Nano- and Macro-scale Phase Field Modeling of Phase Transformations

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Despite significant success in modeling microstructure formation during martensitic phase transformations in papers by Khachaturyan et al., Jacobs et al., and Lookman and Saxena et al., there are numerous unsolved problems. The following basic problems of modeling of martensitic phase transformations at the nanoscale based on the Ginzburg-Landau approach are discussed:

1. New thermodynamic potentials for stress-induced martensitic phase transformations, both for small [1,2] and large [3,4] strains. These potentials were designed by requiring that they describe the experimentally observed features of martensitic phase transformation in shape memory alloys and steels, specifically, a constant or weakly temperature dependent transformation strain tensor and stress hysteresis, and transformation at non-zero tangent elastic moduli. They include all temperature-dependent thermomechanical properties of the austenite and martensitic variants and describe phase transformations between austenite and martensitic variants and between martensitic variants for arbitrary crystal structures.

2. Phase transformations in nanosize sample: surface effect, new microstructures, new functionally graded nanophases, barrierless surface-induced nucleation [5,6].

3. Finite element algorithm and modeling martensite microstructure evolution for small and large strains, for two- and three-dimensional problems, and for quasi-static and dynamic formulations [4,7-9]. The most sophisticated problems for large strains are solved using finite element code "FIDESYS" [10].

4. Introducing an athermal threshold in phase field modeling [7,9] (Fig. 1). Previous phase field approaches could not describe stable two-phase equilibrium and rate-independent hysteresis.

Fig. 1. Examples of stationary microstructures in a NiAl single nanocrystal obtained as a result of cubic-to-tetragonal phase transformation, stabilized by the spatially oscillating stress field of defects [7,9].

Sample size in Ginzburg-Landau simulations is limited by necessity to resolve few nm diffuse interface. Alternative phase field approach is developed for the scale from 100nm and without upper limit [11,12]. It is based on micromechanically derived constitutive equations for the representative volume consisting of austenite and mixture of two martensitic variants divided by plane interface [13]. It describes evolution of crystallographic parameters under complex loading. Universal (i.e.
independent of the constitutive equations) driving force for interface reorientation is derived. The relations between the rates of single and multiple interface reorientation and propagation and the corresponding driving forces are derived, which take into account athermal and viscous interface friction. It was found that under complex loading, an instability in the interface normal leads to a jump-like interface reorientation that has the formal features of the energetics of a first-order transformation [13]. Martensitic microstructure evolution in a single and polycrystalline sample under uniaxial loading is found using finite elements method [11,12] (Fig. 2).

![Fig. 2. Distribution of concentration of martensite (left), martensitic variant 1 (center), and martensitic variant 2 (right) in polycrystalline macroscopic sample [11,12].](image)

Similar approach is developed for stress- and temperature-induced melting with application to melting of aluminum nanoparticles, without and with alumina shall. The effect of surface pre-melting, heating rate, surface tension and stresses is analyzed.

References