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Coupling of Atomistic and Meso-scale Phase-field Modeling of Rapid Solidification[1] J. BELAK, P.E.A. TURCHI, M.R. DORR, D.F. RICHARDS, J.-L. FATTEBERT, M.E. WICKETT, F.H. STREITZ, M. TANG, N. MOELANS, Lawrence Livermore National Laboratory — Recently, phase-field models have been introduced to model the crystallography during polycrystal microstructure evolution [1,2]. Here, we assess these models with molecular dynamics and phase-field simulations that overlap in time and space. Large parallel computers have enabled MD simulations of sufficient scale to observe the formation of realistic microstructure during pressure driven solidification [3]. We compare the two methods by calculating the phase field order parameter (quaternion) from the atomic coordinates and drive the evolution with the MD. Results will be presented for the solidification of tantalum. [1] R. Kobayashi and J.A. Warren, Physica A, **356**, 127-132 (2005). [2] T. Pusztai, G. Bortel and L. Granasy, Europhys. Lett, 71, 131-137 (2005). [3] F. H. Streitz, J. N. Glosli, and M. V. Patel, Phys. Rev. Lett. 96, 225701 (2006).

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