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Structure of Molybdenum Under Dynamic Compression to 1 TPa

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— Molybdenum (Mo) is a refractory 4d transition metal that is widely used as a standard in static and dynamic high-pressure experiments. However, there are significant unanswered questions and unresolved discrepancies about the melting curve and high-pressure phase stability of this fundamental material. Similar questions surround the melting curve and phase stabilities of other transition metals including Ta and Fe, and so a better understanding of Mo has broad implications for high-pressure science and geophysics. Here we use x-ray diffraction to determine the crystal structure of molybdenum under both shock and ramp compression to pressures as high as 1 TPa. Under shock loading, we find that Mo remains in body centered cubic (BCC) structure until melting begins at near 390 GPa. Our results are in good agreement with recent theoretical calculations and recent re-measurement of sound speeds along the Hugoniot. We also carried out x-ray diffraction measurements of ramp-loaded molybdenum up to 1050 GPa. Our x-ray diffraction patterns are consistent with the persistence of the BCC phase up to the highest pressure achieved. The measured densities under ramp loading are intermediate between those achieved under shock compression and those expected from extrapolation of room-temperature data. We do not observe evidence for the theoretically predicted transition to face centered cubic or double hexagonal close packed phases above 600 GPa.

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