

Abstract Submitted
for the SHOCK15 Meeting of
The American Physical Society

Molecular dynamic study of Shock wave response of bulk amorphous polyvinyl chloride: effect of chain length and force field ANUPAM NEOGI, NILANJAN MITRA, Indian Institute of Technology Kharagpur — Atomistic molecular dynamics in conjunction with multi-scale shock technique is utilized to investigate shock wave response of bulk amorphous polyvinyl chloride. Dependence of chain length on physical and mechanical behaviour of polymeric material at ambient condition of temperature and pressure are well known but unknown for extreme conditions. Non-reactive force fields PCFF, COMPASS and PCFF+ were used to determine applicability of the force field for the study of the material subjected to shock loads. Several samples of PVC with various chain lengths were subjected to a range of shock compression from 1.5-10.0 km/s. Even though dependence of chain length was observed for lower shock strengths but was not for intense shock loads. The principle Hugoniot points, calculated by applying hydrostatic Rankine-Hugoniot equations and as well as multi-scale shock technique, were compared against LASL experimental shock data, demonstrating superior performance of PCFF+ force-field over PCFF and COMPASS. Shock induced melting characteristic and vibrational spectroscopic study were conducted and compared with experimental data to observe differences in response with relation to different force fields, chain length of the material for different shock intensities.

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Date submitted: 30 Jan 2015

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