X-Ray Diffraction at Multi-Megabar Conditions

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Magnesium (Mg) is known to transition from its equilibrium hexagonal-close-packed (hcp) structure to a body-centred cubic (bcc) structure between 45 and 60 GPa [1], with several high-pressure phases predicted above the bcc phase including face-centred cubic [2], simple cubic [3] and simple hexagonal [3]. The latter two are predicted to be electride phases and, as such, the experimental observation of them would be of particular value to future DFT calculations and other theoretical investigations. The aim of this experiment was to statically compress Mg above 2 Mbar in order to either verify or contradict the theoretical results, and in doing so inform future studies of light elements at extreme conditions.

Two diamond anvil cells were prepared with magnesium foil and the pressure was determined from the copper x-ray diffraction signal and its equation of state [4]. We were able to compress magnesium to a V/V_0 of 0.33 at a pressure of 3.11 Mbar which constitutes a significant extension of the explored pressure range as shown in **Error! Reference source not found.** Analysis of the diffraction data is still ongoing, however it appears that magnesium remains in the *bcc* phase up to at least 3.11 Mbar.



Figure 1. The atomic volume of Mg as a function of pressure to 3.11 Mbar (311 GPa) at 300 K. Data from this experiment's two cells are plotted as crosses. Only the bcc phase was studied since our previous investigation in Ref. 1 already mapped the hcp phase. The data from Ref. 1 are plotted as filled symbols, with filled squares showing data in the hcp phase and filled diamonds showing the bcc phase. The dashed line is a proposed equation of state fitted to the bcc phase using the Birch-Murnaghan formalism, which gave K₀=32.5 GPa, and K²=3.99.

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References

- [1] Stinton et al., PRB 2014, 90, 13.
- [2] Li et al., J. Phys. Chem. C 2010, 114, 49.
- [3] Pickard & Needs, Nat. Mater. 2010, 9, 8.
- [4] Sokolova et al., Comput. Geosci. 2016, 94, 162.