\[
h_{\alpha\beta} = h_{\alpha\beta}(\gamma^\alpha, \alpha_{ij}).
\]

(4.7)

Thus, the hardening moduli depend both on slip and on their gradients through Nye’s dislocation tensor that is used as an incompatibility measure. In crystal plasticity theory, Nye’s tensor \( \alpha_{ij} \) can be expressed as

\[
\alpha_{ij} = e_{jkl} u_{i}^{p} = e_{jkl} \sum_{\alpha} \gamma^\alpha_{,k} m_{i}^{\alpha} n_{j}^{\alpha},
\]

(4.8)

where \( e_{jkl} \) is the alternating symbol.

There are however outstanding issues on how Nye’s tensor are calculated under multiple slip (Arsenlis and Parks, 1999). Therefore, another proposal for the incorporation of plastic strain gradients is given in Paper F. The length of the slip gradient vector is utilized as a parameter that influences the hardening modulus for each slip plane, accordingly,

\[
h_{\alpha\beta} = h_{\alpha\beta}(\gamma^\alpha, l \sqrt{\gamma^\alpha_{,i} \gamma^\alpha_{,i}}),
\]

(4.9)

where \( l \) is an internal length scale.
4.5 Macroscopic properties

When a micromechanical model can be used to homogenize a material behavior the model is good. To achieve this, macroscopic properties of the model need to be evaluated. In principle, there are two ways of evaluating macroscopic properties from a finite element model. Firstly, one could do a summation of all stresses and strains in all the elements, and then calculate the averages. Secondly, boundary conditions can be formulated to simplify the evaluation process, e.g. as described by the periodic boundary condition formulation above. The advantage with the latter approach is that it simplifies the evaluation considerably. Especially large and complex geometries are preferably evaluated in this way, compare Paper B.

4.6 Local properties

The purpose of studying the local behavior within an RVE is to gain further insight of the deformation mechanisms. Generally, local properties are more sensitive to discretization errors and geometric simplifications in comparison to macroscopic properties such as average stresses or strains. Therefore, efforts should be made to create as realistic models as possible before local behavior is studied. Microstructures can e.g. be represented by three-dimensional models as done in Papers B, C, D, F and G. Especially in Paper C, an attempt is made to evaluate average properties within grains of different orientations. This is a very enlightening example of how the average behavior differs only due to a change of orientation even though the material constants are the same.

In Papers E and G, local properties are evaluated on a surface. These are good examples of how numerical data can be compared to experiments.

4.7 Two-dimensional examples

To demonstrate how different geometrical models behave, three different finite element based micromechanical models are presented below. The purpose of all models is to generate periodic cells representing Material 2 and Material 3, that were characterized in Chapter 2. These two materials are ferrite/pearlite steels with pearlite fractions 0.25 and 0.58 respectively. For this purpose, it is assumed that the ferrite and pearlite have the same isotropic elastic properties, $E=202$ GPa and $\nu=0.3$, while the plastic properties differ. The experimental stress-strain curves presented in Paper A for ferrite (Material 1) and pearlite (Material 4) are used as input for the phases’ plastic properties in the FE-models. Furthermore, it is assumed that the ferrite phase behaves in the same way in a two-phase material, as it does as a single phase material. The same assumption also goes for the pearlite structure. The intention is thereafter to model the mixed materials, based on the volume fraction of the constituent phases.

In Paper A, the generation of two-dimensional periodic cells by the Voronoi algorithm for simulation of Material 2 and Material 3 is described in detail. Models are also generated from pictures of microstructures. These micrographs are based on the pictures in Figure 2.2b and Figure 2.2c. By use of the program OOF (Carter et al., 2000), meshes with 7240 and 7165 elements for the two materials resulted. The program contains a mesh generator and a finite element solver. For present purposes, only the mesh generator is utilized, since the mesh is exported to ABAQUS (1998), to enable the use
of elastic-plastic material models and generalized plane strain elements. As a result of this approach, unit cells containing 25% and 81% pearlite were created to represent Material 2 and Material 3.

Some very simple models have also been incorporated in this analysis to investigate if it is worth the effort doing a more sophisticated model. The models have a square unit cell with a circular inclusion. To model Material 2, the matrix represents the ferrite and the circle that fills 25% of the cell represents the pearlite. For Material 3 the internal circle represents the ferrite and the matrix the pearlite which in this case fills 58% of the cell. These models are meshed with the same Matlab (1997) routine as the Voronoi models, which creates a periodic mesh containing 1320 and 1280 elements respectively. In addition, inverted circle models were also created. In these, the minor phase represent the matrix, and the major phase the internal circle.

