THESIS FOR THE DEGREE OF LICENTIATE OF ENGINEERING IN SOLID AND STRUCTURAL MECHANICS

Computational Multiscale Modeling of Pearlitic Steel

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Abstract

The objective of this thesis is to investigate the possibilities to describe the mechanical behavior of a pearlitic steel by using computational homogenization, or multiscale modeling. The proposed model contains three scales: the engineering macroscale, the mesoscale representing the colonies of the pearlite ($\sim 10\mu$m) and the microscale containing the individual cementite lamellae and the ferrite matrix ($\sim 0.1\mu$m).

On the mesoscale of a pearlitic steel, two constituents can be identified in the form of cementite lamellae embedded in a ferrite matrix. These lamellae appear in domains, referred to as colonies, within which the corresponding orientation is ideally constant. The different domains, with their cementite (morphological) orientations but also with their crystallographic orientations of the ferrite, are homogenized in the modeling to obtain a macroscopic behavior of the pearlite. In the appended papers, different orientation distributions have been assumed and their influence on the macroscopic response has been studied. In addition, the number of orientations that should be included in the mesomodel to obtain a representative response has been investigated.

To capture the mechanical behavior of the constituents and their orientations, the mesomodel is linked to a micromodel using different prolongation conditions (both Taylor, Dirichlet and periodic). In the micromodel the ferrite is modeled by using crystal plasticity while the cementite is assumed to behave elastically. The micromodel is rotated depending on what cementite lamella orientation/colony it should represent. In addition, the crystallographic orientations of the ferrite are chosen depending on what colony that is modeled. The influence on the macroscopic response of the size of the micromodel and the prolongation condition from the mesomodel to the micromodel has been examined.

A number of numerical examples are presented within the appended papers illustrating the overall possibility of using the proposed multiscale model to predict the behavior of a pearlitic steel. In particular, both 2D and 3D models are used to show different sources of anisotropy. Finally, it is shown how the proposed multiscale model can be used to predict macroscopic yield surfaces.

Keywords: Multiscale modeling, crystal plasticity, pearlite, FE^2

Preface

The work presented in this thesis was carried out at the division of Material and Computational Mechanics at Chalmers University of Technology during 2009-2012. The research is financially supported by the Swedish Research Council (Vetenskapsrådet).

First of all, I would like to thank my supervisor Professor Magnus Ekh for his invaluable guidance and engagement during my time as a PhD-student. I also want to thank my co-supervisors Doctor Håkan Johansson and Associate Professor Johan Ahlström for their support. Furthermore, I want to thank all of my colleagues for creating such a nice working climate. Last, but certainly not least, I want to thank my girlfriend Elin Dartman for her endless support and understanding.

Göteborg, March 2012

Erik Lindfeldt

Thesis

This thesis consists of an introduction and the following appended papers:

Paper A E. Lindfeldt and M. Ekh. "Multiscale modeling of the mechanical behavior of pearlitic steel". Submitted for international publication (2011)

Paper B E. Lindfeldt and M. Ekh. "On the prediction of macroscopic yield surfaces for a pearlitic steel using computational homogenization". In preparation

The appended papers were prepared in collaboration with the co-author. The author of this thesis was responsible for the major progress of the work in preparing the papers, i.e. planning the papers, developing the theory, developing the numerical implementation and carrying out the numerical simulations.

Contents

Part I
Introduction

1 Background and Motivation

Pearlitic steels are frequently used in applications where the material is subjected to severe deformation, either during the manufacturing process or during operation. One example of the latter is rails which are subjected to very high loads at the contact patch between the rail and the wheel. The loading causes changes in the microstructure which in turn have an impact on the mechanical behavior of the component (see e.g. Wetscher et al. [15]).

By studying the microstructure of pearlitic steels, see Fig. 1.1, it is observed that pearlite is a two-phase material with cementite lamellae embedded in a ferrite matrix. It can also be noted that these cementite lamellae are aligned within domains, denoted colonies (following the definition by Mehl [12]), within which the corresponding orientation is (ideally) constant.

