Anisotropy in pearlitic steel subjected to rolling contact fatigue - modelling and experiments

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CHALMERS UNIVERSITY OF TECHNOLOGY
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Abstract

In rails and wheels subjected to severe rolling/sliding contact, large plastic deformations accumulate in the surface layer. This decreases the fatigue resistance of components and makes this layer prone to formation of common rolling contact related defects. In pearlitic steel railway components, accumulated plastic deformations result in microstructural changes which, in turn, lead to anisotropic characteristic of properties like fracture toughness.

The aim of the thesis is to investigate the influence of material anisotropy on damage mechanisms of pearlitic rail steels subjected to rolling/sliding contact. The interaction between the pearlitic microstructure and cracks in the surface layer of rail samples is studied. Based on microstructural investigations, an anisotropic fracture surface model is proposed to account for the directional dependence of resistance against crack propagation. The fracture surface model is employed in a computational framework where propagation of planar cracks is simulated. The simulation results show that the degree of anisotropy in the surface layer has a significant influence on the crack propagation path. In particular isotropic material characteristics will result in crack propagation towards the surface. This is a fairly benign type of fracture as compared to the transversal rail breaks that may result if the propagation deviates into the bulk material.

To include large plastic deformations and the resulting anisotropy in simulations, a hybrid micro-macromechanical material model for pearlitic steels is proposed. Results from High Pressure Torsion (HPT) tests were used to calibrate the model. In HPT tests, samples are deformed under similar loading conditions to that of the rail–wheel contact i.e. a high compressive force and simultaneous large torsional straining. The HPT deformation procedure is simulated in the commercial finite element package ABAQUS. Numerical results agree well with experimental data demonstrating the high potential of the proposed material model in analyses including large deformations of pearlitic steel. In addition, the influence of different homogenization techniques in the material model is investigated. Two models proposed for a pearlitic colony are calibrated against micro-compression test data. The macroscopic response of a 3D model of pearlitic steel during simple shear deformation is compared with the response predicted by the developed hybrid material model. The hybrid model was found to give stress–strain responses that are qualitatively similar, but around 12% lower in stress magnitudes compared to the other two models. This should be contrasted towards the superior computational performance of the hybrid model.

Keywords: Anisotropy, plasticity, pearlitic steel, Rolling Contact Fatigue, crack propagation, High Pressure Torsion

to Ahmad Larijani & Tehereh Shabnam

whose support and love can fly
3660.21 km and even more:

ای کاش
ای کاش آدمی وطنش را
مثل بنفشه ها
در جعبه های خاک
یک روز می توانست
همراه خویشتن
ببرد هر کجا که خواست
در روشنای باران
در آفتاب پاک

"Think if man could one day
like violets
in soil boxes
take his home with him
wherever he wanted ..."

-Mohammad-Reza Shafiei Kadkani

Preface

The work presented in this thesis was carried out at the Department of Applied Mechanics at Chalmers University of Technology between the years 2009-2014 within the project MU19 "Material anisotropy and Rolling Contact Fatigue in rails and switches". The project is part of the activities within the Centre of Excellence in Railway Mechanics (CHARMEC) and is supported by the industrial partners voestalpine Schienen GmbH, Trafikverket and SLL Trafikförvaltningen.

Acknowledgements

First of all, I would like to thank my main supervisor Professor Magnus Ekh who patiently mentored me during the last five years which I know for fact was not easy at all. I am also very grateful for all the support and encouragement I received from my co-supervisor Professor Anders Ekberg. I believe he is the only professor who can praise you for the smallest things like learning how to say "It goes fine!" in Swedish as if it is a big accomplishment towards winning the Nobel Prize. I would like to express my gratitude to my co-authors Jim Brouzoulis, Martin Schilke, Professor Christer Persson and Erik Lindfeldt at Chalmers University of Technology and also Christoph Kammerhofer, Marlene Kapp and Professor Reinhard Pippan from Erich Schmid Institute of Materials Science. It has been a pleasure to be a part of all of these co-operational works between computational mechanics and material science experts which I hope will continue in future. Furthermore, I want to thank my colleagues at the Divisions of Material and Computational Mechanics and Dynamics especially the hard working PhD students who did not let me feel lonely even for one single weekend at work.

Most importantly, I would like to thank my family in Iran for their unconditional support through these years which made all the difficulties of living so far away from them tolerable. I am also very thankful to Tayyebeh Larijani and Nasser Rajabi who have been my second parents during the last seven years. Last but definitely not least, I wish to thank Martin who showed me what you truly mean by saying "for better and for worse". He being there for me while writing this thesis was definitely a good example of the latter.

Nasim Larijani
Göteborg, May 2014

Thesis

This thesis consists of an extended summary and the following appended papers:

Paper A	M. Schilke, N. Larijani, and C. Persson. Interaction between cracks and microstructure in three dimensions for rolling contact fatigue in railway rails. *Fatigue and Fracture of Engineering Materials and Structures* **37**.3 (2014), 280–289
Paper B	N. Larijani, J. Brouzoulis, M. Schilke, and M. Ekh. The effect of anisotropy on crack propagation in pearlitic rail steel. *Wear* **314**.1–2 (2014). Proceedings of the 9th International Conference on Contact Mechanics and Wear of Rail / Wheel Systems, Chengdu, 2012, 57 –68
Paper C	N. Larijani, G. Johansson, and M. Ekh. Hybrid microemacromechanical modeling of anisotropy evolution in pearlitic steel. *European Journal of Mechanics, A/Solids* **38** (2013), 38–47
Paper D	N. Larijani, C. Kammerhofer, and M. Ekh. Simulation of high pressure torsion tests of pearlitic steel. *To be submitted for international publication* (2014)
Paper E	M. Ekh, N. Larijani, E. Lindfeldt, M. Kapp, and R. Pippan. A comparison of homogenization approaches for modelling the mechanical behaviour of pearlitic steel. *To be submitted for international publication* (2014)

The appended papers were prepared in collaboration with the co-authors. The author of this thesis is responsible for the major progress of the work in papers **Paper B-D** i.e. planning the papers and developing the theory, developing the numerical implementations and carrying out the numerical simulations. In **Paper A** the author of this thesis is responsible for three-dimensional reconstruction of the cracks, and in **Paper E** the author has assisted in developing the theory and numerical implementation and carrying out the numerical simulations.

Contents

Part I
Extended Summary

1 Motivation and background

Current demands on railways in terms of transportation volumes, axle loads, speeds, reliability, competitiveness etc. are often much higher than what the railways were initially designed for. The consequence is that operational loads have increased significantly at the same time as margins for errors have decreased. To meet these requirements, numerous efforts have been put into railway research. One important research goal is to decrease the deterioration of rails and wheels. Development of new materials is one example of such research. The research can also aim at improving the knowledge of actual operational loads and resulting deterioration mechanisms e.g. by improved quantification of wheel–rail contact forces or by analysis of the material behaviour under identified loading conditions. The current thesis mainly focuses on the latter topic. By an increased understanding of the material response and related improvements in predictive capabilities, the development (e.g. new materials) can target key aspects and modified solutions (e.g. regarding wheel–rail geometries) can be analysed through simulations before introduction in field.

The damage mechanisms in rails and wheels can be broadly distinguished as wear, cracking and plastic deformation. Wear is characterized as removal of material from the surface in the form of small particles. Cracking, which consists of initiation and propagation of cracks in the bulk material, is generally distinguished by the type of loading that causes the crack formation. Cracks caused by the repeated mechanical loading between wheel and rail (so-called rolling contact fatigue, RCF) are one of the most common defects in rails and wheels. The maintenance costs associated with RCF related defects are generally very high; e.g. the annual RCF maintenance cost in Deutsche Bahn rail network surpassed €150 million in 2009 [13].

