

Influence of nanoscale parameters on solid-solid phase transformation in Octogen crystal: multiple solution and temperature effect[1)]

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Phase-field (PF) approach [1, 2] has been widely used to captures various phase transitions (PTs) [3–10]. Recently, It has been realized that the finite width of the interface is an important aspect to discover new phenomena [11–14] and can be used to control PTs for different material system [15–19]. However, for most of the cases, such scale parameters have been ignored, and corresponding various scale effects and phenomena could not be studied systematically. In the present study, solid-solid PTs via interfacial molten phase have been considered where solid δ-Octogen (O_1) phase partially or completely melts and re-solidifies into solid β-Octogen (O_2) phase in a propagating solid-melt-solid interface [20–24] Since the transitional molten interface is metastable and temporary, that is why it is called as a virtual melt [17, 25–29]. During virtual melting, two different important dimensionless nanoscale parameters can be defined, e.g., ratios of width and energy of two different interfaces, $\xi_\delta = \delta^{21}/\delta^{s0}$ and $\xi_\Psi = \Psi^{21}/\Psi^{s0}$ which significantly affect the formation of interfacial melt in Octogen [30–32]. These nanoscale parameters ξ_Ψ and ξ_δ can be explicitly defined and easily controlled in our multiphase phase-field (MPF) theory [30–33]. In our current work, we have extended our previous parametric study [31, 32] for different range of nanoscale parameters (ξ_Ψ, ξ_δ) and a MPF parameter Υ_{12} characterizing the interaction of two solid-melt interfaces on the formation of propagating interfacial melt which reveals multiple solutions of barrierless nucleated melt nanostructure and nontrivial nanoscale effects.

Different scale effects and non-trivial phase transformation mechanism has been observed when the solution of Ω has been studied for nanoscale parameters ξ_Ψ and ξ_δ for broad range of non-equilibrium temperature as shown in Fig. 1. For different critical values of the parameters (i.e., ξ_Ψ and ξ_δ) and depending on the energy barrier of the solid-melt interface Υ_{12}, the appearance of propagating interfacial melt can be either continuous-reversible without the hysteresis or jump-like first-order discontinuous transformation with hysteresis.

Our MPF model and simulation results presents a new point of view on solid-solid phase transformation describing the transitive interfacial molten phase for Octogen crystal. The resulted interesting non-trivial evidence of the existence of molten layer in the solid-solid transition way below the melting temperature indicates the general applicability of our MPF model for the case of first-order-like solid-solid transformations and deposition. Additionally, this approach can be utlilized to capture PTs in metallic and amorphous systems [34–36] as well as grain-boundary melting [37–39]. Our developed approach is applicable to various PTs [40] such as surface-induced melting [41], martensitic PTs [42–44] and precipitate evolution [45] etc.

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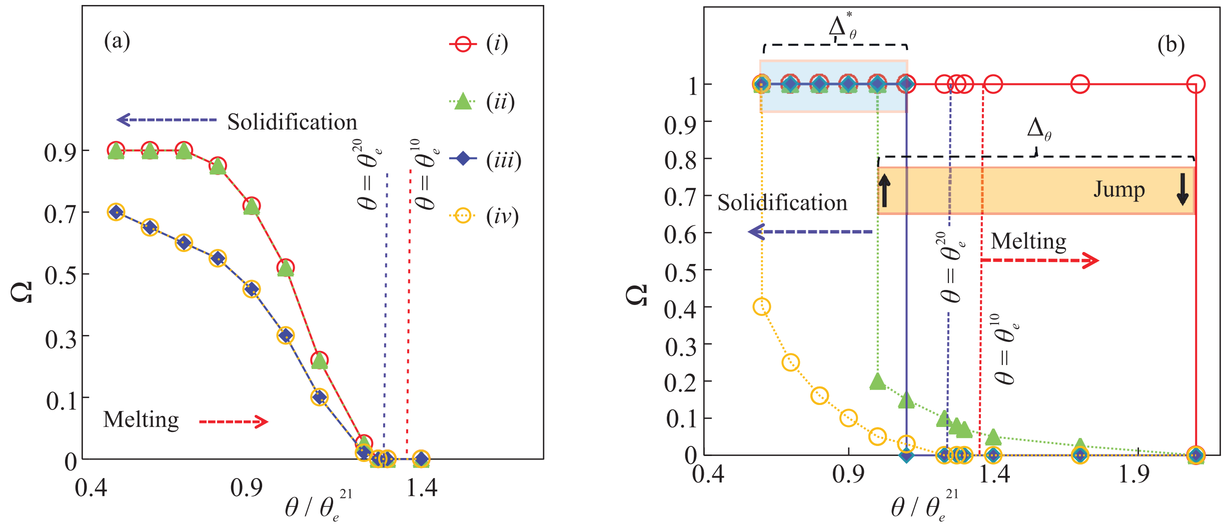

Fig. 1. (Color online) Stationary value of Ω is plotted as a function of θ/θ_e^{21} in the range $0.5 \leqslant \theta/\theta_e^{21} \leqslant 2.4$ for (a) – $\xi_\delta = 0.5$, $\Upsilon_{12} = 1$ and (b) – $\xi_\delta = 1.4$, $\Upsilon_{12} = 10$ for (i) $\xi_\Psi = 2.2$ ($O_1O_0O_2$), (ii) $\xi_\Psi = 2.2$ (O_1O_2), (iii) $\xi_\Psi = 3.7$ ($O_1O_0O_2$), and (iv) $\xi_\Psi = 3.7$ (O_1O_2). Continuous and reversible solution occurs for $\xi_\delta = 0.5$, $\Upsilon_{12} = 1$; while the solution for $\xi_\delta = 1.4$, $\Upsilon_{12} = 10$ represents jump-like first-order transformation with hysteresis loops. All the values of Υ_{12} are in kg/(nm.s^2)

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