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Development of Phase-Field Crystal model free energy functionals based on molecular dynamics D.M. NICHOLSON, Oak Ridge National Lab, J.A. DANTZIG, Univ. of Illinois, SARMA GORTI, Oak Ridge Natioanl Lab, BALA RANHAKRISHNAN, Oak Ridge National Lab, D.D. JOHNSON, Ames Lab — The Phase-Field Crystal (PFC) model represents the density as a continuous function, whose spatial distribution evolves in time at diffusional, rather than vibrational time scales. PFC provides a tool to study defect interactions at the atomistic level but over longer time scales than those achievable with MD. We examine the behavior of the PFC model with the goal of relating the PFC parameters to physical parameters for Fe and Mo, derived from molecular dynamics (MD) simulations (using either classical force fields or on density-functioanl-theory-based Hellmann-Feynman forces). MD and PFC results for diffusion rates, energy and volumes of fusion, and melting points as a function ofvacancy concentration are used to validate free energy functionals used in the PFC model. Acknowledgments: This work was supported by the Center for Defect Physics, an Energy Frontier Research Center funded by the US Department of Energy, Office of Science, Office of Basic Energy Sciences.

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