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COMPUTATIONAL MULTISCALE MODELING OF STEELS ASSISTED BY TRANSFORMATION-INDUCED PLASTICITY

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Summary. *The contribution of the martensitic transformation to the overall stress-strain response of a multiphase steel assisted by a transformation-induced plasticity effect is analyzed in detail. A recently-developed multiscale transformation model is combined with a plasticity model to simulate the response of a three-dimensional grain of retained austenite embedded in a ferrite-based matrix. Results show that the effective hardening behavior of the material depends strongly on the grain orientation and, to a lesser extent, on the grain size.*

1 INTRODUCTION

Among the class of new high-strength high-ductility steels being developed, special attention has been devoted to TRIP steels, whose mechanical behavior is enhanced by a transformation-induced plasticity effect. The improved performance of this class of steels has been attributed to the effect of islands of retained austenite in the initial microstructure. The thermomechanical response of retained austenite depends on sub-grain scale phenomena, particularly its transformation into systems of twinned martensite with different orientations with respect to the original austenite lattice. The sub-grain structures and the corresponding length scales are schematized in Fig. 1.

The effect of the sub-grain structures is accounted for using a recently developed multiscale model for martensitic transformations[1,2,3]. The microstructural information for the phase transformation model is based on the crystallographic theory of martensitic transformations and further includes the anisotropic stiffness of each system of twinned martensite. In addition, the model contains a surface energy term associated to regions close to the habit planes, as shown at the microscale in Fig. 1. The surface energy is indirectly related to the grain size via a length scale parameter. Using these features of the model, it is possible to study the effect of (i) grain orientation and (ii) grain size on the overall response of a TRIP steel.

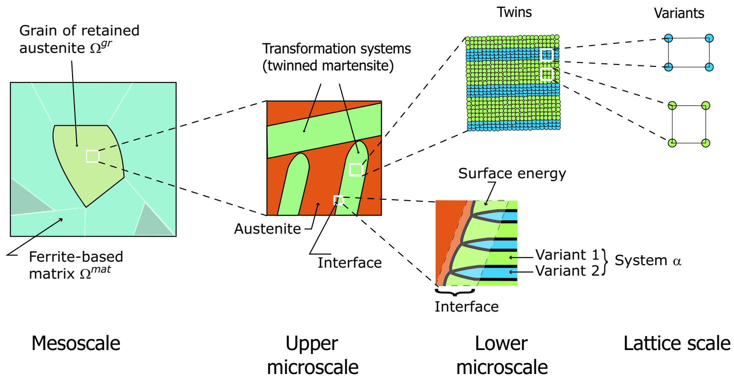

Figure 1: Sub-grain structures and length scales.

2 TRANSFORMATION MODEL

Cubic to tetragonal transformations in multiphase carbon steels (face centered cubic FCC to body centered tetragonal BCT) are characterized by the formation of up to $N = 24$ possible active transformations systems. Each transformation system, denoted with a superscript α, is composed of two (out of three possible) variants of BCT martensite. The transformation systems are described in terms of a shape strain vector $\boldsymbol{b}^{(\alpha)}$ and the normal to the habit plane $\boldsymbol{m}^{(\alpha)}$ (i.e., a vector normal to the austenite-twinned martensite interface). For a stress-assisted transformation, the deformation gradient $\boldsymbol{F}$ in a material point $\boldsymbol{x}$ in a grain of retained austenite Ω^{gr} may be decomposed as $\boldsymbol{F} = \boldsymbol{F}_e\boldsymbol{F}_{tr}$, where $\boldsymbol{F}_e$ is the elastic deformation gradient and $\boldsymbol{F}_{tr}$ is the transformation deformation gradient. The transformation deformation gradient is $\boldsymbol{F}_{tr} = \boldsymbol{I} + \sum_{\alpha=1}^{N} \xi^{(\alpha)}\boldsymbol{\gamma}^{(\alpha)}$, where $\boldsymbol{\gamma}^{(\alpha)} = \boldsymbol{b}^{(\alpha)} \otimes \boldsymbol{m}^{(\alpha)}$ is the transformation strain and $\xi^{(\alpha)}$ is the volume fraction of system α in a reference configuration. The relation between the second Piola-Kirchhoff stress $\boldsymbol{S}$ in a stress-free intermediate configuration and the Green elastic strain $\boldsymbol{E}_e$ is taken as $\boldsymbol{S} = \mathbb{C}\boldsymbol{E}_e$, where the mesoscopic effective stiffness tensor $\mathbb{C}$ is related to lower-scale constitutive information as[1,2,3]

$$\mathbb{C} = \frac{1}{J_{tr}} \left\{ \left(1 - \sum_{\alpha=1}^{N} \xi^{(\alpha)} \right) \mathbb{C}^A + (1+\delta_T) \sum_{\alpha=1}^{N} \xi^{(\alpha)} \mathbb{C}^{(\alpha)} \right\} . \tag{1}$$

