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ICAMS Special Seminar

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Stress- and Surface-induced Phase Transformations: Phase Field Approach

Using the first and second law of thermodynamics, phase field equations for the description of phase transformations are derived for finite strains and lattice rotations. A criterion for the instability of a crystal lattice with respect to a change in order parameters is formulated for homogeneous states. An explicit relation for lattice rotation is derived. The Landau potential for multivariant displacive phase transformations is formulated in terms of elastic strain, temperature, and order parameters for the most general case of large rotations, elastic and transformational strains, as well as nonlinear and different elastic properties of phases [1]. For small elastic strains, essential simplification of the theory is achieved, and the explicit expression for Gibbs potential is obtained [2]. The phase equilibrium and phase transformation conditions are obtained as well. The above theory represents a generalization of our small strain theory [3,4] for a general geometrically nonlinear case and it satisfies all the same conditions necessary for a conceptually correct description of the effects of stress tensors and temperature on martensitic phase transformations. Martensitic phase transformations in NiAl, BN and C are analyzed and the importance of finite-strain corrections is demonstrated. Then this theory, including energy contribution related to the gradient of the order parameters, is further generalized to incorporate description of the surface effects [5,6]. Fully geometrically nonlinear formulation is crucial for this generalization, even if the strains are small. The generalization includes introducing the surface tension at the internal interfaces and external surfaces, correct description of the variant-variant interface energy, as well as description of phenomena related to the variation of the energy of the external surface during phase transformations. Boundary conditions take into account variation of surface energy during transformation and lead to surface-induced pre-transformation and transformations. Some specific problems related to melting are addressed. Various examples and surface-induced phenomena for solid-solid and solid-liquid phase transformations are presented. A similar approach can be applied for twinning and dislocations.

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[3] Levitas V.I., Preston D.L. Part I&II. Physical Review B, 2002, **66**, 134206&134207.

[4] Levitas V.I., Preston D.L. and Lee D.-W. Physical Review B, 2003, **68**, 134201.

[5] Levitas V.I. and Javanbakht M. Physical Review Letters, 2010, ***105***, 165701.

[6] Levitas V.I. and Samani K. Nature Communications, 2011, **2**, 284.