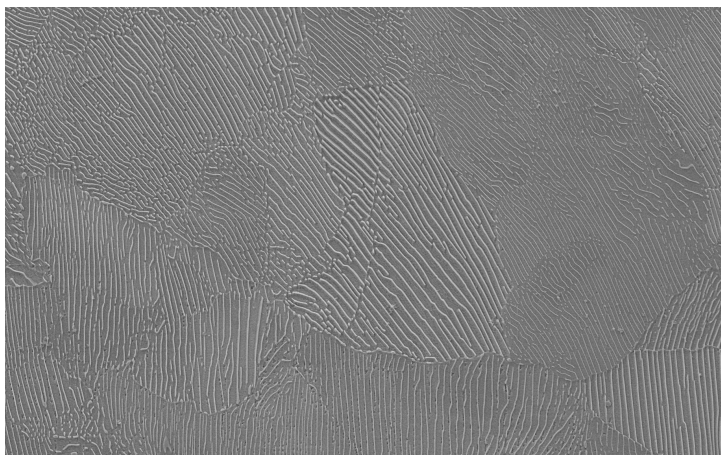

Figure 1.1: *Micrograph showing the microstructure of a pearlitic railway steel (900A). Image: Krste Cvetskovski.*

A random distribution of both the crystallographic orientations and the morphological (cementite lamellae) orientations results in an isotropic macroscopic behavior of the pearlite. However, if the pearlite is subjected to severe deformations then the microscopic orientations tend to align with the deformation which leads to an evolving macroscopic anisotropy (cf. [7, 15]).

Another important characteristic of the microstructure is the cementite lamella spacing s. As found in Alexander [2] the initial yield stress depends on the spacing in a Hall-Petch

type of relation i.e. $\sigma_y \sim s^{-1/m}$ where σ_y is the yield stress and m is an experimentally determined parameter (typically $1 \leq m \leq 2$).

The goal of this thesis is to include the microstructure with its characteristics explicitly in the modeling of the macroscopic behavior of pearlite. To reach this goal, a framework based on computational homogenization, or multiscale modeling, is proposed. The main concepts in the proposed multiscale model are described briefly in the following section.

2 Multiscale Model for Pearlitic Steel

The trend in the field of material modeling is to incorporate physical phenomena in the microstructure by adopting a multiscale modeling technique, cf. [5, 13, 16, 8] and references therein.

In the appended papers, a multiscale model for pearlitic steel is proposed, see Fig. 2.1. The model includes three scales: macroscale, mesoscale and microscale. On the macroscopic length scale the stress and strain relations, obtained by homogenization of the mesomodel, can be used e.g. to analyze the performance of a structural component.

Interactions between colonies, with varying cementite orientation (morphological orientation) and varying crystallographic orientation of the ferrite, are modeled on the mesoscopic length scale ($\sim 10\mu$m). Thus, the mesomodel comprises a number of colonies each related to a specific set of orientations. For both of the appended papers the modeling effort has been focused to the micromodel and therefore only the Taylor assumption has been used on the mesoscale. Clearly, this eliminates the possibility to include effects arising from e.g. fluctuating displacements, the shape of the colonies and interaction mechanisms at the colony borders. However, the impact of the distribution of both crystallographic and morphological orientations can still be accounted for.

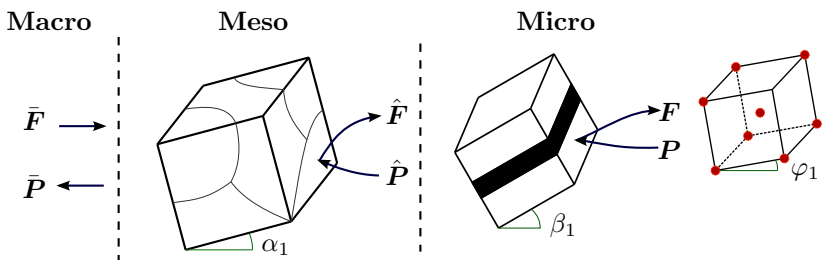

Figure 2.1: *Different length scales used in the prototype model*

On the microscopic length scale ($\sim 0.1\mu$m) the mechanical behavior of the constituents, i.e. ferrite and cementite, is modeled using a crystal plasticity model in the spirit of e.g. [13]. It is assumed that the constituents appear as single crystal domains. The behavior of the cementite is assumed to be elastic in the range of interest. The geometrical shape of the micromodel is chosen in the spirit of [11, 14]. The orientation of the micromodel

is described by the two Euler angles β_1 and β_2 which are controlled by the cementite lamella orientation of the considered colony.

As a means to investigate the validity of the micromodel, the size of the micromodel and the influence of the chosen prolongation condition (Taylor assumption, Dirichlet boundary condition and the periodic boundary condition) are studied. In the cases when fluctuating displacements are allowed the interactions between the constituents are explicitly taken into account.

In the first of the appended papers [9] a simplification to a 2D model is done by assuming a state of plane stress. In the second paper [10], as a means to increase the realism of the model, a general 3D model is used both on the mesoscale and on the microscale.

