XXI ICTAM, 15–21 August 2004, Warsaw, Poland

MULTISCALE MODELING OF STEELS ASSISTED BY TRANSFORMATION-INDUCED PLASTICITY.

S. Turteltaub and A.S.J. Suiker
Faculty of Aerospace Engineering, Delft University of Technology, Kluyverweg 1, 2629 HS Delft, The Netherlands

Summary We develop a multiscale thermomechanical model for retained austenite in carbon steels where the effects of fine-scale substructures, within an austenitic grain, is accounted for via a homogenization procedure and the mesoscale interaction with neighboring phases is modelled numerically via a three-dimensional analysis of a representative mesostructure.

INTRODUCTION

The favorable combination of strength and ductility in carbon steels whose mechanical response is enhanced by a transformation induced plastic behavior (known as TRIP steels) has been attributed to the presence of islands of retained austenite in the initial microstructure. Austenite is a solid phase that usually is unstable at room temperature and zero stress. Nonetheless, with the addition of certain elements (e.g., Si, Al) and under a controlled thermal processing route, it is possible to have regions where austenite is metastable at room temperature. Several models have been proposed to study the contribution of retained austenite; however, there are still many open issues regarding the role of retained austenite on the overall material response of TRIP steels (see, e.g., [2]). In view of this, we develop a multiscale model and focus attention on representative inclusions of retained austenite. We study in detail their contribution to the macroscopic material response under mechanical loads. Additionally, we take into account the effect of other phases in the microstructure and analyze their contribution as well.

MULTISCALE MODEL

The mesoscopic response of TRIP steels depends upon the interaction of several phases present in the mesoscale structure, i.e., ferrite, bainite and retained austenite. The evolution of retained austenite depends on smaller scale phenomena, particularly its transformation into different types of twinned martensite (referred to as “transformation systems”, numbered $\alpha = 1, \dots, 24$). These systems have their own internal structure, formed by body-centered tetragonal variants of martensite. The different scales and structures of interest are shown in Figure 1. We divide the scales of observation into a lattice, lower microscale, upper microscale and finally a mesoscale. To study the behavior of retained austenite in a ferrite-based

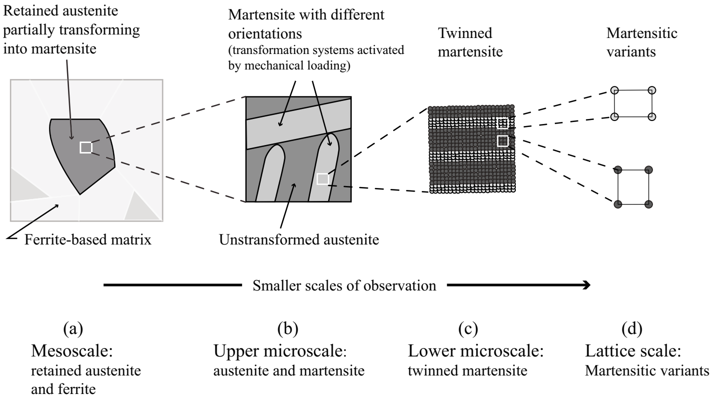
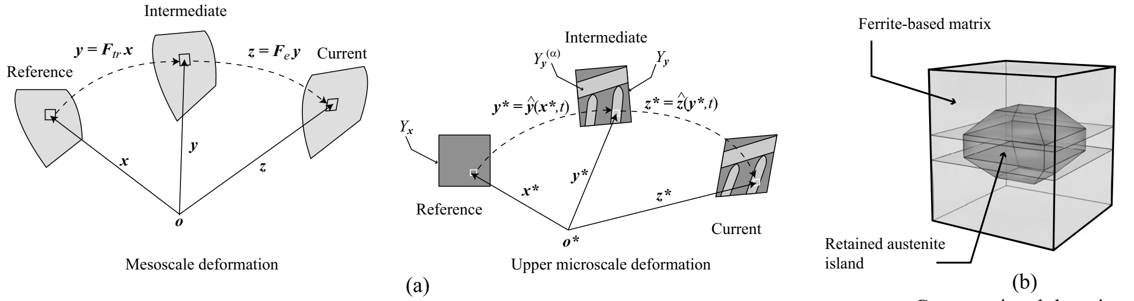


Figure 1. Scales of observation.

matrix at the mesoscale, we first develop a multiscale model that takes into account the thermomechanical response at the various scales of observation as sketched in Figure 1. Subsequently, we perform a numerical simulation of a representative austenite inclusion in a ferrite-based matrix. The model is developed within a three-dimensional, geometrically nonlinear framework. The different configurations and scales are shown in Figure 2a.

