Joint 20th AIRAPT - 43th EHPRG, June 27 - July 1, Karlsruhe/Germany 2005

Molecular dynamics simulations of pressure-induced solidification

Mehul V. Patel and Frederick H. Streitz,
Lawrence Livermore National Laboratory, Livermore, CA, U.S.A,
mehul@llnl.gov

Molten metals subjected to rapid pressurization may undergo a phase transition to a solid phase if the final conditions are chosen appropriately. Specifically, the details of the final structure and the time scales for arriving at that structure should depend on the final magnitude and rate of pressurization. We study these dependencies using large scale atomistic modeling of copper (fcc prototype) and tantalum (bcc prototype). Results of many simulations on copper, modeled using a embedded-atom potential, allow us to construct a time-presssure-transition plot that shows the sensitive dependence of the solidification time on the final pressure. For, Ta, a more complex MGPT potential including up to 4 body interactions is required to adequately capture the d-electron bonding, and the presense of energetically competitive phases in this case results in extended solidification times.

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.