Owing to the small wheel–rail contact patch and the very high contact loads in current railway operations, plastic deformation in rail and wheel surfaces is usually inevitable. Plastic deformation will lead to profile changes in wheels and rails. Furthermore, accumulation of plastic deformation in the surface material is the root cause for surface initiated RCF cracks.

The most commonly used steel type in railways today is pearlitic steel (cf. [41]). In pearlitic steel components, accumulated plastic deformations cause changes in the microstructure of the material. This leads to considerable changes and formation of anisotropy in the severely deformed surface layer which affect properties like yield stress and fracture toughness, cf. [76, 28]. These properties are decisive for fatigue performance of the material. Consequently, initiation and propagation of cracks in the surface layer of wheels and rails are substantially affected by the amount of anisotropy evolved in the material.

Changes in the microstructure and as a result in the behaviour of pearlitic steel under large deformations has been the subject of many research works during years e.g. [43, 44, 68, 69, 79, 76, 28]. In [2, 70, 12, 19] microstructural changes in pearlitic rail steel specifically under rolling contact loading has been studied and some models in the context of RCF analyses are proposed. However, material anisotropy is rarely considered in studies on initiation and growth of RCF cracks. To quantify and predict the amount of developed anisotropy and the related influence on material strength in pearlitic steel subjected to repeated (rolling) contact loading is the core topic of the current thesis.

To this end numerical simulations of rolling contact and models for prediction of material responses are required. The first approaches set out from assumption of elastic contact and idealized contact geometries. Resulting contact pressure distribution under these assumptions was first derived by Heinrich Hertz in 1882 [26]. The resulting stress field in the contacting bodies is calculated analytically for special cases, such as a line contact (contact between a cylinder and a plane) in [38]. In [67] the stress in the center of a circular contact (contact between two spheres or a sphere and a plane) is calculated. For more complex cases the stress field may be approximated utilizing point load formulae of Bossinesq and Cerruti [50, 21]. These approaches give reasonable results for fairly idealized contacts. However, for general contact cases, more refined methods such as those suggested in [31] need to be adopted.

In particular, the analyses mentioned above do not account for plastic deformations. A simplified approach to account for the influence of plastic deformation is the "shakedown map" developed by Johnson [38]. Shakedown maps give an indication on whether plastic deformation is to be expected initially (so-called elastic or plastic shakedown) or throughout the repeated rolling contact loading (ratcheting). The shakedown maps are derived under the presumption of fairly idealised conditions. More general/refined analyses usually require the use of Finite Element (FE) simulations where stress and plastic strain field are calculated by adopting a material model including plasticity and hardening. In particular, a non-linear kinematic hardening mechanism needs to be included to be able to predict continuous plastic strain accumulation (ratcheting).

In order to predict material deterioration (in the form of wear or in the form of crack formation and growth), based on stress field analyses, damage criteria need to be defined and employed. There are several such criteria available in the literature, see e.g. [14] and [48] for reviews.

The influence of anisotropy is generally ignored in currently available models for stress analyses and damage prediction in railway components. Considering the amount of anisotropy (directional dependence of properties) found in both wheels [16] and rail steels [76, 28, 39], it is clear that this is a rather severe simplification. How this simplification affects the accuracy of the analyses will depend on the topic studied. Prediction of RCF crack propagation in rails is an example of analysis where overlooking the anisotropic characteristics of the material can result in unrealistic predictions [47].

Building on results from several previous research projects [4, 34, 65, 8], this thesis explores anisotropic material characteristics of pearlitic steel in the vicinity of the wheel–rail contact. Methods of introducing these material characteristics into predictive models are detailed and implemented in numerical codes. Analysis results are presented and consequences of excluding anisotropic characteristics are demonstrated.

2 Pearlitic microstructure and large deformations

Changes in mechanical properties of pearlitic steel, subjected to large plastic deformations, are generally attributed to changes in its lamellar microstructure and work hardening of the individual phases. Pearlite consists of two phases, ferrite and cementite. While ferrite is relatively ductile, the cementite phase is hard and brittle. These two phases together give a composite-like structure to pearlite in the form of bands of ferrite and cementite (see Figure 2.1). Due to the higher percentage of the ferrite phase, the cementite

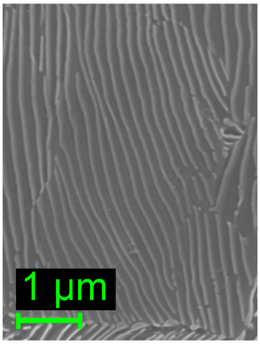
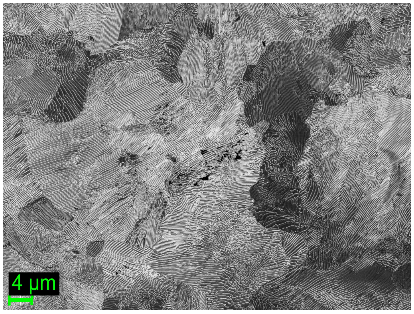
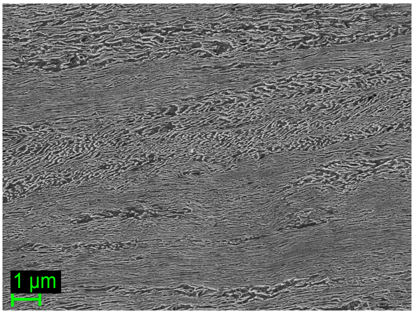


Figure 2.1: *Micrograph of a small pearlitic colony taken by a Scanning Electron Microscope (SEM).*

phase is usually referred to as cementite lamellae. Domains in which cementite lamellae are aligned in a preferred direction, are denoted as colonies. Random orientation of



(a)



(b)

Figure 2.2: *SEM micrographs of pearlitic steel R260 (a) undeformed base material; (b) deformed material in a high pressure torsion (HPT) machine up to an equivalent strain of 500%.*

colonies in an undeformed pearlitic structure (Figure 2.2a), accounts for the isotropy of the mechanical properties on the macroscopic length scale. Under deformation, however, the individual colonies start to re-orient and align in the principal direction of deformation, cf. [30, 68, 76]. This alignment evolves markedly in the microstructure with increasing deformation. At very large deformations, the largest part of the structure is fully aligned while the interlamellar distance is decreased and the lamellae have become thinner and broken (Figure 2.2b). This transformation in the microstructure can be clearly seen in micrographs of the pearlitic structure in rails where alignment decreases with depth below the rail surface, see Figure 2.3.