The periodic boundary conditions presented in Eq. (4.1) were utilized for the Voronoi model, but Eq. (4.2) had to be used on the Micrograph model and circle models, because in these cases the mesh generator did not create a periodic node set.

In addition to the numerical models, also the rule of mixtures for stresses is used to compare the results. This model can be used for predicting the mechanical behavior of two-phase materials. The effective stress \( \bar{\sigma} \) is expressed as,

\[
\bar{\sigma} = \sigma_1 (1 - V_2) + \sigma_2 V_2
\]  

(4.10)

where \( V_2 \) is the volume fraction of pearlite, and \( \sigma_1 \) and \( \sigma_2 \) are the stresses in the ferrite and pearlite at the strain \( \varepsilon \). This expression has also been used in the analysis for comparisons with the experimental results and the finite element models. For Material 2, \( V_2 = 0.25 \) and for Material 3 \( V_2 = 0.58 \).

The experimental results, the data generated by the finite element models and by rule of mixture are presented in Figure 4.8. In the figure, the average uniaxial stress in the loading direction \( \sigma_{xx} \) is plotted versus average strain \( \varepsilon_{xx} \) over the representative cell. The Voronoi results represent averages of 50 simulations for each material, where the standard deviation at \( \varepsilon_{xx} = 2\% \) is smaller than 6.4 MPa for Material 2 and 14 MPa for Material 3. It is evident that there is a quite good agreement between the experimental and most simulated data.

For Material 2, the agreement between the experimental data and the Voronoi and circle model is good at higher strains. The circle model fits quite well to the experiments, while the Voronoi model predicts slightly higher stresses. The Micrograph model and the inverted circle model coincide in the plot, and predict even higher stresses. Compared to the experimental stress at 2% strain, the Voronoi model is 6% and the Micrograph model and inverted circle model are 11% larger.

Unfortunately, none of the models is able to predict the mechanical response of the material around the yield point. One can see that the experimental tensile test data has higher yield stresses than the data generated by the models. This indicates that the fairly complicated microstructure in the two materials plays an important role in the yield point prediction. Possible explanations to the behavior can be that there are either Lüder band formation, or residual stresses in the phases. None of these effects have been incorporated in the models.

For Material 3, all models predict the initial response quite well. The experimental and simulated data capture the same behavior, but as strain increases, the models predict higher stresses than the experiments. Compared to the experimental stress at 2% strain, the Voronoi model is 7% larger, the inverted circle model is 11% larger, the circle model is 15% larger and the Micrograph model is as mush as 40% larger.
An attribute that differs between the three models is the distribution of the two phases. In the circle models, the phases are separated, while they are more connected in the Voronoi and Micrograph models. This fact will influence the local stresses and strains in the models. In Figure 4.9, contour plots of the von Mises effective stress within the unit cells have been plotted for uniaxial tensile loading at an average strain $\varepsilon_{xx} = 2\%$. In all models it is apparent that the harder pearlite phase has the highest stress.

The local $\varepsilon_{xx}$ strain component has been plotted for all models in Figure 4.10. In the figure, it is evident that it is the softer ferrite that takes the highest strain. It is also observed that bands of intense shear in the $45^\circ$-direction develop in the Voronoi and the Micrograph models.

From the local stresses and strains, one can conclude that as long as there is a random microstructure, and the two phases are continuous or close to continuous, the local stresses and strains seem to evolve about the same. But if the softer phase is discontinuous the maximum strain increases, and a discontinuous hard phase decreases the maximum stress.