MESOSCALE THERMOMECHANICS

The variables used to describe the thermomechanical response of retained austenite at a mesoscopic level are the deformation gradient $\boldsymbol{F}$, the entropy η and a set of internal variables $\xi^{(\alpha)}$ that correspond to the volume fractions of the transformation systems. We use information from the nonlinear theory of martensitic transformations at the lattice and the microscales [1] and irreversible thermodynamics, together with a homogenization procedure to determine the mesoscopic form of the transformation deformation gradient $\boldsymbol{F}_{tr}$ and the transformation entropy η_{tr}. The influence of local



(a) Configurations for the meso- and upper microscales

(b) Computational domain

Figure 2. (a) Reference, intermediate and current configurations at the upper microscale and mesoscale levels. (b) Typical island of retained austenite in a ferrite-based matrix for FEM analysis.

carbon concentration in the retained austenite is also included in the transformation deformation gradient. The plasticity induced in the soft ferrite-based matrix surrounding the retained austenite is incorporated in our model via an elastoplastic formulation for large deformations. Since most of the plastic deformation occurs in the matrix, the austenite is assumed not to deform plastically. Consequently, the deformation gradient and the entropy in the austenite are decomposed as

$$\boldsymbol{F} = \boldsymbol{F}_e \boldsymbol{F}_{tr} \ , \qquad \eta = \eta_e + \eta_{tr} \ , \tag{1}$$

where $\boldsymbol{F}_e$ represents the elastic deformation gradient and η_e is the conservative part of the entropy. Through a multiscale analysis we estimate the effective thermomechanical response at a mesoscopic level. We provide constitutive expressions for the second Piola-Kirchhoff stress $\boldsymbol{S}$ in the intermediate configuration and for the temperature θ in terms of the elastic Green-Lagrange strain $\boldsymbol{E}_e = \frac{1}{2}(\boldsymbol{F}_e^T \boldsymbol{F}_e - \boldsymbol{I})$ and the entropy η_e, respectively, as well as the internal variables. The effective stiffness can be expressed in terms of the stiffness $\mathbb{C}^A$ of the austenite, the stiffness $\mathbb{C}^{(\alpha)}$ of each transformation system and the internal variables that measure the evolution of the transformation. We develop a similar formula for the effective specific heat in terms of the specific heats h^A and h^M of austenite and martensite respectively. The surface energy is included by means of an expression that depends on the martensitic volume fractions. All this information is used to construct a Helmholtz potential that characterizes the material behavior. The evolution of the distinct phases is described by a kinetic law. A key ingredient in the model is the expression for the transformation driving force. With the decomposition for the entropy given by (1), one can obtain thermal analogues for the mechanical terms of the transformation driving force for each transformation system α (twinned martensite). The driving force for each α has been derived as [3]

$$\begin{aligned} f^{(\alpha)} = \det(\boldsymbol{F}_{tr}) \boldsymbol{F}_e^T \boldsymbol{F}_e \boldsymbol{S} \boldsymbol{F}_{tr}^{-T} \cdot \boldsymbol{\gamma}^{(\alpha)} + \tfrac{1}{2} \left(\mathbb{C}^A - (1 + \operatorname{tr} \boldsymbol{\gamma}^{(\alpha)}) \mathbb{C}^{(\alpha)} \right) \boldsymbol{E}_e \cdot \boldsymbol{E}_e \\ - \frac{\chi}{l_0} \left(1 - 2\xi^{(\alpha)} \right) + \rho_0 \theta \frac{\lambda_T^{(\alpha)}}{\theta_T} + \rho_0 (h^M - h^A) \left(\theta \ln \frac{\theta}{\theta_T} - (\theta - \theta_T) \right) \ , \qquad \alpha = 1, \ldots, 24, \end{aligned} \tag{2}$$

where $\boldsymbol{\gamma}^{(\alpha)}$ is the shape strain of system α, χ is the surface energy of an austenite-twinned martensite interface, l_0 is a characteristic length of platelets of twinned martensite, ρ_0 is the mass density in the reference configuration, $\lambda_T^{(\alpha)}$ is the latent heat for system α and θ_T is the transformation temperature. Additional details of the model can be found in [3].

SIMULATIONS

We perform three-dimensional numerical simulations of a domain, shown in Figure 2b, formed by a ferrite-based matrix and an island of retained austenite. Details of the numerical implementation can be found in [4]. We explore the transformation of retained austenite into martensite as a function of lattice orientation and we quantify the plastic deformation induced by this transformation. The detailed analysis of the TRIP effect at the mesoscale will be used to determine optimal microstructures for the next generation of high-strength, high-ductility steels.

References

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