Abstract Submitted
for the SHOCK11 Meeting of
The American Physical Society

Melting property of Mo at high pressure ZHANG GONGMU, LIU HAIFENG, SONG HAIFENG, DUAN SUQING, ZHAO XIANGENG, Institute of Applied Physics and Computation Mathematics — DAC experiments showed Mo is stable in a bcc structure up to the pressure of at least 500 GPa at normal temperature . Shock wave experiment identified the first transition at 200GPa as that of bcc to a new solid phase(perhaps fcc). We conducted ab initio molecular dynamics simulations to reveal the effect of different solid structures for melting temperature. We use three methods: Z method, single phase method and two phase coexistence MD simulation, the simulations at different volumes and atoms arranged initially in an ideal bcc or fcc lattice. The Z method and two phase MD method can avoid superheating. The results show that the melting temperature of bcc solid is higher than fcc about 500K-1000K, the Z method and two phase MD simulation describe the two mechanisms (homogeneous and heterogeneous) of melting but with the same melt temperatures ,which are lower than single phase method about 10%, this result indicates that melting mechanisms don't impact the melting temperature in equilibrium melting. Our melting curve is substantially higher than the one determined in diamond anvil cell experiments, agree with the shock wave measurement.

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Date submitted: 02 Feb 2011 Electronic form version 1.4