Pis'ma v ZhETF, vol. 113, iss. 4, pp. 263 – 264 

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

*A. M. Roy*[2)]

*University of Michigan, Materials Science and Engineering, Ann Arbor, MI 48109, USA*

Submitted 25 November 2020
Resubmitted 30 December 2020
Accepted 11 January 2021

DOI: 10.31857/S1234567821040078

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 $\delta$-Octogen ($\mathsf{O}_1$) phase partially or completely melts and re-solidifies into solid $\beta$-Octogen ($\mathsf{O}_2$) 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 $\xi_\Psi$ and $\xi_\delta$ 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 ($\xi_\Psi$, $\xi_\delta$) and a MPF parameter $\Upsilon_{12}$ 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 $\Omega$ has been studied for nanoscale parameters $\xi_\Psi$ and $\xi_\delta$ for broad range of non-equilibrium temperature as shown in Fig. 1. For different critical values of the parameters (i.e., $\xi_\Psi$ and $\xi_\delta$) and depending on the energy barrier of the solid-melt interface $\Upsilon_{12}$, 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.

The support of LANL (Contract # 104321) and National Science Foundation (Grant # CMMI-0969143) are gratefully acknowledged. The author is grateful to Dr. V. I. Levitas from Iowa State University for his kind guidance and discussion.

Full text of the paper is published in JETP Letters journal. DOI: 10.1134/S0021364021040032

1. L. Q. Chen, Annu. Rev. Mater. Res. **32**, 113 (2002).
2. I. Steinbach, Model. Sim. Mat. Sci. Eng. **17**, 073001 (2009).
3. A. Artemev, Y. Jin, and A. G. Khachaturyan, Acta Mater. **49**, 1165 (2001).
4. A. Basak and V. I. Levitas, Acta Mater. **139**, 174 (2017).
5. V. I. Levitas, A. M. Roy, and D. L. Preston, Phys. Rev. B **88**, 054113 (2013).
6. A. M. Roy, JETP Lett. **112**, 173 (2020).
7. A. M. Roy, App. Phys. A **126**, 576 (2020).
8. V. I. Levitas and M. Javanbakht, Phys. Rev. B **86**, 140101 (2012).
9. A. Basak and V. I. Levitas, Appl. Phys. Lett. **112**, 201602 (2018).
10. V. I. Levitas and K. Samani, Phys. Rev. B **89**, 075427 (2014).

[1)] Supplementary materials are available for this article at DOI: 10.1134/S0021364021040032 and are accessible for authorized users.

[2)] e-mail: e-mail: arunabhr.umich@gmail.com

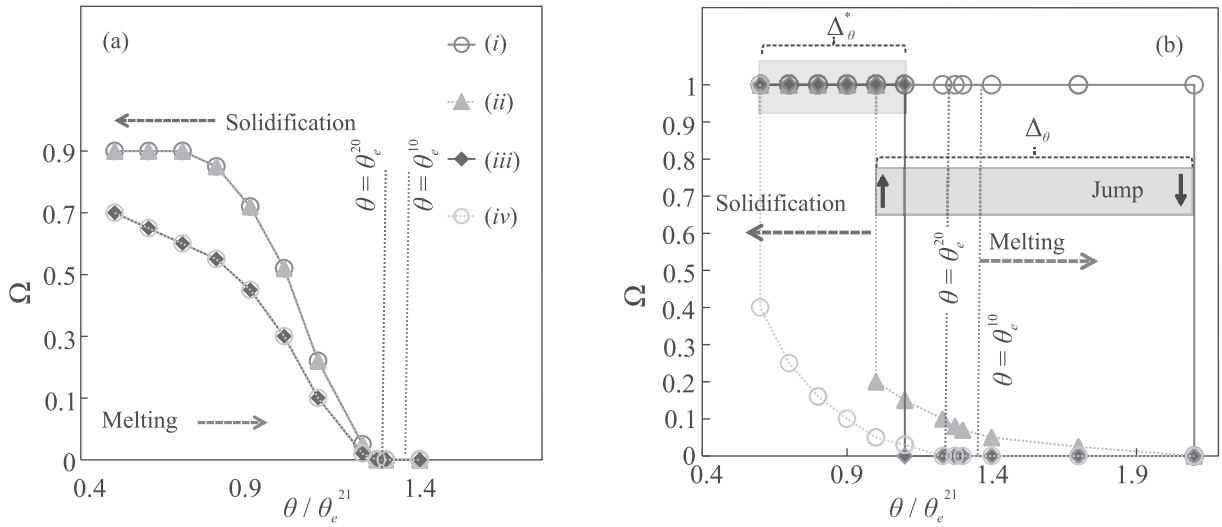


Fig. 1. (Color online) Stationary value of Ω is plotted as a function of $\theta/\theta_e^{21}$ in the range $0.5 \leqslant \theta/\theta_e^{21} \leqslant 2.4$ for (a) – $\xi_\delta = 0.5$, $\Upsilon_{12} = 1$ and (b) – $\xi_\delta = 1.4$, $\Upsilon_{12} = 10$ for (i) $\xi_\Psi = 2.2$ ($\mathsf{O}_1\mathsf{O}_0\mathsf{O}_2$), (ii) $\xi_\Psi = 2.2$ ($\mathsf{O}_1\mathsf{O}_2$), (iii) $\xi_\Psi = 3.7$ ($\mathsf{O}_1\mathsf{O}_0\mathsf{O}_2$), and (iv) $\xi_\Psi = 3.7$ ($\mathsf{O}_1\mathsf{O}_2$). 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 $\Upsilon_{12}$ are in kg/(nm.s$^2$)


