Stress-assisted martensitic transformations in steels: A 3-D phase-field study

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Abstract

A 3-D elastoplastic phase-field model is developed for modeling, using the finite-element method, the stress-assisted martensitic transformation by considering plastic deformation as well as the anisotropic elastic properties of steels. Phase-field simulations in 3-D are performed by considering different loading conditions on a single crystal of austenite in order to observe the microstructure evolution. The thermodynamic parameters corresponding to an Fe–0.3% C steel as well as the physical parameters corresponding to commercial steels, acquired from experimental results, are used as input data for the simulations. The simulation results clearly show the well-known Magee effect and the Greenwood–Johnson effect. The results also show that even though the applied stresses are below the yield limit of the material, plastic deformation initiates due to the martensitic transformation, i.e. the well-known transformation-induced plasticity (TRIP) phenomenon. It is concluded that the loading conditions, TRIP as well as autocatalysis play a major role in the stress-assisted martensitic microstructure evolution.

1. Introduction

The mechanical properties of steels are determined by their microstructure and the constituent phases. In particular the high strength of steels can be attributed to martensite, a desirable high-strength constituent in many commercial steels. Some special steels, e.g. transformation-induced plasticity (TRIP) steels, are known for their ability to enhance their mechanical properties "in service" by means of martensite formation under applied stress. The high strength of the martensitic phase can be attributed to the strong solid-solution hardening effect of carbon and to the complex martensitic microstructure formed by the rapid diffusionless martensitic transformation. Hence in order to understand the microstructure–property relations of steels, it is essential to understand thoroughly the

martensitic transformation and the martensitic microstructure evolution under various thermomechanical conditions.

Martensitic transformation, despite being a widely studied phase transformation, is still intriguing to the scientific community. Based on the mode of formation, martensitic transformation in steels can be classified as: athermal, i.e. by rapid quenching of steel; isothermal, i.e. by holding the steel at a constant temperature close to the martensite start temperature; stress-assisted, i.e. by application of stress that is below the yield limit of the steel; and strain-induced, i.e. by plastic deformation of steel.

Several theoretical works have been performed to understand the formation of athermal [1,2], isothermal [3,4] as well as stress- and strain-induced martensite [5–8] and have significantly contributed to our understanding of the overall transformation. Studies have also been performed to understand some of the complexities, associated with the transformation, such as martensite nucleation [2,9], autocatalysis [10,11], morphology [12,13] and crystallography [13–15]. These studies have clearly established that, from

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a morphological point of view, martensite can be formed in the form of laths and plates, depending on the alloy composition [12], and from a crystallographical point of view martensite can be formed in 24 different crystallographic variants, which can be grouped into three main groups known as Bain groups [14,15].

The martensitic transformation behavior under different stress states has been well studied, both experimentally and theoretically [6,7,16–23]. Two important phenomena, i.e. the Greenwood–Johnson effect [17] and the Magee effect [18], have been identified as occurring during the martensitic transformation under applied stress. The Greenwood–Johnson effect, which can be considered to be the origin of the TRIP phenomenon, corresponds to the plastic accommodation of internal stresses that arise due to the martensitic transformation. The Magee effect corresponds to the variant selection mechanism under applied stress, i.e. for a given stress state only the variants with the best orientation with respect to the applied stress are favored. Several micromechanical models [20,22,6,8,24] have been developed in order to explain the above-mentioned aspects. However, the microstructure evolution under different stress states needs further in-depth studies.

Recent advances in modeling the microstructure evolution by using the phase-field method [25–27] seem promising and should aid the study of the martensitic transformation. Several works have been performed to study the martensitic transformation by using the phase-field method [28–41]. In the present work the above model in Ref. [37] is modified and extended to study the stress-assisted martensitic transformation occurring in a single crystal of an Fe–C steel. Different loading conditions, on an elastoplastic material, are considered in order to study their effect on the microstructure evolution. The finite-element method, which allows a straightforward and transparent formulation of the equations, is applied to solve the phase-field as well as the continuum mechanics equations.

