

Abstract Submitted  
for the MAR05 Meeting of  
The American Physical Society

**Rapid pressure-induced solidification of molten metals** MEHUL PATEL, FREDERICK STREITZ, Lawrence Livermore National Laboratory — The process in which a molten metal subjected to sudden pressurization transforms into a solid is studied by large scale molecular dynamics simulations. Specifically, copper and tantalum are modeled as prototypical fcc and bcc metals. Copper interactions are described by an EAM potential, while tantalum is described with a more sophisticated MGPT potential including up to 4-body interactions. Questions about the structure of the final solidified state as well as the mechanisms (ie, metastable intermediaries) involved in getting there are answered by these atomistic simulations, and recent algorithmic and computational advances have allowed for studies of increasing system sizes and simulation times. In particular, the effects of varying physical parameters such as the magnitude and rate of pressurization on the total solidification time will be discussed.

Work performed under the auspices of the U.S. DOE at the University of California/Lawrence Livermore National Laboratory under contract W-7405-ENG-48

Mehul Patel  
Lawrence Livermore National Laboratory

Date submitted: 05 Dec 2004

Electronic form version 1.4