In (1), $\delta_T = \boldsymbol{b}^{(\alpha)} \cdot \boldsymbol{m}^{(\alpha)}$ is the volumetric expansion due to the phase transformation and $J_{tr} = \det \boldsymbol{F}_{tr}$. The terms $\mathbb{C}^A$ and $\mathbb{C}^{(\alpha)}$ refer to, respectively, the microscale stiffnesses of austenite and transformation system α of martensite. In turn, $\mathbb{C}^{(\alpha)}$ can be related to the stiffness of each variant of martensite and its orientation in the transformation system[1,2]. The evolution of the transformation from austenite to system α of martensite is taken to be governed by the following kinetic relation between the transformation driving force $f^{(\alpha)}$ and the rate of change $\dot{\xi}^{(\alpha)}$ of the volume fraction: $\dot{\xi}^{(\alpha)} = \dot{\xi}^{(\alpha)}_{\max} \tanh \left(\langle f^{(\alpha)} - f^{(\alpha)}_{\text{cr}} \rangle / (\nu^{(\alpha)} f^{(\alpha)}_{\text{cr}}) \right)$, where $\dot{\xi}^{(\alpha)}_{\max}$, $\nu^{(\alpha)}$ and $f^{(\alpha)}_{\text{cr}}$ are material parameters and $\langle a \rangle = (|a| + a)/2$. The driving force for the transformation is[1]

$$f^{(\alpha)} = J_{tr}\boldsymbol{F}_e^T\boldsymbol{F}_e\boldsymbol{S}\boldsymbol{F}_{tr}^{-T} \cdot \boldsymbol{\gamma}^{(\alpha)} + \frac{1}{2}\left(\mathbb{C}^A - (1+\delta_T)\mathbb{C}^{(\alpha)}\right)\boldsymbol{E}_e \cdot \boldsymbol{E}_e - \frac{\chi}{l_0}\left(1 - 2\xi^{(\alpha)}\right) + f_{th}^{(\alpha)}$$

for $\alpha = 1, \ldots, N$, where $f_{th}^{(\alpha)}$ is a thermal term (constant for isothermal processes), χ is the surface energy per unit area and l_0 is a length scale parameter. The parameter l_0 can be related to the average size d_0 of a grain of retained austenite and the average thickness to width ratio c of plates of twinned martensite as[2] $l_0 \sim (c/2)d_0$.

In a material point $\boldsymbol{x}$ inside the ferrite-based matrix Ω^{mat} the deformation gradient is decomposed as $\boldsymbol{F} = \boldsymbol{F}_e\boldsymbol{F}_p$ where $\boldsymbol{F}_p$ is the plastic deformation gradient. The plastic deformations in the ferrite-based matrix are modelled by a large-strain, J_2-plasticity formulation with isotropic hardening.

3 SIMULATIONS

Several quasi-static uniaxial loading simulations were conducted on a grain of retained austenite embedded in a ferrite-based matrix. The computational domain and boundary conditions are shown in Fig. 2a. The grain of retained austenite occupies 16% of the total volume, which is a typical average value for multiphase steels. The domain was discretized using 1771 linear tetrahedrons. The transformation model was implemented using a fully-implicit backward Euler discretization scheme for the stress update within the framework of finite deformations[3]. A robust search algorithm was used in the return mapping algorithm for detecting the transformation systems activated during loading and a sub-stepping algorithm was implemented to accurately satisfy the completion of the transformation process. The computation of the consistent tangent operator was performed through a numerical differentiation method.

The evolution of the transformation, measured in terms of the volume fraction of retained austenite $\bar{\xi}_A$, is shown in Fig. 2b as a function of the logarithmic strain $\bar{e}_{11}$ averaged over the entire domain. The distinct cases correspond to two crystal orientations ($[100]_A$ and $[111]_A$, see Fig. 2a), each for three selected values of the length scale parameter l_0. Increasing values of l_0 can be correlated with larger grain sizes for fixed aspect ratios of martensitic plates. It can be observed from the figure that, at 10% strain, the grains oriented in the $[100]_A$ direction have almost fully transformed into martensite. In contrast, the grains oriented in the $[111]_A$ direction have not fully transformed, in particular the smallest grain that is related to $l_0 = 0.0125\mu$m. The axial Cauchy stress $\bar{T}_{11}^{gr}$ is shown in Fig. 2c as a function of the axial logarithmic strain $\bar{e}_{11}^{gr}$, averaged over the grain of retained austenite. As shown in the figure, the onset of the phase transformation occurs at higher local stress levels for decreasing grain sizes, in accordance with experimental results. When averaged over the entire domain, this effect is less noticeable as shown in Fig. 2d. In contrast, the crystal orientation plays a more significant role compared to the effect due to the grain size. From Figs. 2c,d, it can be observed that the orientation $[111]_A$ provides the highest increase in effective hardening behavior.