2. Elastoplastic phase-field model

A diffusionless phase transformation, such as the martensitic transformation, can be modeled using the Cahn–Allen equation [42], also known as the time-dependent Ginzburg–Landau (TDGL) kinetic equation [28]. The microstructure evolution can be simulated by predicting the time-dependent variation of the phase-field variable, which in turn is related to the minimization of the Gibbs energy G of the system with respect to phase-field variable η_p as:

$$\frac{\partial \eta_p}{\partial t} = -\sum_{q=1}^{q=v} L_{pq} \frac{\delta G}{\delta \eta_q} \tag{1}$$

where $\frac{\delta G}{\delta \eta_q}$ is a variational derivative that serves as a driving force for the formation of martensite denoted by the phase-field variable η_q that is dependent on the position vector $\mathbf{r}$, v is the total number of martensite variants and L_{pq} is a kinetic parameter.

The phase transformation of austenite (face-centered cubic crystal, fcc) into martensite (body-centered tetragonal crystal, bct) causes asymmetry in the crystal structure and thereby gives rise to three possible orientations of the tetragonal martensitic phase, i.e. the longest axis of the bct oriented along either of the three Cartesian coordinate axes. Thus in order to represent the three possible orientations, three phase-field variables, i.e. η_1, η_2, η_3, need to be considered in the model and hence three phase-field equations, i.e. for $p = 1, 2, 3$ and $v = 3$ in Eq. (1), need to be solved at each time step.

It has to be emphasized that these three orientations are equivalent to the Bain groups, i.e. the three main martensite variant groups that represent all the 24 different crystallographic martensite variants, usually considered in the microstructural characterization of martensite [14]. Each of the above three variants (orientations) is governed by a Bain strain tensor $\epsilon_{ij}^{00}(p)$, i.e. compression along one of the coordinate axes and expansion along the other two axes of fcc.

From a thermodynamic point of view, the Gibbs energy of a system undergoing stress-assisted martensitic transformation consists of the following parts:

$$G = \int_V \left(G_v^{chem} + G_v^{grad} + G_v^{el} + G_v^{appl} \right) dV \tag{2}$$

G_v^{chem} corresponds to the chemical part of the Gibbs energy density of an unstressed system at the temperature under consideration. G_v^{grad} is the extra Gibbs energy density caused by the interfaces. The transformation of cubic austenite into tetragonal martensite induces elastic strain energy density G_v^{el}, into the material. G_v^{appl} is the extra Gibbs energy density that arises due to the externally applied stress.

2.1. Chemical energy

The chemical part of the Gibbs energy density G_v^{chem}, expressed as a Landau-type polynomial [30,37], is given by:

$$G_v^{chem}(\eta_1, \eta_2, \eta_3) = \frac{1}{V_m} \left[\frac{1}{2} A (\eta_1^2 + \eta_2^2 + \eta_3^2) - \frac{1}{3} B (\eta_1^3 + \eta_2^3 + \eta_3^3) \right.$$
$$\left. + \frac{1}{4} C (\eta_1^2 + \eta_2^2 + \eta_3^2)^2 \right] \tag{3}$$

By considering the driving force ΔG_m, i.e. the difference in the Gibbs energies of austenite and martensite, and the Gibbs energy barrier ΔG^* terms in the above equation, the coefficients are modified [37] as: $A = 32\Delta G^*$, $B = 3A - 12\Delta G_m$ and $C = 2A - 12\Delta G_m$. ΔG^* is expressed as $\Delta G^* = \frac{V_m \beta}{2\delta^2}$. V_m is molar volume, δ is thickness of the interface and β relates to interfacial energy and is discussed in the following section.

2.2. Gradient energy

The gradient energy density term, G_v^{grad} as presented in Refs. [30,37] can be expressed as: