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Simulations of Rapid Solidification in Metals at High Pressure¹

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Although computer simulation has played a central role in the study of nucleation and growth since the earliest molecular dynamics simulations almost 50 years ago, confusion surrounding the effect of finite size on such simulations have limited their applicability. Modeling molten tantalum in systems ranging from 64,000 to 131,072,000 atoms on the BlueGene/L computer, I will discuss the first atomistic simulations of solidification that demonstrate independence from finite size effects during the entire nucleation and growth process, up to the onset of coarsening. Using both our new results and historical data, we show that the observed maximal grain sizes for systems smaller than about 8,000,000 atoms are functions of the simulation size, following the predictions of finite size scaling theory. For larger simulations, a crossover from finite size scaling to more physical size-independent behavior is observed.

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