

Abstract Submitted
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Sound velocity in shock compressed molybdenum obtained by ab initio molecular dynamics TYMOFIY LUKINOV, ANATOLY BELONOSHKO, Royal Inst of Tech, SERGEY SIMAK, Linkping University — The sound velocity of Mo along the Hugoniot adiabat is calculated from first principles using density-functional theory based molecular dynamics. These data are compared to the sound velocity as measured in recent experiments. The theoretical and experimental Hugoniot and sound velocities are in very good agreement up to pressures of 210 GPa and temperatures of 3700 K on the Hugoniot. However, above that point the experiment and theory diverge. This implies that Mo undergoes a phase transition at about the same point. Considering that the melting point of Mo is likely much higher at that pressure, the related change in the sound velocity in experiment can be ascribed to a solid-solid transition.

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