Abstract Submitted
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Application of the Phase-Field Crystal Model for Quantitative Materials Modeling[1] TAPIO ALA-NISSILA, Helsinki Univ. of Tech., Finland — The recently proposed Phase-Field Crystal (PFC) model [1] can be used to model materials on microscopic length but diffusive time scales. The model can be related to the classical density functional theory of liquids [2] allowing modeling of solidification, phase segregation, grain growth, elastic and plastic deformations in anisotropic systems with multiple crystal orientations. In this talk, I will discuss recent progress on using the PFC model and its extensions to describe quantitative modeling of selected properties of BCC Fe [3].

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[2] K.R. Elder, Nikolas Provatas, Joel Berry, Peter Stefanovic, and Martin Grant, Phys. Rev. B **75**, 064107 (2007).
[3] A. Jaatinen, C. V. Achim, K. R. Elder, and T. Ala-Nissila, Phys. Rev. E **80**, 031602 (2009).

[1]Work done in collaboration with: C. Achim, K.R. Elder, L. Granasy, E. Granato, A. Jaatinen, M. Karttunen, and S.-C. Ying.

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