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Analysis of banded microstructures in multiphase steels assisted by transformation-induced plasticity

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The influence of the spatial distribution of the austenitic phase on the effective mechanical properties of a multiphase steel assisted by transformation-induced plasticity is analyzed using a numerical homogenization scheme. Representative three-dimensional volume elements with distinct microstructures are created applying a newly-developed algorithm based on the generation of a multilevel Voronoi tessellation; this approach allows for straightforwardly incorporating grains with complex, non-convex shapes in the microstructure. The effective macroscopic response of the samples is computed under the formulation of a set of non-redundant, periodic boundary conditions, which warrants a consistent transition between the microscopic and macroscopic scales. A sample in which austenitic grains are clustered within a ferritic matrix by means of a band-like region is compared to a sample with austenitic grains being randomly dispersed within the ferritic matrix. It is found that the banded microstructure may be detrimental in comparison to the dispersed microstructure, since it allows substantial plastic localization to occur in the ferritic matrix, which in turn diminishes the strengthening effect provided by the austenitic phase.

1. Introduction

A thorough understanding of the link between the microstructural characteristics of a heterogeneous multiphase material and its macroscale response is critical for the enhancement of its mechanical properties. A specific class of technologically-important multiphase materials are those assisted by the transformation-induced plasticity mechanism. This class of steels, commonly referred to as TRIP steels, are characterized by a microstructure containing ferrite as the most dominant phase, complemented by retained austenite, bainite, and occasionally a small amount of thermal martensite, see e.g., [1–7]. The key constituent for steels assisted by transformation-induced plasticity is the retained austenite, which is metastable at room temperature, but may transform into martensite under the application of mechanical and/or thermal loading. The transformation process increases the effective strength of the steel, since the martensitic product phase is significantly harder than the austenitic parent phase and the ferrite-based matrix. It further increases the ductility of the steel, due to plastic deformations induced in the ferritic and bainitic phases by a volumetric expansion of the transforming austenitic phase. These two microstructural mechanisms essentially characterize the TRIP-effect, and therefore have been taken into account in various macroscopic and microscopic continuum models developed during the last four decades [8–23].

The microstructure of a multiphase steel can be modified by changing its processing route [24,25]. For TRIP steels this may significantly improve the effective material properties, since specific microstructural characteristics, such as the initial volume fraction of austenite, the carbon concentration in the retained austenite, and the crystallographic texture, appear to substantially influence the stability of the retained austenite, and, consequently, the overall mechanical response [26]. The grain size also affects the macroscopic properties, as analyzed in detail by means of both continuum models and discrete models [27,28].

Although the macroscopic properties of a multiphase steel clearly show a dependency on the initial volume fraction of austenite, it is not yet well understood how the *spatial distribution* of the austenite grains contributes to this aspect. For this purpose, two distinct, technologically-relevant microstructural morphologies are analyzed and compared in the present communication, namely (i) a benchmark microstructure with isolated, randomly-distributed austenitic grains embedded in a ferritic matrix and (ii) a microstructure where austenitic grains are clustered in a plate-like region (or band) within a ferritic matrix. The benchmark distribution is typically encountered in cold-rolled TRIP steels that are

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subsequently subjected to a two-step annealing (intercritical annealing followed by isothermal heat treatment), where retained austenite appears in grains wedged between ferritic grains. Conversely, austenitic grains clustered in a band-like region may appear during hot-rolling (i.e., high-temperature mechanical deformation during processing), whenever the banded morphology is not completely removed during further heat treatment, see [29]. The relevance of banded morphologies on the mechanical response of ferrous alloys has been discussed in [30–32]. Their effect on the effective strength was analyzed in [33] by means of a discrete dislocation-transformation model, where it was found that a microstructure composed of randomly-distributed grains of austenite is advantageous, as it delays the onset of plastic localization in comparison to banded microstructures. The present study is based upon a continuum approach which, compared with the above-mentioned discrete model, allows to extend the analysis to a three-dimensional setting as well as to a larger range of deformations, i.e., beyond the onset of plastic deformation. Accordingly, a more comprehensive insight is obtained into the strengthening effect caused by the austenitic phase and the role played by its spatial distribution.

In order to establish a direct link between the spatial distribution of austenite and the macroscopic properties of a multiphase steel, simulations are conducted on banded and dispersed microstructures while keeping all other relevant microstructural features the same (i.e., initial volume fraction of austenite, average crystallographic orientation, carbon content, etc.). The constitutive models used for ferrite and austenite are summarized in Section 2. A multilevel Voronoi algorithm for generating microstructural computational samples of an aggregate of grains is presented in Section 3. The samples are subjected to non-redundant, periodic boundary conditions, which warrants a consistent transition between the microscopic and macroscopic scales. The samples are used in a convergence analysis to establish the required size of a representative volume element for the determination of the macroscopic properties. The effect of a banded microstructure is analyzed in Section 4 based on a comparison with benchmark simulations for dispersed microstructures. Conclusive remarks are provided in Section 5.

