



# Numerical investigation of the interaction between the martensitic transformation front and the plastic strain in austenite



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## ABSTRACT

Phase-field simulations of the martensitic transformation (MT) in an austenitic matrix which has already undergone the plastic deformation are carried out. For this purpose the elasto-plastic phase-field approach of incoherent MT developed in a previous work [Kundin et al., 2011. A phase-field model for incoherent martensitic transformations including plastic accommodation processes in the austenite. *J. Mech. Phys. Solids* 59, 2082–2012] is used. The evolution equation for the dislocation density field is extended by taking into account the thermal and athermal annihilation of the dislocations in the austenitic matrix and the athermal annihilation at the transformation front. It is shown that the plastic deformation in the austenite caused by the MT interacts with the dislocation field and the MT front that leads to an inhomogeneous increasing of the total dislocation density. During the phase transformation one part of the dislocations in the austenite is inherited by the martensitic phase and this inheritance depends on the kinetics and the crystallography of MT. Another part of dislocations annihilates at the transformation front and decreases the dislocation density in the growing martensite. Based on the simulation results the specific type of phenomenological dependency between the inherited dislocations, the martensite phase fraction and the plastic deformation is proposed.

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## 1. Introduction

The morphology of the martensitic microstructures is strongly related to the mechanical properties of steel and other metallic alloys. It is important to predict the formation of the martensitic microstructure precisely. Furthermore, during the MT the incremental elastic strain energy is reduced by the formation of a heterogeneous array of different orientation variants of the martensitic phase and by plastic accommodation. The development of appropriate models allows to calculate the strains which are associated with the phase transformation. The understanding and control of localized plasticity and its interaction with the transformation front is quite essential e.g. for TRIP-steels and shape memory alloys (Dadda et al., 2008; Graessell et al., 2000).

Recently, phase-field (PF) models have been extensively studied as a powerful tool for predicting microstructural evolution and applied to the martensitic transformation. Khachaturyan and co-workers developed the phase-field microelasticity (PFM) theory (Wang and Khachaturyan, 1997; Jin and Khachaturyan, 2001), which integrates the microelasticity into the phase-field model employing the fast Fourier transform algorithm. The model was further applied to investigate the

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MT in single crystals (Artemev et al., 2001) and polycrystalline systems (Artemev et al., 2002) as well as in multilayer systems under applied stresses (Artemev et al., 2000). It has been successfully applied to various coherent phase transformations including the prediction of many complicated strain-induced morphological patterns (Wen et al., 2000; Chen, 2002; Shen and Wang, 2005; Zhang et al., 2007). Resolving the individual martensite plates the PF approach differs from the phenomenological martensitic transformation modeling of irreversible processes in various representations: local, crystalline and mean-field (Kubler et al., 2011; Ostwald et al., 2011, 2012; Fischer and Reisner, 1998; Fischer et al., 2000; Idesman et al., 2000; Kaganova and Roitburd, 1989), which are widely used in the simulation of shape memory alloys and TRIP-steels due to their simplicity and efficient incorporation of elasto-plastic effects on mesoscale. To understand the mechanism of nucleation and the growth conditions of martensitic plates inside an inhomogeneous plastic strain field, a number of theoretical models were developed (Olson and Cohen, 1986; Cherkaoui and Berveiller, 2000). These models include the dislocation theory of the martensitic interfacial structure and introduce a driving force of interface propagation in inelastic materials.

Besides the coherent phase transformations the MT in technical alloys is usually associated with plastic strains. The effect of plasticity, which can be represented as the generation and motion of dislocations during the MT, is very complex. On the one hand, if the MT is caused by applied loads, the evolution of the plastic deformation reduces the driving force of the transformation. On the other hand, a local plastic relaxation allows the accommodation of strains caused by the MT and the nucleation and growth of new martensitic variants. Finally, statistically stored dislocations are an irreversible structural change which affect the energy landscape by their own elastic fields. Thus, a general phase-field model for MT should include not only the driving forces originating from the elastic fields, but also the effects resulting from the plastic strain fields.

