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Multiscale modeling of failure initiation in a ferritic–pearlitic steel

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ABSTRACT

A representative volume element (RVE)-based strategy for modeling the hardening and failure behavior of a ferritic–pearlitic steel at different length scales – mesoscale and microscale – is presented. At first, pearlite properties were considered to be isotropic and homogeneous. Micrographs taken on the undeformed material were transformed to a finite element mesh by using the software OOF2, a public domain FE-analysis software created at the National Institute of Standards and Technology (NIST) for the investigation of microstructures. Boundary conditions of the RVE were defined based on the macroscopic deformation history of a region of interest of an axisymmetric impact extrusion part. Crack initiation in pearlite is modeled within the extended finite element method (XFEM) framework. Pearlite cracking modeled at the mesoscale corresponds well to the observed cracks on SEM-micrographs. In a further approach, the crystallographic orientation of ferrite as well as various distributions of cementite lamellae were considered to take the inhomogeneous structure of the pearlite into account. For this purpose, in the framework of RVE computation, a spectral solver of the code DAMASK (Düsseldorf Advanced Material Simulation Kit, an open source crystal plasticity general purpose solver) was applied to model strain localizations at grain level. X-ray measurements were carried out to determine the orientation of ferrite grains and to determine the parameters of the applied crystal plasticity material model (critical resolved shear stress and slip hardening parameters). Investigations showed that the orientations of cementite lamellae have a significant influence on strain localization. The concept of coupling the FE-method to simulate the macroscopic behavior of the material and the spectral solver to achieve a high resolution of the microstructure in the framework of RVE computations leads to an efficient strategy regarding computational time and modeling of the microstructure.

1. Introduction

Modeling of the material behavior at different length scales is one of the most important research topic in engineering and material sciences. This is because the requirements to develop products which are e.g. lighter, safer or of high strength and ductility are increasing continuously. These requirements influence the complexity of the materials directly and therefore their numerical modeling as well, [58]. Thus, in addition to the extensive developments in material modeling, sophisticated numerical methods to solve large problems are needed. Nowadays, one of the most prominent solvers in solid mechanics – regarding general domains and loading conditions – is the finite element method (FEM). However, on the other hand, if the computation is focused on representative volume elements (RVE), much more efficient solvers could be applied, e.g. spectral solver, [42,13,38].

1.1. RVE and micro mechanical modeling

Recent investigations in the field of RVE and micro mechanical modeling especially cover topics of: local strain hardening, local shear localization and softening phenomena, local micro mechanical cluster effects, modeling of hardening behavior based on chemical composition etc. Various empirical and physically based models have been developed and applied to a large range of materials, see e.g. [56,28,24,39,53,21,37,48]. A very informative overview of the modeling of dual phase steels with an emphasis on micro mechanical and RVE modeling is given by Tasan et al. [51].

Tasan et al. [53] investigated strain localization and damage in dual phase steels by performing in-situ experiments and crystal plasticity simulations. The strain distribution was measured by microscopic-digital image correlation techniques (μDIC). The presented results showed, that the characteristics of the dual phase microstructure (fractions of ferrite and martensite, grain size etc.) strongly affect the strain localization process. It was emphasized that larger ferrite grains deform plastically earlier than smaller ones. The process led to pronounced deformation bands. Damage

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incidents were observed in the boundary of these zones. It was concluded that optimal mechanical behavior can be achieved by grain refinement and martensite dispersion.

Jia et al. [21] investigated local shear banding in face centered cubic crystals by means of crystal plasticity finite element simulations. It was shown that the initiation of shear banding depends on the initial orientation of the crystals and their mechanical properties. Simulations on copper-oriented single crystals, considering different boundary conditions and sample geometries, showed different shear banding behaviors for the same boundary conditions but different sample geometries.

Raabe et al. [37] presented results regarding local effects associated with local hard to soft mechanical transitions. It was concluded that the strain path follows soft crystals and avoids hard crystals. Further, it was highlighted that strain localization takes place at triple points and at most grain boundaries. Additional investigations were published by Sachtleber et al. [46].

The direct combinations of full field models and corresponding local image correlation methods were presented by Zhao et al. [62]. For this purpose, during the deformation of an oligocrystal aluminum sample, the histories of strain localization, surface roughening and in-grain fragmentation were recorded. Experimental investigations and crystal plasticity finite element simulations showed that surface roughening profiles are related to the localization of strains at macro level as well as to the intra-grain interaction. In addition, it was reported that the grain topology and microtexture significantly influenced the origin of the strain heterogeneity.

