Abstract Submitted
for the 4CF07 Meeting of
The American Physical Society

How does a crystal melt? SHENG-NIAN LUO, Los Alamos National Lab, QI AN, Univ. Sci. Tech. China, LIANQING ZHENG, Florida State Univ. — Melting is one of the most important yet poorly understood phenomena. Nucleation and growth of melt play a key role in melting processes, and occur at sub-ns and sub-ns scales which essentially preclude direct observation of the initial stages of melting. Inherent defects also complicates the whole process. An indispensable first step is to understand the melting of an initially defect and surface free solid, namely, homogeneous nucleation. A natural tool to decipher the physics of melting is molecular dynamics simulations on a simple system. We have conducted such simulations on Cu described by an accurate embedded atom method potential on system sizes ranging from 10^3 to 10^6 atoms. The structural evolution of the system is characterized with local and global order parameters, and the evolution of liquid, with cluster analysis. The size distribution of liquid nuclei is thus quantified for a single run. As fluctuations are ubiquitous and critical for phase transitions, we adopt the mean first passage time method to obtain statistically from 100 MD runs the critical nucleus size, Zeldovich factor and steady state nucleation rate. The nucleation and growth of melt, with the aid of fluctuations, are demonstrated by the simulations; classical nucleation theory can describe the nucleation process with reasonable accuracy, if the solid−liquid interface is properly considered. We also present shock wave induced melting of Cu single crystals.

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Date submitted: 10 Sep 2007 Electronic form version 1.4