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Multi Phase Phase-Field Approach for Virtual Melting: A Brief Review

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Abstract

A short review on a thermodynamically consistent multiphase phase-field approach for virtual melting has been presented. The important outcomes of solid-solid phase transformations via intermediate melt have been discussed for HMX crystal. It is found out that two nano scale material parameters and solid-melt barrier term in the phase-field model significantly affect the mechanism of PTs, induces nontrivial scale effects, and changes PTs behaviours at the nano scale during virtual melting.

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Phase-field (PF) approach[1,2] has been widely used to captures various solid-solid phase transitions (PTs).[3–11] Lately, it has been discovered that the finite-width interface plays a crucial role in controlling PTs for the different material systems[12,13] such as PTs via intermediate molten state (IM) which has been observed experimentally hundreds of degrees below the thermodynamic melting temperature in HMX.[14,15] Such a transitional, metastable interface is called a virtual melt.[16–19] Additionally, it has been found that such virtual melt induces nontrivial scale effects, and changes phase transformation behaviours at the nanoscale.[20] Previously, a PF model was developed to describe solid-solid PT via IM in hyperspherical order parameter which is limited for n=3 phase-system.[20] More recently, a multiphase phase-field (MPF) theory has been proposed for generalized n phase-system to capture such intriguing PT mechanism during virtual melting.[21] This MPF model is thermodynamically consistent and satisfies all thermodynamic stability conditions.[21–24] One of the advantages of the MPF model is that, for each of the propagating solid-melt and solid-solid interfaces, the analytical solutions for width, energy, and velocity can be derived.[21,22,25] Thus, interface material properties can be fully calibrated and characterized for all interfaces. In the aforementioned MPF model, two dimension less parameters at the nanoscale [e.g., ratios of width and energy of two different interfaces, k_E (or Δ_ψ) and k_δ (or Δ_Γ)] can be explicitly defined and controlled during PT. These parameters significantly

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affect the formation and stability of virtual melt during solid-solid PT in HMX.[21–24] The MPF approach has been employed to investigate the appearance and corresponding thermodynamic, and structure of IM for a three-phase system.[22,24] Additionally, a detailed study on barrierless melt nucleationin HMX has been reported for propagating IM.[23] The kinematics and energetic of appearance of IM have been detailed.[25] It is found out that the nano scale material parameters and solid-melt barrier termin the MPF model significantly affect the mechanism of PTs, induces nontrivial scale effects, and changes PTs behaviours at the nano scale during virtual melting.[22,24,23,26]

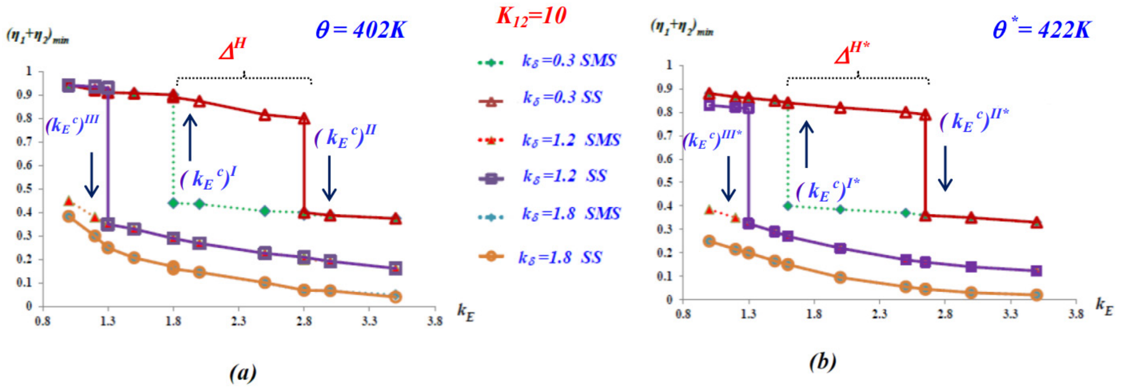

Fig.1: $(\eta_1 + \eta_2)_{min}$ has been shown as a function of k_E at (a) θ = 402 K and (b) θ^* = 422 K for K_{12} = 10^{10}J/m^3. Reprinted from[22] with the permission of AIP Publishing, 2021