Sachtleber et al. [46] proposed an experimental approach for the investigation of the strain heterogeneity during plastic deformation of a coarse-grained recrystallized polycrystalline aluminum. During a plane strain compression test, the microstructure of the material was determined by EBSD analysis, whereas the distribution of plastic surface strains was determined by means of photogrammetry. Amongst others, it was shown, experimentally, as well as by means of crystal plasticity finite element simulations, that remarkable strain gradients within grains can occur. Further, the influence of initial crystal orientations on the resulting strain pattering was highlighted.

Woo et al. [61] e.g. considered a dual-phase steel to determine the relationship between the crystallographic orientation of ferrite and martensite on the localization of strain. For the sake of simplicity, circular martensite particles with one orientation were modeled in the framework of the RVE computation, whereas for the ferrite phase two orientations were considered. The hardening behavior of each phase was modeled based on empirical yield curves to define the necessary information for the CP-FEM. It was reported that the crystallographic orientation of ferrite significantly influences the localization of shear strain.

Full field micro mechanical simulations of dual phase steels considering the complete texture were presented by Tasan et al. [52]. A strong strain partitioning among the ferrite regions was observed. Moreover, it was shown by both, experiments as well as simulations (performed with DAMASK), that plastic strain is especially high at submicron bands oriented 45–50° with respect to the loading direction. It was also highlighted that in many cases localization bands develop at the center of ferrite grains. Kadkhodapour et al. [22] investigated local hardening effects of ferrite in dual phase steels. It was observed that the hardness of the ferrite matrix increases in the region of the martensite interface. The mechanism of local hardening due to geometrically necessary dislocations was analyzed.

1.2. Modeling of pearlite

Ferritic–pearlitic steels, investigated also in the framework of this study, show a complex microstructure. One of the biggest challenges in modeling such microstructures are the pearlite regions containing cementite lamellae. A direct discretization of the cementite lamellae within FEM modeling is not appropriate, because of the high resolution required. This would lead to a very high number of elements and therefore to an increase of computational time and memory as well. Different approaches are presented in literature to take the pearlitic structure into account, mainly based on homogenization techniques, see e.g. [2,29,59]. A direct modeling approach of the cementite lamellae was presented by Berisha et al. [7] based on the spectral solver provided by DAMASK, [43]. Further details of the investigation are discussed in the current paper.

The hardening behavior of fully lamellar pearlitic steels was investigated e.g. by Hu et al. [19], using phenomenological and Taylor-type micromechanical models. Ferrite as well as cementite were modeled separately. Further, a global random distribution of the cementite lamellae is considered and the interlamellar spacing inside one cementite colony is assumed to be constant. In addition, reorientation of cementite lamellae was modeled based on March theory as explained in [60]. It was shown that the Taylor-type model delivers better results than the phenomenological one.

Experimental investigations regarding the influence of the cementite morphology on hardening behavior of a fully pearlitic steel were presented by Tomota et al. [55]. It was reported that specimens containing spheroidized cementite lead to low strength and high ductility of the material, and that a smaller interlamellar spacing might lead to an extension of the post necking region.

2. Mesoscopic modeling of hardening and failure

Modeling of hardening behavior of ferrite and pearlite based on grain size and interlamellar spacing of cementite lamellae is described in Section 2.1, whereas modeling of failure in the framework of XFEM is given in Section 2.2. The main steps of the presented strategy in the framework of RVE-modeling of hardening and failure behavior are given in Appendix A.

2.1. Modeling of hardening behavior of ferrite and pearlite

The hardening behavior of a material is determined, in general, based on uniaxial tensile tests or uniaxial compression tests. The investigated material shows a uniform elongation of ≈0.12. In order to achieve higher strains, compression tests at room temperature were also performed. Cylindrical specimens with a diameter of 5 mm and a height of 10 mm were manufactured by electrical discharge machining (EDM). The yield curve of the performed compression tests is shown in Fig. 3. The measured yield curve describes the averaged hardening behavior of the material, which consists of ferrite and pearlite. The chemical composition is given in Table 1.

However, in order to model the ferrite phase and pearlite structure separately, various procedures are presented in the literature. In this study, the approximation presented by Rodriguez and Gutierrez and Gutierrez [41,16] is used to describe the hardening behavior of ferrite:

$$\sigma_{eq}^{ferrite} = \sigma_0 + \alpha M \mu \sqrt{b} \sqrt{\frac{1 - \exp\left(-Mk\varepsilon_{eq}\right)}{kL}} \tag{1}$$

where, $\sigma_{eq}^{ferrite}$ is the flow stress, α a constant close to 0.33, M the Taylor factor $(=3)$, μ the shear modulus $(=80,000\,\text{MPa})$ and $b = 2.5 \cdot 10^{-10}$ m the magnitude of the Burgers vector. Various modeling approaches regarding the dislocation mean free path L are discussed in the literature. Devincre et al. [12] presented detailed investigations on dislocation mean free path based on three