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Non-equilibrium Molecular Dynamics simulations of Cu solidification LUIS ZEPEDA-RUIZ, BABAK SADIGH, JON BELOF, Lawrence Livermore National Laboratory — The development of predictive theories for the study of non-equilibrium phase transitions occurring in dynamic materials processes, such as shocks, requires a multi-scale approach that spans from the atomistic to the continuum scale. For this purpose, we present results of Non-equilibrium Molecular Dynamics (NEMD) simulations of solidification of Cu from the melt for both, thermal cooling and compression conditions. Our simulations show a transition from spinodal-like to nucleation-dominated phase transition as a function of both cooling and compression rates. In addition, the appearance and evolution of different Cu phases are presented. This work is performed under the auspices of the U. S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

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