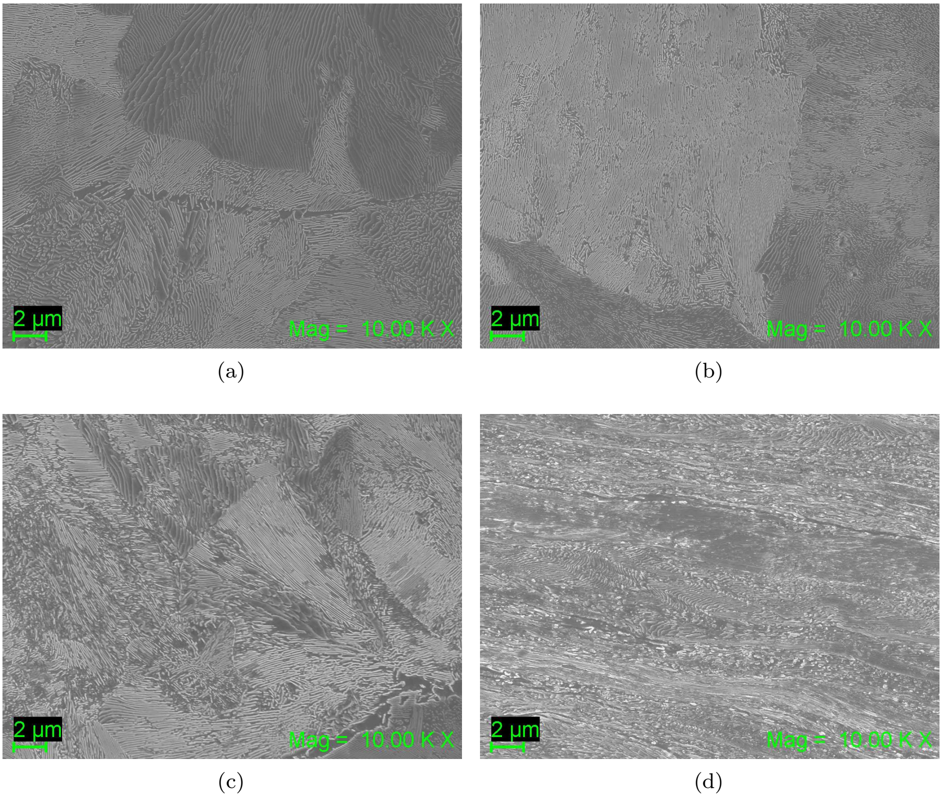
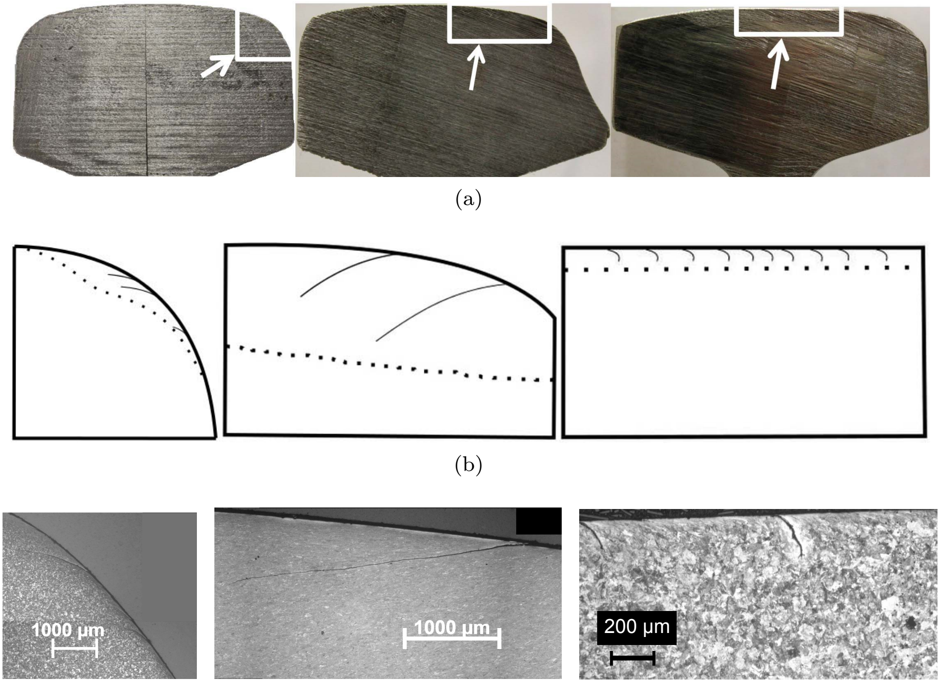


Figure 2.3: *SEM micrographs of the structure of pearlitic rail steel R350HT at depths of (a)* 2 mm*; (b)* 1 mm*; (c)* 500 µm*; (d)* 100 µm *below the running band of the rail.*

3 Anisotropy and RCF cracks in rails

Plastic deformation and resulting crack formation occur, to higher or lower extent, in the surface layer of all rails, cf. [27]. Rails have been investigated in laboratories to analyse the correlation between plasticity and cracks with the main purpose of explaining initiation and crack growth in the deformed surface layer, cf. [12, 23, 19]. In **Paper A** the interaction between cracks and microstructure in three different pearlitic steel rail samples was studied. Investigation of the RCF cracks show that the main direction of the cracks generally coincides with the direction of the plastic flow (see Figure 3.1). The depth of



(a)

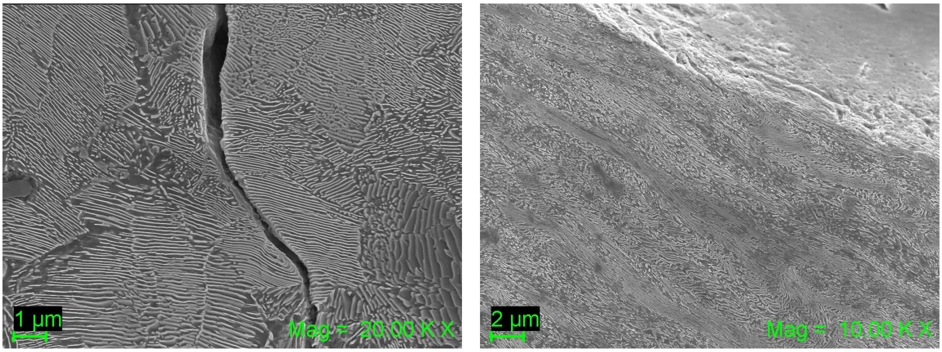
(b)

(c) (d) (e)

Figure 3.1: *Rail samples (from left to right) of the rail grade R350HT tested in a full scale test rig, 900A/900B taken from a curve close to Falköping and R350HT taken from a curve in the Stockholm local traffic network ;(a) Investigated area with RCF cracks; (b) Schematic representation of the transverse plastic flow indicated as solid lines and the border of the plastically deformed area indicated by the dashed line; (c)-(e) typical cracks found in the investigated areas.*

the plastically deformed surface layer and the amount of alignment of the microstructure varies with the contact loading and the rail grade (original microstructure of pearlitic steel). However, once the plastic deformation is present, it is clear that the cracks grow in the direction with the lowest resistance against crack propagation.

Studies on changes in the mechanical properties of heavily deformed pearlitic rail steels, by equal channel angular pressing and High Pressure Torsion (HPT), reveal a significant degree of anisotropy in fracture toughness and fatigue crack propagation rate, cf. [28, 76]. Fracture toughness has been found to be lower (and crack propagation rate higher) for a crack propagation parallel with the aligned microstructure than perpendicular to it. From this it is likely that fatigue crack propagation resistance is much lower for propagation parallel with the alignment of the microstructure than in the perpendicular direction. Micrographs along the path of the rail surface cracks confirm this (see Figure 3.2). Cracks



(a) (b)

Figure 3.2: *SEM micrographs along the path of a crack in the surface layer of a rail sample (tested in a full scale test rig) at the depth of (a) 900* µm*; (b) 100* µm.

propagate parallel to the aligned lamellae in the deformed microstructure close to the surface. However, when the crack grows deeper into the rail, where the alignment in the microstructure is less pronounced, the propagation progresses along colony boundaries and even through colonies. This implies that the weakest path in an undeformed structure is more random. Therefore, even propagation through cementite lamellae is occasionally preferred in such a structure. Based on these observations an *anisotropic fatigue crack growth threshold surface* model is proposed in **Paper B**. Here the fatigue crack growth threshold value $\mathcal{G}_{\mathrm{th}}$, which is a measure of resistance against crack propagation, is defined as a function of direction φ:

$$\mathcal{G}_{\mathrm{th}}(\varphi) = \mathcal{G}_{\mathrm{th},1} + (\mathcal{G}_{\mathrm{th},2} - \mathcal{G}_{\mathrm{th},1})(1 - \exp(-A\,|\sin(\varphi)|)) \qquad \text{for} \qquad 0 < \varphi < 2\pi, \tag{3.1}$$

where $\mathcal{G}_{\mathrm{th},1}$ and $\mathcal{G}_{\mathrm{th},2}$ are the lowest and highest values of fatigue crack growth threshold at a point in the material. In a fully aligned microstruture these represent the resistance against a propagation in the direction of alignment of the microstructure and in the perpendicular direction. Note that experimental results in [28, 76] indicate that, during a transition from an undeformed pearlitic microstucture to a fully aligned microstructure, the resistance against crack propagation in the direction of alignment is reduced and the resistance in the perpendicular direction increases. Figure 3.3 illustrates the fatigue crack growth threshold surface returned by Equation 3.1 for cases of isotropy and anisotropy.