### 4.8 Computer resources

In micromechanical modeling of materials, computers are essential. My experience regarding this issue is “moderate is sufficient”. In doing finite element simulations the internal memory is often the limiting factor, while speed and parallelization is less important. Most of the simulations in this thesis have been performed by one processor on Melker (Sun Ultra Enterprise 450). Some simulations have been performed on my
Figure 4.9: Contour plot of von Mises effective stress after uniaxial tensile loading by an average strain $\gamma_{x}$ of 2%. (a) Voronoi model (Material 2 and Material 3); (b) Micrograph model (Material 2 and Material 3); (c) Circle model (Material 2 and Material 3).
Figure 4.10: Contour plot of the local $\varepsilon_{\text{xx}}$ strain after uniaxial tensile loading by an average strain $\varepsilon_{\text{xx}}$ of 2%. (a) Voronoi model (Material 2 and Material 3); (b) Micrograph model (Material 2 and Material 3); (c) Circle model (Material 2 and Material 3).
own workstation (SunBlade 100), while the representativity simulations were made on Kallsup2 (IBM SP/2 Nighthawk). The advantage with Melker is its 4 GB of internal memory. Thus, fairly large models can be simulated. The crystal plasticity simulations were exclusively simulated on Melker. Generally, about 40 increments take about 10 hours, i.e. simulations can be run over night. Unless a great number of simulations are performed this is a sufficient pace. It gives one the time to evaluate data and analyze the results. However, when many simulations are performed computer time becomes important. Therefore, the representativity simulations were made on a supercomputer. A finite element code will however not parallelize very well. In Figure 4.11 a parallelization study of the representativity cell is shown, and compared to ideal parallelization. It is doing well on 2 processors, moderate on 4 and poor for larger numbers of processors. This is due to the large amount of communication between parts that are on different processors. In the present study, 4 processors were used, since they were available. Each three dimensional simulation then took about 15 minutes.

![Figure 4.11: Parallelization of the representativity cell on Kallsup2. Actual CPU time compared with ideal parallelization.](image-url)
Chapter 5

Discussion and outlook

Over the years the ability to do advanced micromechanical modeling of materials, especially modeling of microstructures, has increased. Since microstructures contain a lot of data, models easily become very large and complex. It is therefore easy to realize what the increased computer capacity the last 20 years has done. Today one solves problems, that 20 years ago were too large, in the matter of seconds. By this revolution in computer capacity also the complexity of the investigated problems has increased. In the future, even larger problems will most probably be solved. Thus, the ability to make good research lies in the field of formulating the problems. It is important to consider the most appropriate mechanisms in defining the problem. The mechanisms should also be based on a solid physical background before equations are formed.

The ideas and proposed models presented in the thesis have at least one thing in common. The microstructure of materials is used to gain more information about the material. Models have been created to investigate effects of loading, morphology, elastic and plastic properties etc. These effects can be difficult to test by experiments. It can e.g. be difficult to test a material under biaxial loading, but fairly simple in a numerical model. Special care has been made to create geometrical models that have resemblance to actual microstructures. Geometrical models have been created by the Voronoi algorithm. As the algorithm is used in three dimensions, models with enormous complexity can be formed. Even though the models can look complicated to handle they are straightforward to deal with numerically. This is however due to great freeware software that is available at the Internet. As a matter of fact when complicated problems are solved, the greatest solutions can be found out there. Even though the actual problem is not available, similar problems often have an existing solution. The Voronoi algorithm is utilized in several diverse areas, such as: molecular classification, circuit layout, pattern identification and speech coding.

The size of the representative cell in micromechanical modeling is often determined by the computer capacity. However, details regarding the size determination are often fuzzy. One important issue that has not been considered in the thesis is how loading is prescribed. Periodic boundary conditions and periodic cells have been applied in the present work. Thus, edge effects are avoided. Another alternative is to prescribe stresses and/or strains along the outer boundaries. But, if that is the case boundary layer effects will result. The macroscopic properties will then be altered, and local properties can not be studied in the vicinity of the boundaries. Exactly how the macroscopic properties are affected has not been studied here. One thing is however certain, a larger cell than necessary needs to be modeled. In this thesis, a concept that work very well for
modeling of microstructures and that can be improved to have a user friendly interface has been developed. The boundary conditions can easily handle any combination of average stress and strain components.

Modeling of materials from microstructure is important since the microstructure easily is revealed and used to characterize the material. A great challenge lies in the approach where a grain structure is considered (as done in several papers here). From the revealed microstructure, it is also possible to predict the macroscopic properties when size, constituents, morphology and other relevant parameters are known. On the opposite, it is possible to go down to smaller scales to study certain aspects in more detail, but then the coupling to macroscopic properties are lost. Therefore, the aim in micromechanical modeling of materials should be to improve the models, rather than increasing the complexity. Detailed studies are however very important background information for the creation of appropriate models.

By now we have the ability to do continuum modeling down to the grain level, as shown in this thesis. To create even better micromechanical models the aim should be to improve the constitutive equations. As shown, non-local plasticity theories can predict a size effect that has been observed in materials science for a very long time. The interest in non-local continuum mechanics theories has however just recently increased. This is mainly due to the earlier difficulties in doing advanced models. Now when it becomes possible to implement non-local theories the important task lies in determining how they should be formulated, and details in the implementations can also become important. The main objective must be to compare numerical work with experiments. If the theories are not able to predict classical experimental findings, they will not last long. It is also very important to get a physical background to proposed models. When a model with a rigid physical basis that predicts experimental work exists, then we can start to understand deformation mechanisms within grain structures.

