Abstract Submitted
for the SHOCK17 Meeting of
The American Physical Society

Application of the ab initio Z method to the melting of Al and Mg

SHAILESH MEHTA, AWE — Density functional theory based molecular dynamics has been used to investigate the accuracy of the Z method. The melt curve of Al is calculated to 3 Mbar and found to be in very good agreement with experiment. This is in contrast to a previous ab initio Z method calculation and an explanation is put forward to explain the failure of other work to achieve satisfactory agreement. Results will also be shown on work being performed to calculate the hcp-bcc-liquid triple point of Mg, by locating the intersection of the hcp and bcc melt curves.

Shailesh Mehta
AWE

Date submitted: 22 Feb 2017 Electronic form version 1.4