Abstract Submitted
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No solid-solid phase transition in Mo before melting: experiment and theory[1] XIULU ZHANG, Laboratory for Shock Wave and Detonation Physics Research, IFP, CAEP, ZHONGLI LIU, College of Physics and Electric Information, LYNU, KE JIN, FENG XI, YUYING YU, YE TAN, CHENGDA DAI, LINGCANG CAI, Laboratory for Shock Wave and Detonation Physics Research, IFP, CAEP — Whether there is a solid-solid phase transition plays an important role in shaping the phase diagram of Mo. Previous sound velocity measurements suggested one at 210 GPa[Phys. Rev. Lett. 62, 637(1989)], but the latest results [J. Nguyen, et al., In Shock Compression of Condensed Matter-2011] did not support it. In our work, adopting the "reverse impact" method[J. Geophys. Res. 100(B1), 529 (1995)] and the "overtake" method[Rev. Sci. Instrum. 53, 245(1982)], we obtained new data in the pressure range from 38 GPa to 160 GPa. Together with the latest results, it can be concluded that a solid-solid phase transition does not occur in Mo under shock loading pressures from 38 GPa to 240 GPa. With the crystal structure prediction techniques based on the genetic algorithms and density functional theory calculations, two metastable structures C2m and I4mmm are found, but we did not reproduce fcc phase of Mo in our searches. As their energy is much higher than that of bcc Mo, it is unlikely that they are more stable than bcc Mo at high temperatures. This is consistent with C. Cazorla's conclusion that fcc is less stable than bcc[Phys. Rev. B 85, 064113(2012)], and theoretically support the conclusion of our sound velocity measurements.

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