The non-local theory implemented here, where gradients only enter in the hardening relation, is fairly straightforward to implement. This is because an existing FE-code only needs little modification. Since only the hardening relations are affected, there is no need to change the equilibrium equations. Therefore, traditional solvers can be used. In other non-local formulations where new equilibrium equations are introduced, the implementation is more complicated. However, interesting work lies ahead that will increase the general knowledge about non-local theories, and especially the use of them.

With micromechanical modeling of grain structures it is possible to gain knowledge about deformation mechanisms in the micrometer range. If one can predict macroscopic properties by models like this, then there is an industrial interest in modeling. If new materials can be engineered from results based on simulations, then more adequate experimental work can be performed from the beginning. Instead of buying/making materials by trial and error more specific demands can be stated if the desired microstructure and properties are known. It is therefore my opinion that the industry should make greater efforts in continuum modeling of microstructures. There is an initial effort to create appropriate tools, but thereafter modeling can be very straightforward. Models are easily changed in the matter of hours to cover new aspects.

In this work the finite element method has been utilized exclusively. The method is easily applicable to micromechanical problems, since solvers and constitutive equations are implemented in commercial programs. Thus, only the problem formulation needs to be considered in creating models. However, FEM is very computer intensive and parallelizations of the codes give only moderate improvements. The question then arises to what extent FEM can be utilized in modeling of microstructures. As larger
models with more grains are considered, more memory is needed. Whether large models will increase the knowledge of materials is questionable, since the amount of data increases considerably. Many people will use FEM to model microstructures, but my opinion is that a stage will be reached where no further scientific information is gained. This is mainly due to the character of deformation. Consider a grain structure, where the grain boundaries present obstacles for dislocation movements, i.e. contribute to hardening under plastic deformation. Thus, around grain boundaries there is great activity, while the grain interior is fairly unaffected. If the deformation characteristics is known within the grains, i.e if dislocation activity could be caught in a continuum model, then it would be sufficient to model only the grain boundaries, or other obstacles. What is needed then is correct constitutive equations. One needs to characterize the stress and/or strain gradients that appears in materials, and incorporate those in the equations. Large scale problems could then be solved more easily, without an excessive amount of data from points that play a smaller role in the deformation. But to reach that stage there are several obstacles that need to be passed (probably through the finite element method).

Within the field of micromechanical modeling of metals through grain structure more work is interesting. I believe that interesting results can be achieved within these fields:

- Experimental investigation of surfaces (and also of bulk material). Analysis of the character of the deformation within grains, and particularly the effect of grain boundaries. Several surface analysis techniques are now becoming available in many labs, such as: AFM, EBSD, speckle methods etc.

- Development of phenomenological models to explain the size effect in a continuum description.

- Implementation of non-local plasticity theories.

- Development of numerical methods as a complement to the finite element method.

If one leaves the mechanical properties, similar approaches and problems will probably also be of interest in the study of magnetic and electrical properties.
Chapter 6

Summary of appended papers

Paper A:
Micromechanical Modeling of Ferritic/Pearlitic Steels

A two-dimensional micromechanical model based on the Voronoi algorithm is presented to model two-phase ferritic/pearlitic steels. Special care is taken to generate periodic grain structures as well as periodic finite element meshes. The model is evaluated by generalized plane strain finite element calculations. Periodic representative cells are generated with the desired volume fraction pearlite. Loading by an arbitrary combination of average stresses or strains is possible by application of periodic boundary conditions.

Uniaxial tension tests are performed on pure ferrite and pearlite specimens, as well as on materials containing 25% and 58% pearlite. Modeling of the two-phase materials were performed by use of the stress-strain curves of the pure phases, in the description of the plastic properties. Comparisons between generated data and experiments at a loading strain of 2% show good agreement.

Moreover, local stresses and strains are studied within the different unit cells. In addition, the model is used to investigate the plastic behavior under biaxial loading. It is shown that Hill’s yield criterion gives a good fit to the numerical data.

