Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Anisotropic shock response of single crystal titanium: Molecular dynamics investigation ANUPAM NEOGI, NILANJAN MITRA, Indian Institute of Technology Kharagpur — A comprehensive atomistic simulation study has been done to investigate anisotropic shock response of single crystal α Ti upto 350 GPa of shock pressure. Details characterization of the shocked microstructure, including hexagonal closed packed α-to-ω martensitic phase transformation, has been done from mechanistic perspective by analyzing radial distribution function, neighbor based structural identification, x-ray diffraction etc. Four different interatomic potentials, Finnis-Sinclair (FS) many-body potential, embedded atom method (EAM) potential, 2NN-MEAM potential and spline-based modified embedded atom method (MEAM) potential, has been chosen to explore the capability, accuracy and applicability of these interatomic potentials for typical dynamic shock study i.e. in high pressure applications.

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Date submitted: 22 Nov 2016 Electronic form version 1.4