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Comparison of the Phase Field Crystal Free Energy Functional and the Second Order Density Functional Theory of Freezing AKUSTI JAATINEN, CRISTIAN ACHIM, JARI JALKANEN, TAPIO ALA-NISSILA, Laboratory of Physics, Helsinki University of Technology, Espoo, Finland, KEN ELDER, Department of Physics, Oakland University, Rochester, Michigan, USA — We present a numerical study of the recently established connection between the phenomenological free energy functional of the phase field crystal model (PFC) and the second-order density functional theory of freezing (DFT) [1]. We have used liquid state structural data of iron and copper near their melting points to study their freezing properties by both DFT and PFC functionals. The results obtained by the two functionals differ from each other significantly, DFT being superior to PFC in predicting crystal structures, density profiles and coexistence densities. We conclude that the fitting procedure outlined in [1] does not provide quantitatively accurate predictions of phase diagrams. [1] K. R. Elder, N. Provatas, J. Berry, P. Stefanovic and M. Grant, Phys. Rev. B 75, 064107 (2007)

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