Paper B:
Three-Dimensional Periodic Voronoi Grain Models and Micromechanical FE-Simulations of a Two-Phase Steel

A three-dimensional model is proposed for modeling of microstructures. The model is based on the finite element method with periodic boundary conditions. The Voronoi algorithm is used to generate the geometrical model, which has a periodic grain structure that follows the original boundaries of the Voronoi cells. As an application, the model is used to simulate two-phase ferrite/pearlite steels. It is shown that periodic cells with only five grains generate representative stress-strain curves. The model is compared with uniaxial tensile tests as well as with a two-dimensional model.
Paper C:
Anisotropy and texture in Thin Copper Films - an Elasto-Plastic Analysis

The role of elastic anisotropy on the stress inhomogeneity and effective behavior of columnar grained textured Cu thin films have been analyzed within a continuum framework. The analysis is based on a three-dimensional model of a film/substrate system. The film exhibits a fiber texture with (111), (001) and randomly oriented grains. Mainly two load cases have been considered. Biaxial loading of a film deposited on a silicon substrate and tensile loading of a film deposited on a polyimide substrate. The stress distributions in the (111) and (001) grains were generally found to be very different when subjected to biaxial loading and quite similar when subjected to tensile loading. When plastic behavior is invoked, a structural hardening effect is observed. The plastic behavior differs significantly between biaxial and tensile cyclic loading respectively. A new orientation dependent hardening law is proposed. This hardening law causes the plastic hardening behavior to be orientation dependent and scale with elastic anisotropy. The newly proposed hardening law is demonstrated on a film with small grain aspect ratio.

Paper D:
Number of grains necessary to homogenize elastic materials with cubic symmetry

A numerical model based on the finite element method is presented for modeling of microstructures. The model uses a discrete version of the Voronoi algorithm to partition the mesh into grains. The model is utilized to study representativity of grain structures. The number of grains needed in a representative volume element (RVE) is evaluated for materials with cubic symmetry and random texture. It is shown that the number of grains needed depend on the anisotropy, and a simple expression that relates anisotropy and the number of grains is suggested.

Paper E:
Comparison of Surface Displacement Measurements in a Ferritic Steel Using AFM and Non-Local Plasticity

An attempt to experimentally study deformation characteristics around grain boundaries and analyze the presence of strain gradients is presented. The evolution of surface profiles is studied by AFM at relatively small strains. The results indicate that this method can be used to draw conclusions about the deformation characteristics, e.g. in large grains the surface profile seems to vary within a grain. This latter effect can be seen as an indication of the inhomogeneous deformation occurring within large grains. The results are also compared with FEM calculations using a non-local crystal plasticity theory that incorporates strain gradients in the hardening moduli.
Paper F:
Incorporating Strain Gradients in Micromechanical Modeling of Polycrystalline Aluminum

It is a well known fact that polycrystals exhibit a grain size dependence. Traditional continuum models can however not catch this effect. Lately, there has however been an increased interest in the development of non-local theories, that can account for the size effect. In this work a non-local crystal plasticity theory is implemented, where slip gradients enter in the hardening modulus. A new proposal of how the gradients can be incorporated in the hardening modulus is presented. The non-local theory is used in a three-dimensional finite element model to model Aluminum (Al). A representative volume element (RVE) containing a random grain structure is used to model the material by the finite element method (FEM). Thus, the mesh is partitioned into a periodic grain structure by a discrete version of the Voronoi algorithm. The model is used to simulate uniaxial tension, by using periodic boundary conditions to constrain the model. The non-local theory contains an internal length scale $\lambda$ that needs to be set in the model. As the simulations are compared to reported experimental data on Al, the internal length is set. The coupling between the microstructure and the numerical model is discussed, and the proposed hardening relation is justified. It is shown that a model containing 30 grains predict the grain size effect well. But cells containing 15, 45 and 60 grains are also investigated. It is shown that the size effect can be predicted by changing the size of the periodic cell, and also by changing the number of grains in the cell.

Paper G:
Numerical Investigation of the Effect of Non-Local Plasticity on Surface Roughening in Metals

A non-local crystal plasticity theory that incorporates strain gradients in the hardening relation has been implemented. It is proposed that a gradient term enters the hardening modulus through a square-root dependence, which introduces an internal length scale. The relation has resemblance to the Hall-Petch relation. Simulations of polycrystalline materials are performed through a numerical finite element model that partition the mesh into grains through a discrete version of the Voronoi algorithm. Numerical simulations of a surface and its roughness are performed since it mimics experimental work, and comparisons to experiments are made. The effect of microstructure, the internal length scale, anisotropy and hardening is presented.
Bibliography


