Abstract Submitted
for the SHOCK13 Meeting of
The American Physical Society

Embedded atom model for tin and MD simulation of tin shock loading and melting FILIPP SAPOZHNIKOV, GENNADY IONOV, VLADIMIR DREMOV, RFNC-VNIITF, Snezhinsk, Russia, LAURENT SOULARD, CEA/DAM, France — The goal of the work was to develop an interatomic potential, that can be used in large-scale classical MD simulations to predict tin properties near the melting curve, the melting curve itself, and the kinetics of melting and solidification when shock and ramp loading. According to phase diagram, shocked tin melts from bcc-phase, and since the main objective was to investigate melting, the EAM was parameterized for bcc-phase. The EAM was optimized using isothermal compression data (experimental at T=300K and ab initio at T=0K for bcc, fcc, bct structures), experimental and QMD data on the Hugoniot and on the melting at elevated pressures. The Hugoniostat calculations centered at β-tin at ambient conditions showed that the calculated Hugoniot is in good agreement with experimental and QMD data above β-BCT transition pressure. A series of calculations of overcooled liquid in pressure range corresponding to bcc-phase showed crystallization into bcc-phase. Since the principal Hugoniot of tin originates from the β-tin that is not described by this EAM the special initial state of bcc samples was constructed to perform large-scale MD simulations of shock loading.

Filipp Sapozhnikov
RFNC-VNIITF, Snezhinsk, Russia

Date submitted: 07 Feb 2013 Electronic form version 1.4