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Formation of Molybdenum Deuteride at High Pressure: A Neutron Diffraction Study

The locations and occupancies of deuterium atoms in molybdenum deuteride were studied using time-of-flight neutron powder diffraction under pressures up to ~ 6.2 GPa. The sample was synthesised in situ by reacting molybdenum powder with deuterium gas, introduced via an offline high-pressure gas-loading technique, and compressed using a Paris–Edinburgh press. Above ~ 4 GPa, diffraction data revealed the formation of a hexagonal deuteride phase. We confirmed the $P6_3/mmc$ symmetry and determined the over-stoichiometric deuterium content to give a composition of $\text{MoD}_{1.15}$, showing that our data are highly sensitive to deuterium positions and occupancies. The refined atomic positions and interatomic distances provide insight into D–Mo interactions and the origin of non-stoichiometry.

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