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Pressure Induced Solidification of Ta and Cu: A Comparison
DAVID RICHARDS, JAMES GLOSLI, FREDERICK STREITZ, Lawrence Livermore Natl Lab — Using powerful computers such as Blue Gene/L it is now possible to use classical molecular dynamics to simulate pressure induced solidification at size scales that are free of finite size effects. We present a comparison of the nucleation, growth, and coalescence of clusters during pressure induced solidification in large scale MD simulations of liquid Ta and Cu. We extract growth and nucleation rates from our simulations, as well as cluster size distributions that can be compared against the predictions of simple models. This work 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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