In the above mentioned MPF model, order parameter's(η_i) evolution has been described by Ginzburg-Landau(G-L)equations,[21,22]

$$\frac{1}{L_{i0}}\frac{\partial \eta_i}{\partial t} = -\frac{\partial \psi^l}{\partial \eta_i} + \beta_{i0}\nabla^2\eta_i + \beta_{ij}\nabla^2\eta_j;\ ;\forall i \neq j;$$

where ψ^l is the local part of the Helmholtz free energy $\psi^\theta=\psi^l+\psi^\nabla$ (see[21,22] for detail). In Fig.1, different scale effects and non-trivial phase transformation mechanism has been observed when the influence of k_E (or Δ_ψ) which characterizes the energy of two different interfaces on the appearance and disordering of IM has been explored for two different non-equilibrium temperatures where $\xi_\phi=(\eta_1+\eta_2)_{min}$ indicates the disordering. For different critical values of k_E (i.e., k^C_E) and depending on the energy barrier of the solid-melt interface K_{12}(or $\Sigma_{\delta\beta}$), two different solutions exist for k_E <k^c_E For relatively low k_δ (or Δ_Γ):one is solid-melt-solid interface solution with high disordering of IM at the interface, and another one is solid-solid interface solution with lowd is ordering of IM at the interface. At first critical value $k_E=(k_E^c)^I$, jump occurs between solid-melt-solid initial condition(SMS) solution to less disordered IM solution. Whereas, at second critical value $k_E=(k_E^c)^{II}$, second jump occurs from solid-solid initial condition(SS) solution to high disordered IM solution. Hence, the solution of propagating inter facial melt can be either continuous-reversible without the hysteresis or jump-like first order discontinuous transformation with hysteresis. In Fig.2, the influence of temperature on the appearance of propagating interfacial melt has been explored where ξ_ϕ indicates the disordering. From the simulation results, it is clear that increasing temperature θ increases the disordering ξ_ϕ of inter facial melt for all Δ_ψ, Δ_Γ(or k_E, k_δ). For relatively small Δ_Γ, the solution of ξ_ϕ is continuous-reversible for both solid-melt-solid and solid-solid initial conditions. However, for relatively large Δ_Γ, one is a solid-melt-solid interface solution with a high disordering of IM at the interface during solidification and another one is a solid-solid interface solution with low disordering of IM at the interface during melting at some critical value of temperature. These two different solutions correspond to two different nanostructures that produce a" hysteretic region". From the numerical result, it is evident that the appearance of nucleated melt can form much below thermodynamic melting temperature and different Δ_ψ and Δ_Γ control the width of the temperature hysteresis curve and melt formation temperature. The appearance of such nontrivial multiple solutions of IM could not be captured by the simplified thermodynamic descriptions which did not consider interface width as a scale parameter (i.e., k_δ), thus, can only predict a single solution of IM and the formation of IM (or melt) can only possible for k_E>2 close to thermodynamic equilibrium melt temperature.

Summarizing, the numerical results from the MPF model indicate a new perspective of solid-solid PT via transitive virtual melt in HMX. The penalizing potential in MPF formalism significantly controls the existence of virtual melt by limiting the pure solid-solid interface solution in order parameter space. Hence, these two scale parameters and penalizing term K_{12} (or $\Sigma_{\delta\beta}$) influence the formation of virtual melt much below the thermodynamic melting temperature. The presented MPF model demonstrates the general applicability of this formalism to capture first-order jump-like PT as well as second-order continuous PTs. In addition, such MPF approach can be utilized to capture various PTs[27] such as martensitic PTs,[9–11,28–40] evolution of nano voids,[41–44] surface-induced melting,[45–47] grain boundary premelting,[48–53] interface modelling in composite,[55] and crack propagation,[56,57]

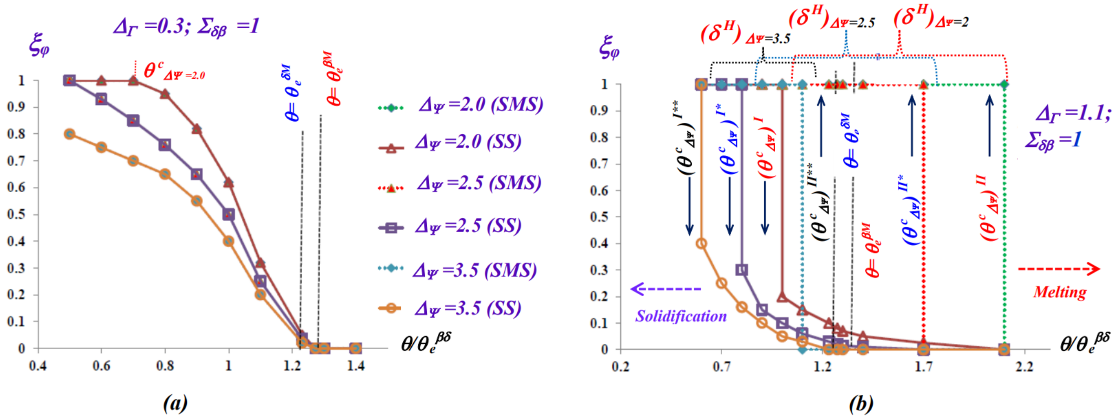

Fig. 2: (η_1 + η_2)$_{min}$ has been plotted as a function of θ for different Δ_Γ for $\Sigma_{\delta\beta}$ = 1. Reprinted from[23] with the permission of Elsevier, 2021

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Conflict of Interests

The authors declare no competing interests.

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