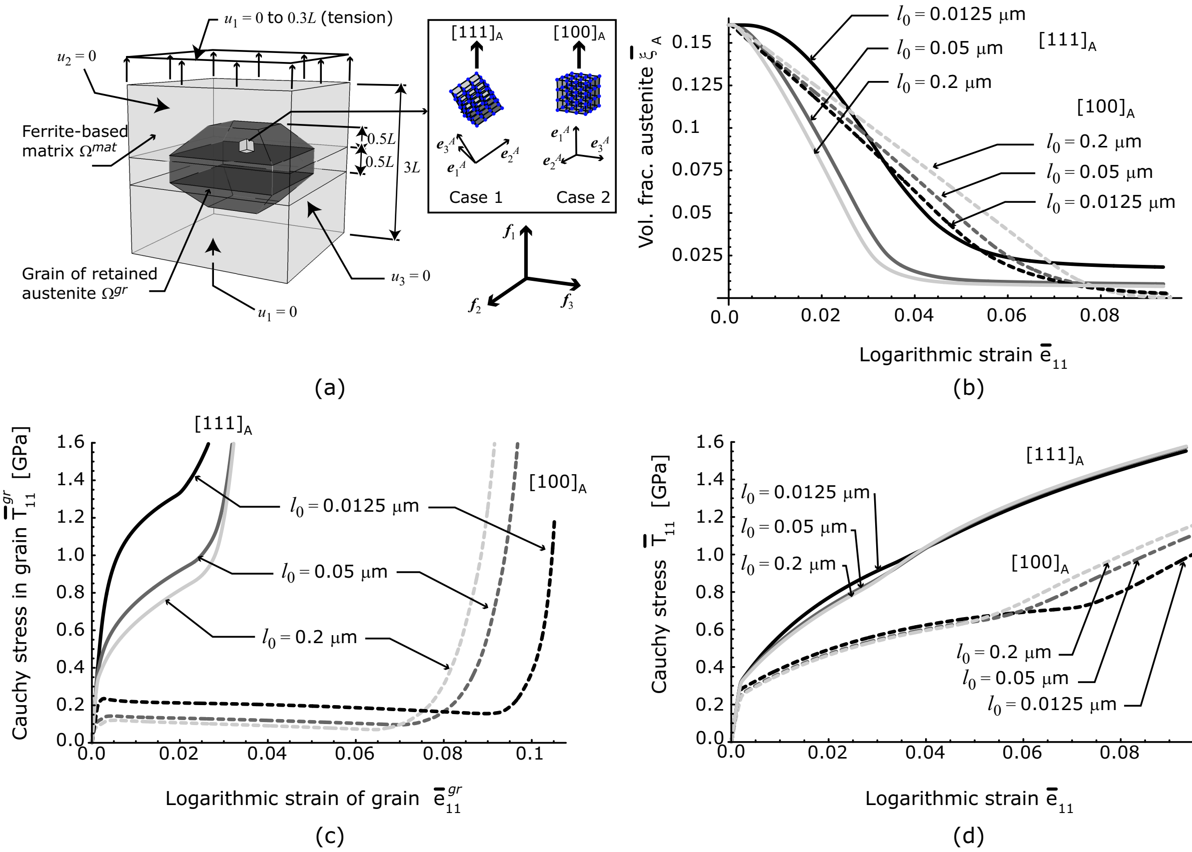

Figure 2: (a): Grain of retained austenite Ω^{gr} in a ferrite-based matrix Ω^{mat}. The inset indicates the different grain orientations. (b): Average volume fraction of austenite $\bar{\xi}_A$ as a function of the axial logarithmic strain $\bar{e}_{11}$ averaged over entire domain for two grain orientations and several values of the length scale parameter l_0. (c): Axial Cauchy stress $\bar{T}_{11}^{gr}$ vs. axial logarithmic strain $\bar{e}_{11}^{gr}$ averaged over grain of retained austenite. (d): Axial Cauchy stress $\bar{T}_{11}$ vs. axial logarithmic strain $\bar{e}_{11}$ averaged over entire domain.

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