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A molecular dynamic investigation for shock induced phase transition of water NILANJAN MITRA, ANUPAM NEOGI, Indian Institute of Technology Kharagpur — Atomistic equilibrium molecular dynamics (EMD) was carried out to investigate shock induced phase transition of bulk liquid water. Multi-scale shock technique (MSST) was utilized to investigate low ($U_S = 2.5km/s$) to strong ($U_S = 6.5km/s$) intensity shock response on an extended flexible three point model up to 100 ns. The thermodynamic pathway of phase transition from liquid water to ice VII was investigated using temporal variation of thermodynamic state variables, power spectrum analyses of O-H bond vibration along with temporal evolution of pair correlation function between O-O, O-H and H-H atoms. Static structure factor along with pair-distribution function extended up to 20 Å was calculated and compared against the ideal ice VII to get information regarding long range ordering. Bragg reflection at different crystal planes were evaluated to investigate percentage of crystallinity of the shocked sample. Specific questions answered in this work involves: What is the exact time frame after the passage of shock at certain intensity in which nucleation of solid phase can be observed? Is it a complete or partial phase transition? Are external nucleators essential for this transformation? What is the percentage of crystallinity of the nucleated phase?

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