The degree of anisotropy at each material point in the surface layer is related to the degree of alignment in the microstructure. By employing knowledge about how the alignment of the microstructure varies with depth, changes in crack propagation resistance over the surface layer can be illustrated as in Figure 3.4. In **Paper B**, a 2D crack propagation model, formulated in terms of a *crack-driving force* based on the concept of material forces (see [51, 22]), is adopted for simulation of crack propagation, cf. [66,

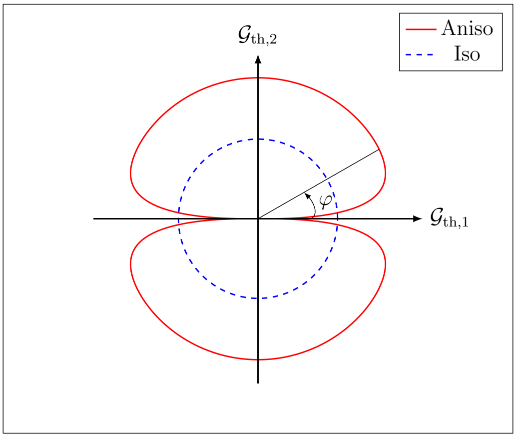


Figure 3.3: *Fatigue crack growth threshold surface for an anisotropic and isotropic structure.*

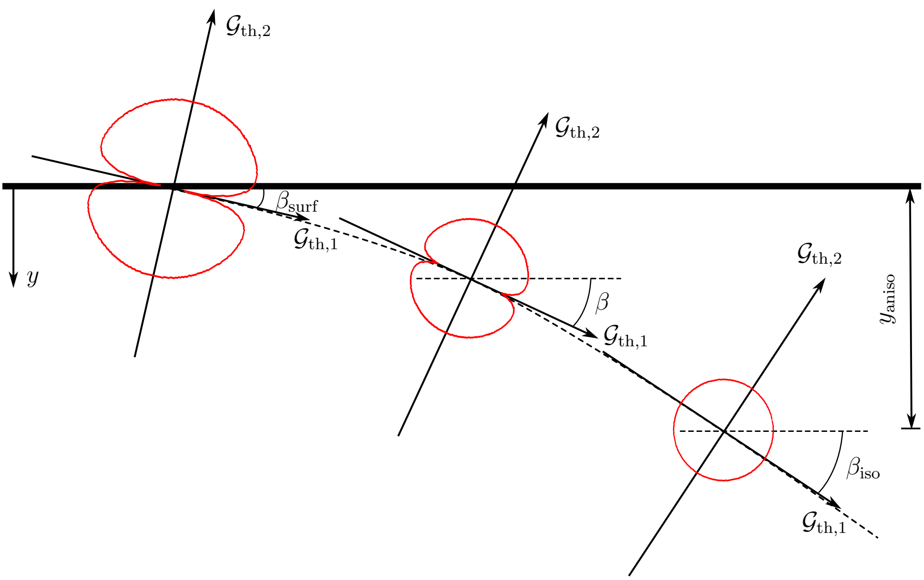


Figure 3.4: *Variation of fatigue crack growth threshold surface over the anisotropic surface layer.*

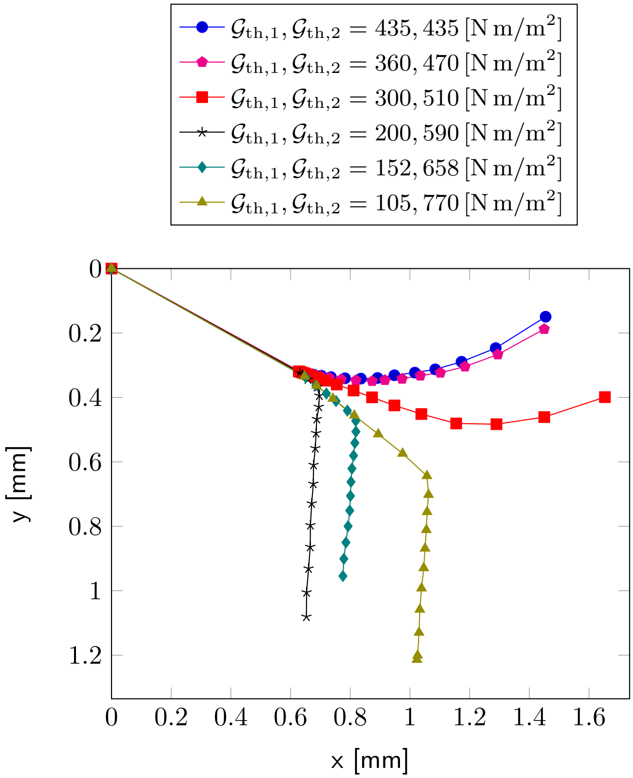


Figure 3.5: *Crack paths for different degrees of anisotropy with the initial crack length* $a_0 = 0.7\,\mathrm{mm}$ *and thickness of anisotropic layer* $y_{\mathrm{aniso}} = 1\,\mathrm{mm}$.

9]. Numerical simulations of crack growth that incorporated the developed fatigue crack growth threshold model were carried out for a simple 2D model of wheel–rail contact. The results show that the degree of anisotropy (in terms of directional dependent fatigue crack growth threshold properties) has a substantial influence on the direction of propagation of cracks in the surface layer (see Figure 3.5). In addition, the results show that cracks in a surface layer with a high degree of anisotropy tend to grow downwards into the rail while cracks in a more isotropic surface layer tend to propagate towards the surface. The latter case would imply detachment of surface material which is fairly benign. The former, on the other hand, could imply transverse fracture of the rail which may cause a rail break with severe consequences. Field observations have shown that both of the cases happen in pearlitic steel rails (see Figure 3.6). Analyses in the context of numerical prediction of RCF could give an assessment of the probability of a downward propagation if the amount of deformation-induced anisotropy could be predicted.

(a) (b)

Figure 3.6: *(a) Transverse propagation of a rail crack resulting in a rail break (Image courtesy Jan-Olof Yxell, Chalmers); (b) Running surface of the same rail with cracks and detached pieces (probably due to upward propagation of cracks).*

4 Material model

Prediction of evolution of anisotropy and large plastic deformations in pearlitic steel requires a constitutive model designed to capture changes in material's behaviour due to re-orientation and alignment of cementite lamellae on the microscopic level. Therefore, in **Paper C** a macroscopic material model is formulated to predict large irreversible deformations and evolution of anisotropy in pearlitic steel.

Different models have been proposed in literature for prediction of the behaviour of pearlitic steels. Depending on the adopted approach, the models can be divided into two main groups: phenomenological based models and microstructure based models. The phenomenological based models employ empirical equations that are formulated based on the correlations found between microstructural factors and the macroscopic behaviour of material, cf. [1, 6]. These models are usually computationally inexpensive. However, they can not predict the influence of interactions between the constituents on micro-scale.

