Abstract Submitted
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Towards a kinetics model for dynamically driven liquid-solid transitions built from atomistic simulations[1] LORIN X. BENEDICT, LUIS ZEPEDA-RUIZ, TOMORR HAXHIMALI, SEBASTIEN HAMEL, JON L. BELOF, Lawrence Livermore National Laboratory — We discuss the development of a kinetics model for the liquid-to-solid transition in Cu as modeled by the Mishin et al. EAM Cu potential [1]. Starting from a determination of the multiphase EOS of this system, and a series of MD simulations in which solidification was observed by quenching and pressurizing at various rates, we describe our initial attempts to fit a kinetics model to be used in continuum simulations. The phenomena of nucleation and growth of the fcc phase, as well as the appearance and effects of bcc wetting layers, are discussed. This work is performed under the auspices of the U. S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

[1] Y. Mishin et al., Phys. Rev. B vol.63, 224106 (2001).

[1]Phase Transition Kinetics Program

Lorin Benedict
Lawrence Livermore National Laboratory

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