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Phase field-elasticity analysis of austenite–martensite phase transformation at the nanoscale: Finite element modeling

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ABSTRACT

In the present work, a nonlinear finite element method is utilized to solve the coupled system of time-dependent phase field and elasticity equations for phase transformations (PTs) at the nanoscale in the Cartesian coordinate system. The Galerkin residual weighted method is used to derive the finite element equations. The alpha family and the explicit methods are used for time discretization. Since the local free energy includes a 3rd degree polynomial in terms of the phase order parameter the kinetics Ginzburg-Landau equation is a nonlinear function of the order parameter. Thus, the Newton-Raphson method is used to linearize the nonlinear equation. Linear triangle elements have been used in the self-developed FEM code. Stability and mesh and time step independence of the solutions have been discussed. The system of equations and the numerical procedure are verified using the existing analytical solutions. For the phase field equation, the isolated boundary condition is considered everywhere, imposing the constant surface energy over the simulation domain. Examples of austenite (A) to martensite (M) phase transformations in 2D for a single martensitic variant are presented including planar/nonplanar interface propagation, martensitic nucleus growth and reverse phase transformation under thermal and different mechanical loadings. The A-M interface velocity, width and energy have been obtained. The threshold stresses for the growth of a martensitic nucleus in an austenitic matrix under uniaxial and biaxial loadings and for reverse PTs are calculated. It is found that the numerical results are in a good agreement with the transformation work based criterion. The developed FEM code represents a proper and accurate tool to study the PTs including nucleation, growth and propagation of transformed phase, reverse PTs and equilibrium and stability conditions for PTs. A further development of the numerical procedure provides a powerful tool for the study of more complicated PTs-related phenomena in 2D and 3D.

1. Introduction

Martensitic phase transformation (MPT) is defined as a first-order, displacive, and diffusionless transformation which creates nano and microstructures of different complexities and mechanical properties in various materials such as shape memory alloys, steel and ceramics. During this transformation, austenite (A) phase which has a cubic lattice and is stable at high temperatures transforms to martensite (M) which has a lower-symmetry, such as tetragonal or rhombic, lattice and is stable at low temperatures. Mechanical loading, reducing temperature and varying surface energy are the main reasons for such a transformation in small scales. The deformation caused by martensitic or any other types of displacive PTs is defined by a transformation strain tensor. There are three possible martensitic variants which are perpendicular to each other and the strain tensor components of each variant is obtained by permutation of those of other variants [1,2].

In contrast to the theories which assume some geometry for martensitic nano/microstructures [3–8], the phase-field method (PFM) is broadly used for modeling of MPTs without any assumption on solution geometry [9–31].

In the PFM, each martensitic variant is described by an order parameter η_i, and its evolution is described by the phase field or the Ginzburg-Landau (GL) equations. These equations linearly connect the rate of change of η_i to the thermodynamic driving forces conjugate to η_i which are the functional derivatives of the free energy with respect to η_i. Considering stresses, martensitic nanostructures can be resolved by solving the coupled system of the GL and elasticity equations. The result can consist of different phases where between any of two contacting phases, there exists a diffusive interface within which η_i smoothly varies from the value of one phase to that of the contacting phase. The PFM has been broadly used for modeling of various types of PTs in different scales in many materials. A 3D Landau theory for multivariant stress-

