Aerospace Engineering Graduate Preliminary Oral Exam:

A diffuse interface approach to phase transformation via virtual melting

On behalf of Professor Valery Levitas,
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This work represents development of the first phase field models and detailed study solid-solid transformations via intermediate melting within nanometer size interface. Such phase transformations can occur in different materials, including HMX energetic crystals, PbTiO3 nanowires, complex pharmaceutical substances, electronic and geological materials, as well as colloidal, and superhard materials. A thermodynamically consistent phase field model for three phases is developed using two polar order parameters. It includes the effect of energy and width of solid-solid and solid-melt interfaces, interaction between two solid-melt interfaces, temperature, mechanics, and interface stresses. The derived thermodynamic potential satisfies all the equilibrium and stability conditions for homogeneous phases. The HMX energetic crystal is used as the model material and numerical simulations are performed using COMSOL and Cystorm high performance computing facility. Depending on parameters, the intermediate melt may appear and disappear by continuous or discontinuous barrierless disordering or via critical nucleus due to thermal fluctuations. The intermediate melt may appear during heating and persist during cooling at temperatures well below what it follows from sharp-interface approach. For some parameters when intermediate melt is expected, it does not form, producing an intermediate melt free gap. Elastic energy promotes barrierless intermediate melt formation in terms of an increasing degree of disordering, interface velocity, and width of intermediate melt. Drastic reduction (by a factor of 16) of the energy of the critical nuclei of the intermediate melt within the solid-solid interface caused by mechanics is captured. Interfacial stresses surprisingly increase nucleation temperature for the intermediate melt. Interfacial stresses alter the kinetics of phase transformation, resulting in formation of new interfacial phases and drifting of a thermally activated spontaneous phase transformation to a stable phase.