2. Micromechanical modeling of multiphase TRIP steels

The microstructures considered in the present analysis consist of an aggregate of ferritic grains (primary phase) and metastable retained austenitic grains (secondary phase). Upon loading, the austenitic grains may partially or totally transform into martensite. The goal is to determine the collective response of the aggregate of grains, where separate constitutive models are used for each phase. The main characteristics of the models are summarized in this section and the interested reader is referred to relevant publications for further details.

2.1. Elasto-plastic-transformation model for austenitic grains

The elastoplastic response of the austenitic phase and its possible transformation into martensite is simulated using the model originally developed by Turteltaub and Suiker [15–17] and subsequently extended by Tjahjanto et al. [34] and Yadegari et al. [35]. The model assumes that, upon loading, a region inside each grain (i.e. at the sub-grain length scale) may undergo a plastic deformation through slip and/or a sudden change in crystalline structure (i.e., a martensitic phase transformation). The transformation of austenite, which possesses a face-centered cubic (FCC) structure, into twinned martensite, composed of pairs of body-centered tetragonal (BCT) martensitic variants, is described according to the theory of martensitic transformations [36]. The distinct pairs of (twinned) martensite, referred to as "transformation systems", are characterized by two vectors, namely the habit plane normal and the shape strain vector. The transformation model is coupled to a crystal plasticity model to simulate sub-grain interactions in the austenite caused by transformation and plastic deformation [34]. Plastic deformation at the sub-grain level is described by slip occurring along active slip systems. Following the approach used in crystal plasticity, individual slip systems are characterized by a pair of vectors that represent the slip plane normal and the slip direction.

The sub-grain length scale behavior of a collection of slip systems and transformation systems is translated to the mesoscale (grain-level) by considering the weighted average of the active systems accounting for the corresponding inelastic mechanisms. This averaging procedure is performed within sub-regions in the grains, which allows for simulating non-homogeneous plastic deformations and/or transformations inside individual grains. The response contribution caused by the martensitic transformation is obtained upon time-integration of the rate of change of the volume fractions of the individual transformation systems. This set of rates is denoted as $\dot{\boldsymbol{\xi}} = \left(\dot{\xi}^{(1)}, \ldots, \dot{\xi}^{(N)}\right)$, where $\dot{\xi}^{(\alpha)}$ represents the rate of change of the volume fraction of the αth martensitic system within a sub-region inside a grain and N is the total number of available transformation systems. The contribution of plasticity to the deformation is determined from the rate of slip in each system, i.e., from $\dot{\boldsymbol{\gamma}} = \left(\dot{\gamma}^{(1)}, \ldots, \dot{\gamma}^{(M)}\right)$, where $\dot{\gamma}^{(i)}$ denotes the rate of slip in the ith system and M is the total number of slip systems in the underlying material. Although the martensite is assumed to deform only elastically, the model takes into account the amount of plastic slip that occurred in the austenite prior to transformation.

The rates of change of transformation and plastic slip upon loading are modeled using a formulation that is thermodynamically-consistent with respect to the dissipation inequality. The isothermal model used in the present simulations is derived from a thermomechanical formulation using a constant homogeneous temperature such that the thermal deformation gradient is equal to identity [35]. Combining the formalism proposed by Onsager [37] with the so-called Coleman–Noll procedure [38], the terms in the dissipation inequality are expressed as a sum of products of affinities (i.e., driving forces) and fluxes (i.e., rates of change of martensitic volume fractions and plastic slip) for each inelastic mechanism. The model includes evolution equations between fluxes and affinities, known as the "kinetic relations". In particular, the transformation of the austenitic phase into martensite is described by a tangent hyperbolic function that relates the rate of transformation of each individual transformation system to the driving force of the transformation system. Similarly, the plastic deformation in the austenite is governed by a power law that relates the plastic slip rate of each individual slip system to the corresponding plastic driving force. The evolution of plastic slip resistance is accounted for by a hardening power law. The kinetic relations are complemented by nucleation criteria describing the onset of inelastic deformation. Detailed expressions for the driving forces and the kinetic relations can be found in [15,17,34,35].

At the mesoscale (grain-level), the kinematical description of the austenitic phase is based on a large deformation framework where the deformation gradient at a given material point is multiplicatively decomposed as

$$\mathbf{F} = \mathbf{F}_{\mathrm{e}}\mathbf{F}_{\mathrm{p}}\mathbf{F}_{\mathrm{tr}}, \tag{1}$$

with $\mathbf{F}_{\mathrm{tr}}$ is the transformation deformation gradient, $\mathbf{F}_{\mathrm{p}}$ the plastic deformation gradient and $\mathbf{F}_{\mathrm{e}}$ is the elastic deformation gradient. The mesoscale Cauchy stress tensor $\mathbf{T}$ is determined from the elas-