The microstructure based models formulated for multi-scale modelling have attracted much attention during the last years. In these models, the starting point is a representative model on micro- or meso-scale that can capture the behaviour of the constituents and their interaction. This representative micro- or meso-scale model is utilized to solve for the macroscopic response of the material by some homogenization procedure. In general, Finite Element Method (FEM) is used to solve for the fluctuating displacement field of a Representative Volume Element (RVE) that is subjected to proper boundary conditions, see e.g. [81]. An advantage of this type of models is that they can be used to predict a specific behaviour in the material caused by microstructural changes, where even effects like shape and volume fraction of microstructural components can be included. Some models of this type, proposed for carbon steel, have given promising results, cf. [64, 75]. However, it is obvious that an FE simulation utilizing such a model (i.e. multi-scale modelling) is highly time-consuming and requires high computational efforts. Moreover, calibration of such a model is usually very difficult considering the limited number of experiments that can return the material parameters on the micro-scale.

A common approach for modelling anisotropy is to introduce structural tensors in the governing equations (e.g. free energy and/or yield function) as described in e.g. [5]. By adopting this approach, evolution of anisotropy, e.g. due to large plastic deformations, can be attributed to evolution of the structural tensors. This is discussed and employed to model evolution of anisotropy in e.g. biological tissues, fibre-reinforced composites and during metal forming in [62, 52, 58, 72]. Another main approach is based on formulation of a constitutive law for the plastic spin to describe evolution of the anisotropic properties in the material, as described and used in e.g. [20, 42, 29]. These two main approaches to model evolving anisotropy using structural tensors are described and compared in [25]. In [35, 37] a micromechanical based model was proposed to model evolution of anisotropy in pearlitic steel. The macroscopic model was obtained through analytical homogenization of the microscopic model using a closure assumption taking into account re-orientation of cementite lamellae. The material model in **Paper C** is proposed in the spirit of these recent works, while a different homogenization technique is utilized.

4.1 A hybrid micro-macromechanical model

The model proposed in **Paper C** is a thermodynamically consistent macroscopic model based on the microstructural texture development in the pearlite that causes evolution of anisotropy. Therefore, it can be called a hybrid model. Similar concepts have been employed to model anisotropy e.g. in biological tissues and polymers, cf. [24, 53]

In this hybrid model the evolution of anisotropy on the macroscopic length scale in pearlitic steel is captured via modelling the alignment of the microstructure during deformation. The re-orientation of cementite lamellae within the pearlitic microstructure is assumed to be of *areal-affine* type. The assumption of areal-affine re-orientation states that

$$\boldsymbol{n}_\mu = \boldsymbol{F}^{-\mathrm{t}} \cdot \boldsymbol{n}_{\mu 0} / |\boldsymbol{F}^{-\mathrm{t}} \cdot \boldsymbol{n}_{\mu 0}|, \tag{4.1}$$

where $\boldsymbol{n}_\mu$ represents the current normal orientation of cementite lamellae in a pearlitic colony (see Figure 4.1) and $\boldsymbol{n}_{\mu 0} \doteq \boldsymbol{n}_{\mu | t=t_0}$ is the corresponding initial orientation. This assumption is adopted since the the normal vector $\boldsymbol{n}_\mu$ of the cementite lamellae strives to be perpendicular to the material flow during deformation.

Assuming that plastic flow is mainly caused by shearing of the ferrite phase between the cementite lamellae, the yielding of a pearlitic colony μ is proposed to be governed by

$$\Phi_\mu \doteq \frac{\tau_\mu^2}{Y_\mu} - Y_\mu, \tag{4.2}$$

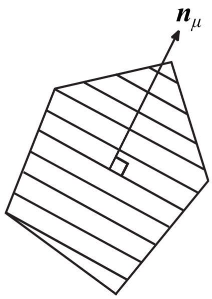


Figure 4.1: *A schematic of a pearlitic colony with the representative normal* $\boldsymbol{n}_\mu$.

where Y_μ is the elastic limit of a single pearlitic colony and τ_μ is a scalar stress measure of Schmid-type representing the shear stress between the cementite lamellae. Considering the finite thickness of ferrite between the cementite lamellae and the evidence on development of plasticity even in the cementite phase, the yield function is extended as follows

$$\Phi_\mu \doteq \frac{\zeta\,\tau_\mu^2 + (1-\zeta)\,\tau_{\mathrm{vM}\mu}^2}{Y_\mu} - Y_\mu \leq 0, \tag{4.3}$$

where ζ is a parameter controlling the portion of the material that yields due to shear in the ferrite phase parallel with the cementite lamellae plane and $\tau_{\mathrm{vM}\mu}$ is the equivalent von Mises stress.

The corresponding macroscopic yield function is motivated by homogenization of the micromechanical yield function

$$\Phi = \frac{\zeta\left\langle\tau_\mu^2\right\rangle + (1-\zeta)\left\langle\tau_{\mathrm{vM}\mu}^2\right\rangle}{Y} - Y, \tag{4.4}$$

where Y is the macroscopic yield stress. The possible orientations for the cementite lamellae within the pearlitic microstructure in 3D space can be represented by normal vectors pointing at the surface of a unit sphere. Therefore, the operator $\langle\bullet\rangle$, which returns the homogenized quantity of the variable $\bullet$, is here defined as a surface integral over a unit sphere (cf. [54]). The material model is formulated in a large strain setting and includes isotropic and kinematic hardening.

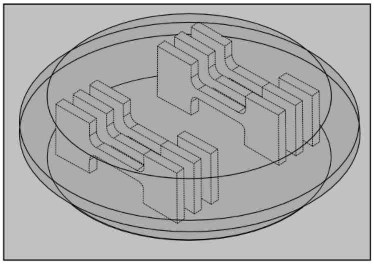
As mentioned earlier, kinematic hardening needs to be included in material models to capture the ratcheting response of the material (i.e. directional plastic strain accumulation under cyclic loading) and also to capture the Bauschinger effect(i.e. reduction of the elastic limit during reversed loading). Modelling of these phenomena in engineering materials generally requires non-linear kinematic hardening laws. A suitable non-linear kinematic hardening law, which can give realistic shapes of the stress–strain curves under cyclic loading, was proposed by Armstrong and Frederick in 1966 [33]. This type of kinematic hardening is discussed and utilized to model large strain plasticity in e.g. [74, 36, 10, 63, 73]. In the current work, multiple kinematic hardening models of Armstrong-Frederick type are adopted with the large strain formulation proposed in [36, 37].

4.2 HPT tests and calibration of the hybrid model

High Pressure Torsion (HPT) is a severe plastic deformation process whereby samples are subjected to a high compressive force and simultaneous torsional straining. This technique has gained much attention over the last 20 years mostly as a metal forming process [80]. Due to the high hydrostatic pressure during this type of torsion test, the fracture strain is increased. Thereby it is possible to apply extremely large torsional deformations on the HPT samples, cf. [7] and obtain exceptional grain refinements to the nanometer level. Different studies on changes of mechanical properties of rail materials under large plastic deformations have been carried out with the help of HPT tests, cf. [28, 77, 39]. Since the loading condition is similar to that of the rail–wheel contact, deformation of pearlitic steel samples in HPT tests produces a microstructure similar to that found in the plastically deformed surface layer of rails (see Figure 2.2).

