Micromechanical modeling and simulations of transformation-induced plasticity in multiphase carbon steels

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The presence of a metastable austenitic phase in the microstructure of low-alloyed, multiphase carbon steels has been identified to be responsible for their good combination of strength-ductility characteristics. Metastable austenitic grains may transform to martensite upon the application of thermal and/or mechanical loadings. In addition to the improvement of the effective strength due to a harder martensitic phase, transformation of retained austenite to martensite is accompanied by relatively large shape and volume changes, which induces elasto-plastic deformations in the neighboring region, and generate the so-called transformation-induced plasticity (TRIP) effect. A thorough understanding of the mechanism of the TRIP effect is, therefore, important for further improvement of the strength and ductility performance of multiphase steels. In the present thesis, the mechanism of the TRIP effect is systematically studied by means of micromechanical modeling and simulations. For this purpose, the following two single-crystalline models have been developed:

First, a crystal plasticity theory for body-centered cubic (BCC) metals is formulated and implemented for describing the elasto-plastic deformation in the ferritic phase, which is presented in Chapter 2. The model is constructed within a finite deformation framework. The non-glide stress effect model proposed by Bassani et al. (2001, Mat. Sci. Eng. A 319–321: 97–101) is adopted, in order to capture the characteristic features of BCC metals, i.e., the asymmetric behavior of slip in twinning and anti-twinning senses, which, at macroscopic scales, corresponds to a tension-compression asymmetry under uniaxial loading. Single-crystalline simulations are performed for various elementary deformation modes (e.g., uniaxial loading, simple shear and plane-stress equibiaxial stretch). The results of the simulations show various effects of the non-glide stress on the overall response of the single-crystalline BCC ferrite. Under uniaxial loading, the model predicts asymmetric behavior in tension and compression, where the magnitude of this effect depends on the crystallographic orientation of the sample. In a (Taylor-type) polycrystalline simulation, the yield stress in uniaxial compression is lower than in uniaxial tension. The opposite trend is observed for samples undergoing plane-stress equibiaxial stretch, i.e., the polycrystalline yield stress in equibiaxial compression is higher than in equibiaxial tension. In general, the non-glide stress effect is less pronounced in simple shear simulations.

Second, in Chapter 3, a single-crystalline elasto-plastic-transformation model is developed for the austenitic phase. This model is based on the multiscale martensitic phase transformation model of Turteltaub and Suiker (2006, Int. J. Solids Struct. 43: 4509-4545). In this model, the lower-scale information on martensite microstructures following from the crystallographic theory of martensitic transformation is incorporated. In order to account for plastic deformations in the austenitic phase, the phase transformation model is coupled to a single crystal plasticity model for face-centered cubic (FCC) metals. The coupling between transformation and plasticity is derived using a thermo-mechanically-consistent formulation. Similar to the model for the BCC
ferrite, the kinematics of elastoplastic transformation model are formulated within a finite deformation framework. Furthermore, the overall response of single-crystalline austenite is simulated for three elementary loading modes, i.e., uniaxial loading, simple shear and volumetric extension/compression. The results of the simulations show that the interaction between the transformation and plasticity mechanisms is strongly dependent of the loading conditions, as well as the crystallographic orientation of the sample. Under uniaxial tension and compression, plasticity in the austenitic phase tends to delay (or postpone) the transformation process, where the magnitude of the delay varies with the crystallographic orientation of the sample. Furthermore, transformation is a less preferable mechanism for samples undergoing simple shear. The results of the simulations show that only a small amount of austenite transforms to martensite during simple shear deformation. In contrast, transformation dominates the overall deformation process during volumetric expansion. In addition, neither transformation nor plasticity occurs in the sample during volumetric contraction.

The numerical implementation of the above single-crystalline models is discussed in Chapter 4. This implementation is based on a robust algorithm for the elasto-transformation model presented in Suiker and Turteltaub (2005, Int. J. Numer. Meth. Eng. 65: 1655-1693). The numerical implementation is presented only for the austenitic elasto-plastic-transformation model, since the implementation of the ferritic elasto-plasticity model can be done in a similar fashion by omitting the transformation-related parts. The model is discretized using a fully-implicit Euler backward scheme, and a Newton-Raphson iteration procedure is applied to solve the resulting non-linear equations. The procedure is equipped with a robust search algorithm for identifying the active sets of slip and transformation systems. In addition, a sub-stepping procedure is applied in order to improve the convergence behavior of the numerical algorithm. The consistent tangent operator is computed in a numerical fashion by means of a first-order accurate, finite difference scheme. The numerical algorithm has been implemented in a finite element program. The results of the simulations show that the finite element solution converges upon mesh refinement, where the convergence behavior of the austenite elasto-plastic-transformation model is somewhat slower than that of the ferrite elasto-plasticity model.

In Chapter 5, the response of TRIP steel microstructural samples undergoing uniaxial tensile loading is studied by means of numerical simulations using the micromechanical models described above. The simulations are performed for several samples representing TRIP steels with different microstructural proper-ties, i.e., the initial volume fraction of austenite (phase morphology), the austenite carbon concentration, the austenitic grain size, the austenitic and ferritic crystallographic orientations (microstructural texture) and the strength properties of the ferritic matrix. The overall response (in terms of the effective stress-strain curve and the transformation evolution) of the TRIP steel samples is presented as a function of the individual microstructural properties. The results of the microstructural simulations show that the transformation behavior depends not only on the orientation of the austenitic grains, but also on the crystallographic orientation of the surrounding ferritic matrix. Furthermore, a higher carbon concentration in the austenite results in a higher initial strength, but a lower austenite carbon concentration leads to a faster transformation and, eventually, to a higher effective hardening. The initial austenitic volume fraction only affects the overall stress-strain response at larger deformations, since a higher initial austenitic volume fraction will translate into a martensite-richer microstructure that has a higher effective hardening. Moreover, the austenitic grain size and the strength of the surrounding matrix affect the effective transformation behavior only marginally.

Simulations of macroscopic TRIP steel samples undergoing deep-drawing are presented in Chapter 6. For this purpose, an efficient averaging scheme based on a weighted-Taylor assumption has been developed. This averaging scheme is implemented together with the single-crystalline models into a finite element pro-gram. Information on the crystallographic texture of the sample is incorporated in the finite element simulations in accordance with a statistical reconstruction of the sample orientation distribution function (ODF). The results of the simulations indicate that transformation occurs mostly at the bottom edge of the cup, which
experiences the largest tensile deformation. Although the overall features of the transformation during deep-drawing are well captured, the rate of transformation in the homogenized model falls short to that predicted by the direct FEM simulation. Furthermore, the individual contributions of the austenite and ferrite to the anisotropy of the material can be distinguished from the earing profile.

In Chapter 7, the transformation behavior during thermal loading (or cooling) is investigated for samples with different microstructural properties. Accordingly, the single-crystalline models described above are modified in order to explicitly account for the effect of thermal expansion/contraction. The prediction of the models shows a qualitatively good agreement with recent experimentally-observed transformation behavior of single austenitic grains in TRIP steel microstructures in the sense that the dependencies on carbon concentration and grain size are well predicted, but their values are rather different.

In a nutshell, this thesis represents a comprehensive analysis of the microstructural behavior of multiphase TRIP steels. The analyses are performed by means of micromechanical modeling and simulations. The results provide valuable insight for the further development of TRIP-assisted steels.