The plastic activity in the phase-field theory has already been treated by modeling the individual dislocations (Hu and Chen, 2001) and their coupling dynamics (Rodney and Finel, 2001; Rodney et al., 2003; Wang et al., 2001; Zhou et al., 2007; Koslowski et al., 2002). A phase-field model of the evolution of a dislocation system due to the evolution of dislocation order parameters based on the time depending Ginzburg–Landau (TDGL) equation was developed by Wang et al. (2001). At the same time, Koslowski et al. (2002) formulated a phase-field theory of the dislocation dynamics for an arbitrary number and arrangement of dislocation lines based on a general framework for dissipative systems.

The plastic deformation can also be added to the phase-field model by introducing a plastic strain field defined at the mesoscale. A version of this approach has been recently proposed by Zhou et al. (2008, 2010), where the plastic strain is related to the inter-dislocation distance. The evolution of the dislocation phase fields is described by the TDGL equation similar to the evolution of the martensitic phase fields, where the driving force is the elastic shear energy density relaxed by the plastic strain. The difference to the individual dislocation dynamic models is that the model proposed by Zhou et al. describes the evolution of dislocation order parameters related to the slip systems of the crystal.

In recent years a similar approach for the simulations of the evolution of the martensitic phase transformations and the dislocation order parameters by the TDGL equations was developed by Levitas and Javanbakht (2012). The phase-field approach was applied to interaction of the phase transformation and the individual dislocation evolution (Levitas and Javanbakht, 2013, 2014). As a result a number of model problems of the stress-induced phase transformations interacting with the dislocation evolution were solved. It is also important that in the work (Levitas, 2013b) the general phase-field theory for multivariant martensitic phase transformations and explicit models have been formulated for the most general case of large strains. The general thermodynamic approach allows to determine the driving force for the change of the order parameters as well as their boundary conditions for the order parameters. Moreover, it allows to calculate correct interface stresses and to elucidate the importance of the interface width (Levitas, 2013a). Remarkable is that Levitas et al. previously developed a finite-strain-continuum thermomechanical approach to simulate the transformation-induced stress and plastic strain fields (Levitas et al., 2002) based on a theory of martensitic phase transformations developed earlier by Levitas (2000).

Another simplified version of this approach has been derived by Yamanaka et al. (2007, 2009) based on the PF micro-elasticity theory and the elasto-plastic PF model suggested by Guo et al. (2005) which does not take into account different slip systems. In recent years elasto-plastic phase-field models of the martensitic transformation using similar evolution equations for the plastic strain have been developed by Koyama's group (Cong et al., 2012a,b, 2013). This approach also follows Yeddu et al. (2012a,b, 2013) and Malik et al. (2012) for the phase-field modeling of the martensitic microstructure evolution in steels by using the elasto-plastic finite-element method. Further, Yamanaka et al. (2012) proposed a model to describe the austenite-to-ferrite transformation, where the mesoscale crystal plasticity theory is used (Pan and Rice, 1983). They combine the crystal plasticity finite element method with the multi-phase-field method to simulate the austenite-to-ferrite transformation with the diffusion of carbon atoms in low carbon steels.

To describe the plastic deformation in single crystals many models use the crystal plasticity framework in which the evolution of plastic strain is described by means of an elastic driving force. A microstructural strain-hardening model suitable for crystal plasticity simulations developed by Roters et al. (2000, 2010) and Ma and Roters (2004) has recently made remarkable progress and allows the numerical study of deformation processes on the basis of the thermally activated dislocation evolution. The model preserves the crystallographic features of dislocation slip processes and captures the commonly accepted concepts of dislocation processes in the plastic deformation, especially various dislocation interaction processes as interactions of mobile and statistically stored dislocations, the formation of locks and dipoles or the thermal and athermal annihilation in a continuum dislocation density framework. The original concept (Ma and Roters, 2004) for fcc single crystals has been extended to polycrystals, considering grain boundary interactions and geometrically necessary

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