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Interface- and surface-induced phenomena during phase transformations: phase field approach

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ABSTRACT

Thermodynamically consistent phase field theory for various phase transformations (including multivariant martensitic transformations, melting, and twinning), which includes interface stresses, is developed [1–5]. Free energy includes several local polynomials in terms of the order parameters describing phase transformations and depends on their gradient in the current configuration. Theory is formulated in a way that some geometrically nonlinear terms do not disappear in the geometrically linear limit, which in particular, allowed us to introduce expression for the interface stresses consistent with the sharp interface approach. For instance, for nonequilibrium interface these stresses are reduced to a biaxial tension with the resultant force equal to the nonequilibrium interface energy [3–5]. A complete system of equations, including Ginzburg–Landau equations, is presented in the reference and actual configurations. Boundary conditions for the order parameters include variation of the surface energy during phase transformation [1, 2]. Alternatively, finite-width external surface is described by an additional order parameter [6, 7]. This leads to various surface-induced pre-transformations, transformations, and scale-dependent phenomena. Analytical solution for the propagating interface and critical martensitic nucleus that includes distribution of components of interface stresses has been found [4, 5, 8]. Fundamental problem in the interface and surface science on the definition of position of the Gibbsian dividing surface is resolved with the help of static equivalence approach [8]. Even two equations for determination of the dividing surface follow from this principle, which may be contradictory. For the obtained analytical solution for the propagating interface, both conditions determine the same dividing surface, i.e., theory is noncontradictory. For melting, anisotropic transformation strain is introduced to describe stress relaxation within interface and known experimental data [9]. Various problems on evolution of multivariant martensitic structure and twins [1, 3], melting of Al nanoparticles [2, 7, 9] and foils under laser heating [10], and surface-induced phenomena [2,6,7,9] have been solved with finite element method. Numerous new effects and phenomena, including scale effects and morphological transitions, have been revealed.

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