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Modeling Rapid Resolidification of Ta on BlueGene/L FREDERICK H. STREITZ, MEHUL V. PATEL, JAMES N. GLOSLI, Lawrence Livermore National Laboratory — We investigate the rapid, pressure-induced solidification of molten Ta using the ddcMD code on BlueGene/L. Access to this massively parallel computer (the world's largest) has enabled us to investigate solidification at a size scale which is unprecedented - we will directly compare results obtained from simulations ranging from 64,000 atoms to over 16 million atoms. Solidification is indeed found to be "rapid," occuring on a time scale of 100 ps in these simulations before grain coalescence occurs and a coarsening process begins. Finite size effects apparent in simulations of less than 1 million atoms had a dramatic impact on not only the final microstructure but on the the approach to final microstucture as well, even at early times. These results punctuate the need for very large simulations to explore the resolidification process.

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