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In situ high pressure-temperature synchrotron XRD study of Mo with laser-heated diamond anvil cells QIANG ZHOU, XIAOLI HUANG, FANGFEI LI, BINGBING LIU, TIAN CUI, National Lab of Superhard Materials, YUE MENG, HPCAT, APS, NATIONAL LAB OF SUPERHARD MATERIALS COLLABORATION, HPCAT, APS COLLABORATION — In order to understand the behavior of materials at high pressure and high temperature, it is important to have a precise knowledge of pressure (P) -volume (V) -temperature (T) relationship. In this paper, Mo is studied by an integrated technique of diamond anvil cell, laser-heated and synchrotron XRD technologies, providing experimental insight into its behavior at high pressure and temperature. We have measured the cold compression of Mo with the neon pressure media up to 77 GPa, and its thermal expansion up to 94 GPa and 3470 K. The third-order Birch–Murnaghan EoS of Mo at room temperature can be fitted with K_0 =267 GPa, K_0'=3.4, with V_0 =31.32 Å^3. High temperature data have been treated with both thermodynamic and Mie–Grüneisen-Debye methods for the thermal EoS inversion. The results are self-consistent and in agreement with those obtained by previous theoretical data. The crystal structure of Mo is determined up to 94 GPa and 3470 K and no evidence for the predicted transition to a close-packed face-centered cubic (fcc) phase is found.

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