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induced martensitic PTs was proposed in [16–18] where different free energy potentials, kinetics and nucleation process as well as PT equilibrium and stability conditions were discussed and important features of known experimental stress-strain curves involving PTs were described. Total strain related [10–13] and transformation strain related order parameters [14,15,19] were suggested to build different PFMs. The PFM was presented at microscale problems in [19,21]. Levitas et al. introduced an internal friction for the interface motion in [22,23]. A multiscale PFM to MPTs was proposed in [24]. The PF microelasticity was used to simulate heterogeneous nucleation and growth in martensitic alloys [25]. Surface-induced PTs due to the variable surface energy were described in [26,28]. A-M and M-M interface widths and energies were studied in [27] and twin nanostructures were obtained under overcooling. Inertial effect on PTs was studied in [29]. The interface stress was introduced in [28,32,33]. Large-strain based PFM and MPTs simulations were presented in [33,34]. The FCC to BCC martensitic transformation in Fe–Ni polycrystalline alloy with plastic deformation was investigated by the elastoplastic phase-field model in two-dimensions [35]. Analytical solutions for diffuse interface propagation and different models for athermal interface friction were proposed and PTs were numerically studied with the focus on the effect of the athermal friction in [23]. A PFM of displacive transformations was developed [36] in which the free energy is expressed in terms of the transformation strain. Elastoplastic phase-field models were employed to study incoherent butterfly-type PTs including plastic accommodation in Fe–30 wt%Ni [37] and Fe–0.3%C [38] alloys. A PFM was developed to model the phase evolution during the beta to gamma transformation in Zr—Nb [39]. The phase field microelasticity model was used to model FCC → BCT transformations in a steel polycrystalline using the finite element method [40]. A large strain based PFM for multivariant MPTs was proposed, the equilibrium and stability conditions were derived and PTs in NiAl, boron nitride, and graphite to diamond were simulated [34]. Phase field modeling of MPTs was reviewed in [41]. Bainitic PTs were studied using the PFM which model could reproduce the incomplete transformation phenomenon [42]. Stress-induced PTs were modeled in nanotubes, beams and nanosheets with voids using a finite strain mechanics-based phase field model and the transformation induced buckling of nanobeams was discussed [43]. A PFM was developed for the tetragonal-to-monoclinic PT in Zr and the PF equations were solved using the FEM for martensitic twinning mechanism [44]. A thermodynamically consistent PFM for PTs was developed introducing correct interface stresses with the help of some geometric nonlinearities and new expression for the free energy [32,45]. A FPM was developed for modeling of the stress-induced MPT involving plasticity and anisotropic elastic properties of steels and using the FEM [46]. The effect of external loading on the martensitic transformation in polycrystalline steel was analyzed using an elasto-plastic phase field model [47]. *FCC to BCC* MPTs in a polycrystalline were simulated based on the combination of inhomogeneous elasticity model and the phase-field equations [48]. A phase field model was presented to capture both forward and reverse tetragonal to monoclinic transformations and shape memory effect in polycrystalline zirconia [49]. The stress-induced tetragonal-to-monoclinic PT in Zr was investigated using a two-dimensional elastic phase field model [50]. A new phase-field model was proposed which separated nucleation from kinetics; and an evolution law that came from a conservation statement for interfaces [51]. This model was characterized through 1D and 2D numerical solutions [52]. A thermodynamically consistent PFM for stress-induced PTs between different variants were developed [53]. Cyclic phase transformations in the Fe–C alloy were simulated in 2D using a PFM where the stagnant stages were described by a Gibbs-energy dissipation model [54]. Beta to omega PT in Zr—Nb alloys was simulated using a elastoplastic PFM and the 3D FEM [55]. Size-dependent martensitic microstructures considering phase interfaces and twin boundaries were studied in CuAlNi shape memory by a PFM and 2D FEM discretization [56]. Internal stresses associated with MPT in MnCu were obtained using a FPM [57]. A PFM of martensitic PTs was proposed based on pathway tree and was applied to 2D square-to-hexagonal transformations which resulted in successive transformations and subsequent numerous variants [58]. Beta to Delta temperature induced PTs were simulated using a proposed PFM and the FEM of octagen energetic crystal. The key point was a penalizing term that allowed controlling the third phase within the interface between two other phases [59]. Peritectic phase transformation of FeMn alloys was studied utilizing a phase-field method in 1-D and 2-D [60]. A PFM was presented for modeling of the lower bainite including carbon diffusion and carbide formation via the FEM [61]. The strong effect of surface tension and energy on PTs was studied in NiAl studied using a PFM in 2D [62]. A thermodynamically consistent, large-strain, multi-PFM was generalized for the case with anisotropic interface energy and interface stresses and analytical solutions for propagating interfaces and critical nuclei were proposed [63]. A PFM was used for shock-induced solid-solid phase transformation and microstructural evolution [64]. A multi-phase-field model was proposed to simulate the peritectic phase transition in Fe-C alloys [65]. Microstructure evolution in Ferritic-martensitic dual-phase steels (DP) was simulated using a multiphase-field modeling [66]. Analytical and numerical solutions were given for elastic stress within a martensitic twin based on a finite strain phase field approach [67]. Cyclic ferrite-austenite PTs were studied using the multi-PFM and the FDM [68]. MPTs and plasticity under thermal cycling in steels were simulated using a PFM [69]. Thermally and stress-induced MPTs in Mn–Cu SMAs were studied using a non-isothermal PFM where the thermoelastic equilibrium between twinned martensite and austenite was obtained and internal stress field was revealed [70]. Thermomechanical properties of polycrystalline SMAs originated from the temperature and stress-induced martensitic PTs were studied using a PFM where the inertial and the latent heat effects as well as the grain boundary energy change were considered [71]. Bainite-ferrite PT in TRIP steel is modeled using a PFM. [72]. Thermal-, stress and surface induced martensitic transformations were investigated in the presence of defects utilizing the PFM [73–77].

In the present work, a nonlinear finite element method is used to solve the coupled system of time-dependent phase field and elasticity equations for phase transformations (PTs) between austenite (A) and martensite (M) in the Cartesian coordinate system. The Galerkin residual weighted method is used to derive the finite element equations. The alpha family and the explicit methods are used for time discretization. Since the local free energy includes a 3rd degree polynomial in terms of the phase order parameter the kinetics Ginzburg-Landau equation is a nonlinear function of the order parameter. Thus, the Newton-Raphson method is used to linearize the nonlinear equation. Linear triangle elements have been used in the developed FEM code. Stability and mesh and time step independence of the solutions have been discussed. The system of equations and the numerical procedure are verified using the existing analytical solutions. For the phase field equation, the isolated boundary condition is considered everywhere, imposing the constant surface energy over the simulation domain. Examples of cubic to tetragonal phase transformations in 2D for a single martensitic variant are presented including plane interface propagation, martensitic nucleus growth and reverse phase transformation under thermal and different mechanical loadings. The A-M interface velocity, width and energy have been obtained. The threshold stresses for the growth of a martensitic nucleus in an austenitic matrix under uniaxial and biaxial loadings and for reverse PTs are calculated. It is found that the numerical results are in a good agreement with the transformation work based criterion. The developed FEM code represents a proper and accurate tool to study the PTs including nucleation, growth and propagation of transformed phase, reverse PTs and equilibrium and stability conditions for phase transformations under mechanical and thermal loadings in 2D.