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Phase-field approach for stress- and temperature-induced phase transformations that satisfies lattice instability conditions. Part 2. Simulations of phase transformations Si I↔ Si II

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Abstract

A complete system of equations of the advanced phase-field theory for martensitic phase transformations (PTs) under a general stress tensor is presented. Theory includes a fully geometrically nonlinear formulation for the general case of finite elastic and transformational strains as well as anisotropic and different elastic properties of phases. Material parameters are calibrated, in particular, based on the crystal lattice instability conditions from atomistic simulations for martensitic PTs between cubic Si I and tetragonal Si II phases under complex triaxial compression-tension loading. A finite element algorithm and numerical procedure is developed and implemented in the code deal.II. Various 3D problems on lattice instabilities and following nanostructure evolution in single-crystal silicon are solved for compression in one direction under lateral stresses and analyzed. Strong effects of the stress states and local stress hysteresis on the interface width and nanostructure evolution are presented. In particular, the interface width diverges when lateral stress tends to the region in which instability stresses for direct and reverse PTs coincide. Direct and reverse transformations both occur in the unique homogeneous way without hysteresis, energy dissipation, and damage

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