The HPT experiments in **Paper D** were carried out at the Erich Schmid Institute of Materials Science on the standard rail grade R260. The HPT samples were small discs machined from samples extracted from the gauge corner of a newly manufactured piece of rail. The disc samples were deformed in the HPT tool under a pressure of 4 GPa and a torsional shearing corresponding to $\frac{1}{4}$, $\frac{1}{2}$ and 2 revolutions. After the HPT pre-deformation, tensile samples were prepared from the disc at various radii, with the sample axis being parallel to the shear direction, as illustrated in Figure 4.2. Tensile tests

(a)

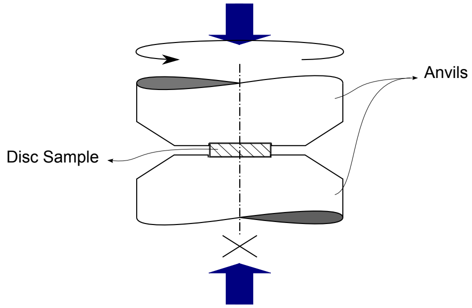


(b)

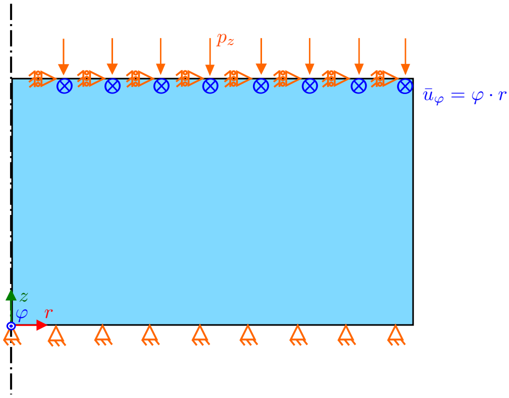
Figure 4.2: *(a) Undeformed and deformed HPT disc samples and tensile test sample; (b) Tensile test samples prepared from the HPT disc.*

were conducted on these samples and the results were used for calibration of the material model proposed in **Paper C**.

In order to calibrate the material model, the pre-deformation of the samples in the HPT machine should be simulated numerically. Simulation of the HPT process has been the subject of a few studies with focus on the qualitative behaviour of material and plastic flow as well as stress state and contact conditions between the sample and the anvils, cf. [7, 78, 40, 11, 71]. However, in **Paper D** the focus was on prediction of stress–strain behaviour of the sample discs made of pearlitic steel after up to at least two revolutions of torsional deformation. The HPT process was simulated in the commercial FE package ABAQUS utilizing an axi-symmetric model of the HPT disc (see Figure 4.3). Good



(a)



(b)

Figure 4.3: *(a) The schematics of loading the disk sample in the HPT machine; (b) Axi-symmetric model of the disk in ABAQUS: Coordinate system, boundary conditions and loads.*

agreement between simulations and experimentally obtained stress–strain curves was achieved (see Figure 4.4). This indicates that the proposed material model in **Paper C** is a good candidate for simulation of large deformation processes and prediction of microstructural evolution in pearlitic steel.

4.3 Comparison of homogenization approaches

4.3.1 Pearlitic colony models

As implied earlier in this thesis, microstructure based models can employ different homogenization techniques to obtain the macroscopic response from micromechanical models. It was mentioned in Section 4.1 that the hybrid model proposed in **Paper C**, was chosen over micromodels designed for multi-scale modelling, due to its superior computational efficiency. However, if this comes at the cost of a considerable precision loss, better alternatives have to be considered.

In the hybrid model, the orientation distribution of the cementite lamellae determines the macroscopic anisotropy characteristics of pearlitic steel. Here the homogenization assumption infers integration over the surface of a unit sphere. The influence of the homogenization assumption (Equation 4.4) on the macroscopic response when adopting hybrid model instead of Equation 4.3 is investigated in **Paper E**. The pearlitic colony model based on Equation 4.3 is denoted as $\hat{f}_{\mathrm{i+1}}$.

Another pearlitic colony model also included in investigations is introduced in [49]. This model is denoted as $\hat{f}_{\mathrm{i}}$. In model $\hat{f}_{\mathrm{i}}$ the cementite and the ferrite are modelled individually by adopting an isotropic elasto-plasticity model. The planes of cementite lamellae and the ferrite in one pearlitic colony are assumed to have infinite width and are modelled

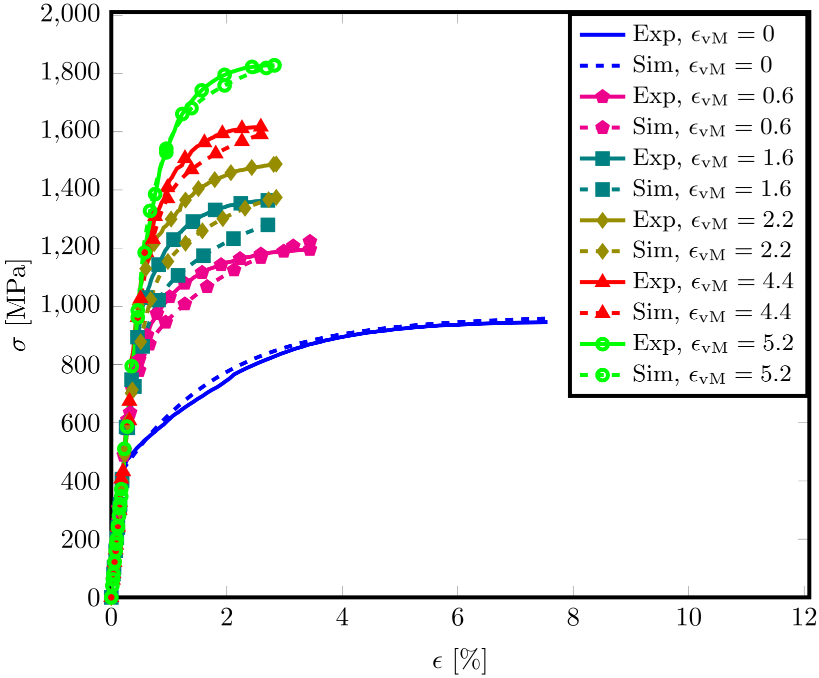


Figure 4.4: *Numerically predicted stress—strain responses from simulation of tensile tests compared to the corresponding curves obtained from experiments.*

according to Figure 4.5. The pearlitic colony response for a given deformation gradient

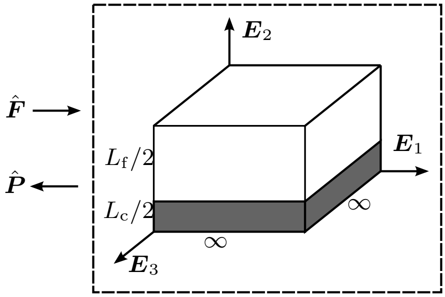


Figure 4.5: *Representative volume of pearlite with half a layer of ferrite ($L_{\mathrm{f}}/2$) and half a layer of cementite ($L_{\mathrm{c}}/2$).*

is obtained by volume averaging the 1st Piola-Kirchhoff stress over the representative volume.

Both of the models $\hat{f}_{\mathrm{i}}$ and $\hat{f}_{\mathrm{i+1}}$ are formulated for a colony with a given normal direction $\boldsymbol{n}_{\mu 0}$. When the models are included in a 3D pearlitic microstructure with a number of colonies, anisotropy due to re-orientation of the lamellae is taken into account in the homogenized stress response.

4.3.2 Micro-compression tests

Micro-compression testing is a promising technique for determining mechanical properties at small length scales. Micro-compression tests on pearlitic pillars have been conducted at Erich Schmid Institute of Materials Science. A fully pearlitic rail steel was deformed by HPT to an equivalent von Mises strain of approximately 15, leading to an ultra fine grain structure in the samples. From these samples micro pillars were milled by a focused ion beam workstation to dimensions of $3 \times 3 \times 6\,\mu\mathrm{m}^3$. The micro pillars were then axially loaded in compression by an electrical conductive diamond flat punch micro indenter mounted inside a SEM as illustrated in Figure 4.6. Considering the dimensions of a pillar, it generally consists only of one random pearlite colony with an inclined orientation if it is cut from an undeformed pearlitic steel sample. This provides the possibility to determine the properties of ferrite, cementite and one pearlitic colony through calibration of the proposed models against test data for different predefined orientations of the pearlite colony.

4.3.3 Macroscopic response of a pearlitic structure

To extend the modelling from individual pearlitic colonies to a pearlitic grain structure with randomly oriented colonies, a 3D RVE, as illustrated in Figure 4.7, is generated in the free (open source) software package Neper, cf. [57].