3 Summary of Appended Papers

- **Paper A: Multiscale modeling of the mechanical behavior of pearlitic steel**.
  Pearlitic steel is a two-phase material with cementite lamellae embedded in a ferrite matrix. In this contribution a representative microscale model is proposed capturing the behavior of the cementite and the ferrite and also the interaction between these phases. The response from the micromodel is coupled by means of computational homogenization to a representative mesomodel containing grains, or colonies, of pearlite. The material parameters of the ferrite and the cementite are identified by calibrating the model to experimental data for the pearlitic steel R260. Different types of prolongation conditions, i.e. how to couple the mesoscale kinematics to the microscale kinematics, are investigated and their results are compared. Finally, investigations are conducted of how many crystallographic directions of the ferrite and how many colonies (i.e. cementite directions) that are needed to obtain a representative mesomodel of the pearlite.

- **Paper B: On the prediction of macroscopic yield surfaces for a pearlitic steel using computational homogenization**.
  In this paper a multiscale modeling framework is used to predict yield surfaces. On the mesoscale a model taking into account the features of the pearlite colonies, i.e. the crystallographic orientations of the ferrite and the cementite lamella orientation, is used. The microscale model includes both the ferrite matrix and the cementite lamellae as well as the interactions between these phases. The model is used to predict yield surfaces for both isotropic and anisotropic mesomodels.

4 Conclusions and Outlook

In the appended papers models, based on the concept of computational homogenization tailored for a pearlitic steel, are proposed. The models are designed to capture physical subscale mechanisms. To be specific, the proposed mesomodel can capture the influence

of the distributions of both crystallographic and morphological orientations. Similarly, on the microscale a micromodel is formulated such that it can capture the mechanical behavior of the constituents of pearlite; cementite and ferrite. Furthermore, when using the Dirichlet or periodic boundary conditions to link the kinematics of the mesomodel to to the kinematics of the micromodel the interactions between the constituents can be explicitly accounted for. As a means to model the mechanical behavior of the constituents, a crystal plasticity model is used for the ferrite while it is assumed that, within the stress range of interest, the cementite can be adequately modeled by assuming an elastic model.

In the first of the appended papers [9], the modeling complexity was limited to a state of plane stress so that a 2D model could be used. By using this model the values for the parameters of the constitutive model were identified using experimental data from [1]. With this model the anisotropic mechanisms, both morphological and crystallographic, were studied. It was then concluded that the crystallographic orientation has a more significant impact on the resulting stress response than the morphological orientation (i.e. cementite orientation). Furthermore, the significance of the size of the mesomodel was studied. This was done by varying the number of orientations and studying the resulting macroscopic stress response. As expected, it was then found that as the number of orientations increases, the stress response converges.

As a means to increase the realism of the model the 2D assumption was replaced in the second of the appended papers [10] by 3D models both on the mesoscale and on the microscale. Using the same material model parameter values as in paper A, the behavior of the 3D model was investigated. By studying the impact of the orientations (now with two angles for each type of orientation) the conclusion from paper A that the crystallographic orientations has a larger impact on the stress response than the morphological orientations was confirmed. In addition, the model was used to predict yield surfaces on the macroscale using an effective plastic strain measure. It was found that it is necessary to allow for a fluctuating displacement field on the microscale to take into account the morphological anisotropy although its importance was found to be of secondary importance. Further studies on how the morphological anisotropy is influenced by the size of the micromodel needs to be conducted.

In the first of the two appended papers the constitutive model parameter values were identified using experimental data pertaining to a standard macroscale experiment. For the future work it would be interesting to compare such a method with in-situ strain measurements on the mesoscale. With such an approach it might be possible to identify the parameters for the constituents directly.

In order to be able to include the mechanisms occurring at colony boundaries with different orientations then the mesomodel would have to be based on an FE solution such that the resulting model would be of FE^2 type. This would of course increase the need for computational power but by using a parallel implementation it might still be a feasible option for studying such effects.

As an alternative approach the mechanisms currently captured in the micromodel could be moved into the mesomodel by resolving it, mesh-wise, down to the constituents. By doing so, the interactions between different grains and the interactions between the constituents would be accounted for in the mesomodel. However, the feasibility of such a model is, in the author's opinion, questionable since it would require a massive

workload to create a mesh for such a model. Furthermore, it would probably render a too computationally costly model.

Another interesting extension of the proposed model would be to include size effects on the microscale by using gradient crystal plasticity, cf. [4, 3]. By using such a model the effects of e.g. dislocation pile-ups at the boundaries between the phases could be included such that the behavior of the micromodel will be affected by the cementite lamella spacing.

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