11. V. I. Levitas, Scr. Mater. **149**, 155 (2018).
12. V. I. Levitas and K. Samani, Nat. Commun. **2**, 1 (2011).
13. V. I. Levitas and M. Javanbakht, Phys. Rev. Lett. **107**, 175701 (2011).
14. A. Basak and V. I. Levitas, J. Mech. Phy. Sol. **113**, 162 (2018).
15. M. A. Caldwell, R. D. Jeyasingh, H. P. Wong, and D. J. Milliron, Nanoscale **4**, 4382 (2012).
16. S. Sinha-Ray, R. P. Sahu, and A. L. Yarin, Soft Matter **7**, 8823 (2011).
17. V. I. Levitas, Z. Ren, Y. Zeng, Z. Zhang, and G. Han, Phys. Rev. B **85**, 220104(R) (2012).
18. V. I. Levitas, Philos. Trans. R. Soc. A **371**, 20120215 (2013).
19. V. I. Levitas, B. F. Henson, L. B. Smilowitz, D. K. Zerkle, and B. W. Asay, J. Appl. Phys. **102**, 113502 (2007).
20. V. I. Levitas, B. F. Henson, L. B. Smilowitz, and B. W. Asay, Phys. Rev. Lett. **92**, 235702 (2004).
21. V. I. Levitas, B. F. Henson, L. B. Smilowitz, and B. W. Asay, Phys. Chem. B **20**, 10105 (2006).
22. B. F. Henson, L. B. Smilowitz, B. W. Asay, and P. M. Dickson, J. Chem. Phys. **117**, 3780 (2002).
23. L. B. Smilowitz, B. F. Henson, B. W. Asay, and P. M. Dickson, J. Chem. Phys. **117**, 3789 (2002).
24. P. Bowlan, B. F. Henson, L. Smilowitz, V. I. Levitas, N. Suvorova, and D. Oschwald, J. Chem. Phys. **150**, 064705 (2019).
25. S. L. Randzio and A. J. Kutner, Phys. Chem. B **112**, 1435 (2008).
26. V. I. Levitas, Phys. Rev. Lett. **95**, 075701 (2005).
27. V. I. Levitas and R. Ravelo, Proc. Natl. Acad. Sci. USA **109**, 13204 (2012).
28. P. Ball, Nature Mater. **11**, 747 (2012).
29. Y. Peng, F. Wang, Z. Wang, A. M. Alsayed, Z. Zhang, A. G. Yodh, and Y. Han, Nature Mater. **14**, 101 (2015).
30. V. I. Levitas and A. M. Roy, Acta Mater. **105**, 244 (2016).
31. A. M. Roy, J. Appl. Phys. **129**, 025103 (2021); doi: 10.1063/5.0025867.
32. A. M. Roy, Materialia **15**, 101000 (2021); doi:10.1016/j.mtla.2021.101000.
33. V. I. Levitas and A. M. Roy, Phys. Rev. B **91**, 174109 (2015).
34. J. Luo, CRC Crit. Rev. Solid State **32**, 67 (2007).
35. J. Luo and Y.-M. Chiang, Annu. Rev. Mater. Res. **38**, 227 (2008).
36. M. Baram, D. Chatain, and W. D. Kaplan, Science **332**, 206 (2011).
37. M. Tang, W. C. Carter, and R. M. Canon, Phys. Rev. B **73**, 024102 (2006).
38. T. W. Heo, S. Bhattacharyya, and L.-Q. Chen, Acta Mater. **59**, 7800 (20011).
39. J. Mellenthin, A. Karma, and M. Plapp, Phys. Rev. B **78**, 184110 (2008).
40. V. I. Levitas, Int. J. Plasticity **102914** (2020); DOI: 10.1016/j.ijplas.2020.102914.
41. V. I. Levitas and K. Samani, Phys. Rev. B **84**, 140103 (2011).
42. V. I. Levitas and M. Javanbakht, Phys. Rev. Lett. **105**, 165701 (2010).
43. A. M. Roy, Mat. Sci. Res. India **17**, 03-06 Special Issue (2020).
44. A. M. Roy, *Doctoral dissertation*, **14635**, Iowa State University, Ames (2015).
45. E. Solomon, A. Natarajan, A. M. Roy, V. Sundararaghavan, A. van der Ven, and E. Marquis, Acta Mater. **166**, 148 (2019).