Deformation in simple shear of this 3D pearlitic model is simulated in the commercial FE package ABAQUS with material models $\hat{f}_{\mathrm{i}}$ and $\hat{f}_{\mathrm{i+1}}$ implemented as user material

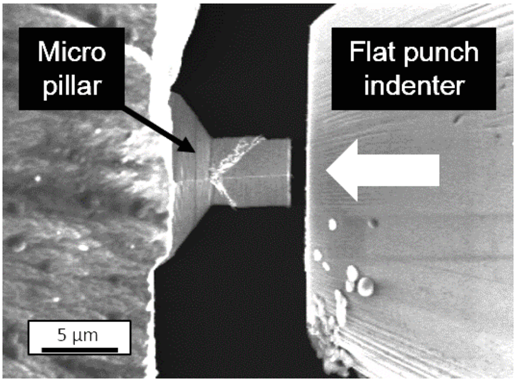


Figure 4.6: *A micro pillar and flat punch microindenter mounted inside a SEM.*

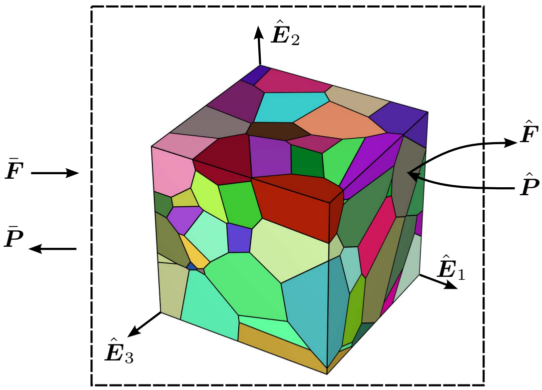


Figure 4.7: *3D pearlitic model with colonies shown in different colours.*

subroutines (UMAT). The comparison of the macroscopic response obtained from the hybrid model and models $\hat{f}_{\mathrm{i}}$ and $\hat{f}_{\mathrm{i+1}}$ (Figure 4.8) indicate that the hybrid model follows the other models qualitatively very well while having the shortest computational time.

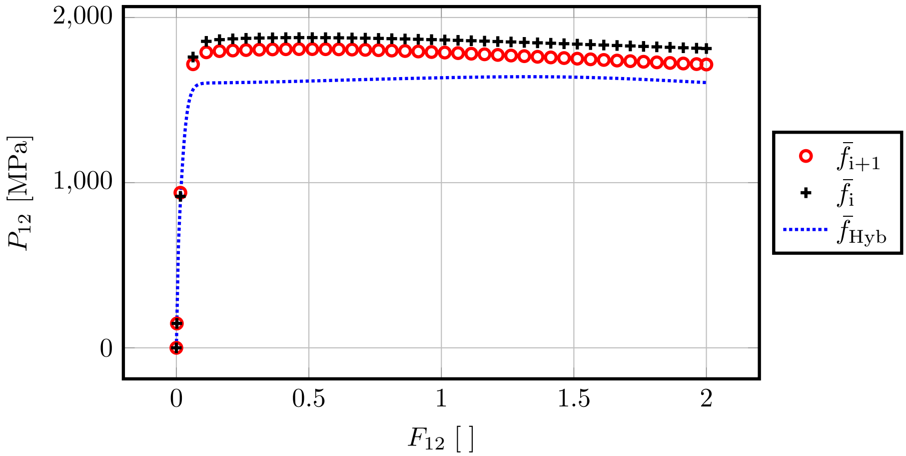


Figure 4.8: *Macroscopic stress response in terms of $\bar{P}_{12}$ for simple shear loading of the 3D pearlitic model with 625 colonies for the pearlitic colony models $\bar{f}_{\mathrm{i}}$ and $\bar{f}_{\mathrm{i+1}}$ together with the corresponding response predicted by the hybrid material model $\bar{f}_{\mathrm{Hyb}}$.*

5 Summary of appended papers

- **Paper A: Interaction between cracks and microstructure in three dimensions for rolling contact fatigue in railway rails.**
  The rail–wheel contact generates plastic deformation and cracks in the top layer of a rail. RCF cracks in rail samples from track and from a full scale test rig were examined. Due to the shear forces arising in the wheel rail contact, the microstructure close to the surface becomes aligned in the shear direction. Thereby, the pearlite becomes anisotropic, and resistance to cracks is lower in certain directions. RCF cracks follow the weakest direction of the microstructure, which in pearlitic railway rails is the aligned pearlite structure or singular weaknesses such as pro-eutectoid ferrites or slags. The deformation of the microstructure is different depending on loading situation and original microstructure (rail grade). Once the plastic deformation is present, the cracks follow the path of the weakest crack resistance. Cracks close to each other can interact or shield each other; it is unclear, however, to what extent. In this paper, a new method is described that allows the presentation of RCF cracks in 3D.

- **Paper B: The effect of anisotropy on crack propagation in pearlitic rail steel.**

One of the main sources of damage in railway components is the large plastic deformations that accumulate in the surface layer under rolling contact loading. Large irreversible deformations in components made of pearlitic steel induce anisotropy in mechanical properties of the material in the surface layer. In the present work the influence of the anisotropic layer on propagation of cracks in rail head is investigated. Based on the concept of material forces, a computational framework for simulation of propagation of planar cracks is formulated where the propagation rate is linked to a crack-driving force. An anisotropic fracture surface model is employed to capture the effect of changes in the resistance against crack propagation in different directions and depths in the surface layer. Results of simulations for cases with different characteristics in the surface layer show that the anisotropic layer has a substantial influence on the crack path.

- **Paper C: Hybrid micro-macromechanical modeling of anisotropy evolution in pearlitic steel.**
  Large shearing and/or stretching of pearlitic steel leads to a re-orientation and alignment of cementite lamellae on the microscopic level. In this paper a macroscopic model formulated for large strains is proposed for pearlitic steel that captures this re-orientation by adopting an areal-affine assumption. The re-orientation of the cementite lamellae influences the macroscopic yield function via homogenization of the normals to the cementite lamellae. Thereby, the re-orientation leads to a distortional hardening of the yield surface. Additionally, the model is formulated in a large strain setting by using the multiplicative split of the deformation gradient and includes non-linear isotropic as well as kinematic hardening. The proposed model is implemented by using a backward Euler technique for the evolution equations together with the integration on the unit sphere to compute homogenized quantities. Finally, numerical results are evaluated and compared to experimental results for wire drawing of pearlitic steel reported in literature.

- **Paper D: Simulation of high pressure torsion tests of pearlitic steel.**
  HPT is a severe plastic deformation method that can transform the characteristic lamellar micostructure of pearlitic steel to a severely deformed and aligned microstructure with respect to the deformation direction. In the current paper, HPT experiment results for the standard rail grade R260 were utilised to calibrate a material model formulated for large deformations to predict evolution of anisotropy due to microstructural changes in pearlitic steel. The HPT deformation procedure is simulated in the commercial FE package ABAQUS. Numerical results agree very well with experimental data demonstrating the high potential of the proposed material model in analyses including large deformations of pearlitic steel e.g. in railway applications and RCF analyses.

- **Paper E: A comparison of homogenization approaches for modelling the mechanical behaviour of pearlitic steel.**
  In this paper different homogenization approaches are adopted for two micromechanical based models of elasto-plasticity in pearlitic steel. Both models are based on the assumption that the yielding is primarily caused by shear of the ferrite

between the cementite lamellae. The orientation distribution of the cementite lamellae determines the macroscopic anisotropy characteristics of pearlitic steel. Properties of the cementite and the ferrite are determined from microcompression tests where the orientation of the cementite lamellae is varied. This is done for both of the micromechanical based models. The first of these models is a micromodel where cementite and ferrite are modelled individually. The second model is a mesomodel where a homogenization approach of a cementite lamella together with the surrounding ferrite is proposed. The anisotropy evolution is assumed to be governed by the re-orientation of the cementite lamellae during the deformation. The most fundamental model that is studied is a 3D grain structure where the fluctuating displacement field within the grain structure is solved by using FEM. The re-orientation of the cementite lamellae is governed by the deformation of the grain structure. In the analytically homogenized models the re-orientation is assumed to follow the areal affine assumption where the normals of the cementite lamellae are convected with the macroscopic deformation gradient. Numerical results for the different models, when subjected to simple shear loading, are given and comparisons of stress–strain response are shown.

