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Interaction between phase transformations and dislocations at the nanoscale. Part 1. General phase field approach

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Abstract

Thermodynamically consistent, three-dimensional (3D) phase field approach (PFA) for coupled multivariant martensitic transformations (PTs), including cyclic PTs, variant-variant transformations (i.e., twinning), and dislocation evolution is developed at large strains. One of our key points is in the justification of the multiplicative decomposition of the deformation gradient into elastic, transformational, and plastic parts. The plastic part includes four mechanisms: dislocation motion in martensite along slip systems of martensite and slip systems of austenite inherited during PT and dislocation motion in austenite along slip systems of austenite and slip systems of martensite inherited during reverse PT. The plastic part of the velocity gradient for all these mechanisms is defined in the crystal lattice of the austenite utilizing just slip systems of austenite and inherited slip systems of martensite, and just two corresponding types of order parameters. The explicit expressions for the Helmholtz free energy and the transformation and plastic deformation gradients are presented to satisfy the formulated conditions related to homogeneous thermodynamic equilibrium states of crystal lattice and their instabilities. In particular, they result in a constant (i.e., stress- and temperature-independent) transformation deformation gradient and Burgers vectors. Thermodynamic treatment resulted in the determination of the driving forces for change of the order parameters for PTs and dislocations. It also determined the boundary conditions for the order parameters that include a variation of the surface energy during PT and exit of dislocations. Ginzburg-Landau equations for dislocations include variation of properties during PTs, which in turn produces additional contributions from dislocations to the Ginzburg-Landau equations for PTs. A complete system

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