6 Conclusions and Outlook

The aim of this thesis is to investigate the influence of material anisotropy on deterioration mechanisms of pearlitic rail steel subjected to RCF loading conditions. In **Paper A** rail samples taken from tracks and tested in a test rig were investigated for common defects in rail head. The interaction between the pearlitic microstructure and cracks grown in the surface layer were studied. A method to show the three-dimensional shape of cracks was presented and the possible interaction between the cracks was discussed. The employed method was based on time-consuming manual work by slicing and viewing a number of cross sections. As a future enhancement more efficient techniques such as X-ray tomography are proposed [3].

In **Paper B**, a fatigue crack propagation law based on the concept of material forces for linear elastic material behaviour was extended to include the effect of anisotropy. Based on microstructural investigations, an anisotropic fracture surface model was proposed to account for the directional dependence of resistance against crack propagation. This was formulated by defining the fracture threshold as a function of the degree and orientation of alignment of cementite lamellae in the microstructure. Parametric studies of crack growth simulations, in a simple 2D model of a wheel–rail contact, showed that the degree of anisotropy in the surface layer has a significant influence both on the path and the rate of propagation of cracks. The results obtained are in good agreement with field observations. Further improvements can include simulation of propagation of shorter cracks with lower initial inclinations from the surface. Such modifications will possibly improve the prediction of crack paths so that they closely resemble the cracks usually found in the surface layer and at the gauge corner of railway rails. More realistic loading conditions (such as bending and thermal loading) can also be included in the future numerical studies. An important extension is to include a more realistic material model that accounts for plasticity, hardening and anisotropy evolution. This requires that the material force can be computed consistently (mesh independent) for an inelastic material under RCF loading which seems to be a delicate challenge, see [8]. The additional extension to 3D simulations is also of interest. To this end the applied re-meshing technique must be replaced by a more computationally efficient method such as an X-FEM technique [55] or a phase field approach [60].

In **Paper C**, a hybrid micro-macromechanical model was developed to predict the evolution of anisotropy in pearlitic steel. The model is formulated in a thermodynamically consistent framework that incorporates large deformations. The proposed model was calibrated against experimental data on wire drawing from [68]. The evolution of the yield limit in these experiments is predicted by the model with a good precision. However, the hardening stage in the stress–strain curves is not predicted as accurately.

The capability of the material model to predict the yield stress and stress–strain response is critical in simulations especially when a significant degree of anisotropy is evolved during deformation. One such case is evolution of anisotropy in the surface layer of rails due to wheel–rail contact loading. This motivates calibration of the hybrid micro-macromechanical model against laboratory experiments on samples heavily deformed in shear. A good example of such experiments is HPT test. In **Paper D**, HPT deformation procedure is simulated with the aim to calibrate the material model against uniaxial tension tests of samples pre-deformed by HPT. This led to improvement of hardening formulation in the material model. Good agreement between model predictions and experimental results was achieved. This indicates that the material model has the potential to be utilized in analyses where large plastic deformations are induced due to high compressive stresses combined with large shear stresses. In order to improve the analyses, instability issues in the numerical simulations of the HPT process should be addressed. Employing remeshing techniques in these simulations as in e.g [71] could resolve this issue and is therefore suggested as a future work.

In **Paper E** experimental information obtained through micro-compression tests on pearlitic steel was utilized to calibrate two pearlitic colony models. The goal in this paper was to demonstrate how experimental information on the micro-scale may be utilized to predict macroscopic behaviour of a 3D model of pearlitic steel. To this end different mesomodels for the ferrite and cementite structure are employed together with different homogenization approaches. In addition, the influence of the choice of mesomodel and homogenization approach on the macroscopic response was investigated. The investigated homogenization approaches were the Taylor assumption and the Dirichlet (linear displacements) boundary conditions. The latter demands FE analysis since it allows for fluctuations of field variables. The analysis was done for both types of colony model and the results were compared with the response predicted by the corresponding hybrid model. The hybrid model adopts simplified homogenization assumptions and is based on integration over the surface of a unit sphere. The comparisons showed that the hybrid model gives qualitatively similar results as obtained with the other homogenization approaches. Although stress levels obtained from the hybrid model were a bit lower. However, the computational efficiency of the hybrid model excels over the other models. For this reason, the hybrid model can be regarded as a very useful material model for pearlite subjected to large strains. Analysis also revealed that simulations featuring the

Taylor assumption and the Dirichlet boundary conditions yielded very similar results. A possible reason for this is the formulations of the colony models. In particular, the model with individual ferrite and cementite models assumes a semi-infinite domain which might lower the influence of colony boundaries. This is suggested to be further investigated in the future. Another interesting topic for future investigations in the semi-infinite colony model is how changes in cementite lamellae distance and its influence on the mechanical behaviour can be accounted for by adopting gradient plasticity modelling, see e.g. [17].

Further investigations can be carried out regarding the effect of anisotropy on initiation of cracks in the rail surface. The proposed material model can be utilised in such analyses. As a starting point, a multiaxial fatigue criterion e.g. Jiang & Sehitoglu [32] can be employed to determine the critical plane in the surface layer of the rail during wheel–rail contact loading. Tuning the degree of alignment in the surface layer of the rail, the effect of anisotropy on crack initiation can be studied. However, the prediction results should be validated by controlled laboratory tests. For example, test rig experiments carried out at voestalpine Schienen GmbH [61] on rail samples could provide the data required for this type of study.

It has been shown that the degree of anisotropy and thickness of the anisotropic surface layer affect the crack growth rate and direction in this layer. An important and very expensive part of the maintenance routines for rails is the removal of RCF cracks by grinding. The procedure consists of removing a very thin ($\approx 200 - 300$µm) layer of the rail head. This usually has to be carried out during nights to avoid any disturbances in the railway traffic. Excessive grinding is also undesirable considering the changes it can cause in the rail profile and as a result in the contact conditions between wheel and rail. In this context an important question would be if there is a detrimental value for the thickness and degree of anisotropy in the surface layer of rails and wheels. An answer to this question could determine the periodicity of necessary grindings and the thickness of the layer that should be removed. This could be explored in a future work by arranging a series of simulations combined with a series of test rig experiments. A rail piece could be tested in a test rig under a known contact loading condition in sequences. The propagation of cracks after each sequence of loading can be followed by a non-destructive method like eddy current or X-ray tomography. The rail and the contact loading could be modelled and the propagation of cracks could be simulated employing a material model that accounts for development of anisotropy. Comparison of the simulation results with the experiments gives the possibility to calibrate and/or validate the models. Finally, this could provide the basis of a tool which can estimate the thickness of the anisotropic surface layer and the depth of surface cracks after a certain amount of traffic in the tracks.

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Part II
Appended Papers A–E

Paper A

Interaction between cracks and microstructure in three dimensions for rolling contact fatigue in railway rails

Paper B

The effect of anisotropy on crack propagation in pearlitic rail steel

Paper C

Hybrid microemacromechanical modeling of anisotropy evolution in pearlitic steel

Paper D

Simulation of high pressure torsion tests of pearlitic steel

Paper E

A comparison of homogenization approaches for modelling the mechanical behaviour of pearlitic steel