Diffraction Studies of Phase Transitions and Strength in Vanadium

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The structural behaviour of vanadium (V) on compression is unique amongst the elements. Static compression studies have observed a subtle bcc-to-rhombohedral transition at ~30-60 GPa, depending on the hydrostaticity of the experiment [1,2]. This transition was confirmed by first principle calculations, which also predicted further transitions at 120 GPa and 280 GPa (at 0 K) to further phases [3,4]. The bcc-to-rhombohedral transition in V arises from a shear instability due to phonon softening, resulting in discontinuities in the elastic constants (including the shear modulus) across the transition [3-6]. This unusual behaviour of the shear modulus has an impact on the pressure dependence of V's strength. Diamond anvil cell (DAC) measurements to 90 GPa have shown that the shear strength of V first increases with pressure up to around 40–50 GPa, and then decreases on further compression [7]. Furthermore, the most recent finite-temperature computational study has predicted that the strength of V will increase with increasing T due to unusual hardening of the shear modulus C44 with T [5].

A recent series of shock-compression experiments on V between 32 GPa and 88 GPa [8], which did not utilise x-ray diffraction, suggested there was evidence of a phase transition starting at 32 GPa and completing at 60 GPa, but, in striking contrast to the DAC results, the strength of the rhombohedral phase above 60 GPa was reported to be higher than that of the bcc phase. Diffraction studies of shocked V on the Orion laser, utilising a plasma x-ray source, have found the strength to be near zero at ~30 GPa [9]. However, it was not possible to determine the strength at higher pressures and temperatures, and it is still unknown, therefore, how the material strength is affected by the bcc-rhombohedral transition.

In vanadium, there is a lack of consensus in literature of the conditions under which the bcc-to-rhombohedral transition occurs, with no direct observation of the reported transition under dynamic compression. Furthermore, there are no published refinements of diffraction data from vanadium above 30 GPa.

Dynamic compression of vanadium foil was carried out using laser-driven-shock-waves at the LCLS XFEL, and we saw little evidence of a transition occurring between 30-60 GPa along the principal Hugoniot. Static compression studies of vanadium foil, powder and single crystals were carried out under both hydrostatic and non-hydrostatic conditions at the Diamond Light Source, ESRF and PETRA synchrotrons. The static studies have suggested that the peak splitting that had previously been used to identify this transition at 30-60 GPa may have arisen from integrating non-circular Debye-Scherrer (D-S) rings distorted by the effects of sample strength rather than from a phase transition. Our recent work on single crystal compression of V hopes to definitively identify and refine the structure of V. These results, coupled with our other foil and powder measurements, aid our understanding of strength effects in V and decouple them from any observed transition, along with comparing the behaviour of V under both static and dynamic compression

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[1] Ding *et al*, PRL **98**, 085502 (2007).
[2] Jenei *et al*, PRB **83**, 054101 (2011).
[3] Lee *et al*, PRB **75**, 180101 (2007).
[4] Lee *et al*, PRB **77**, 134105 (2008).
[5] Wang *et al*, Sci. Reports **6**, 32419 (2016).
[6] Antonangeli *et al*, Sci. Reports **6**, 31887 (2016).
[7] Klepeis *et al*, PRB **81**, 134107 (2010).
[8] Yu *et al*, Appl. Phys. Lett. **105**, 201910 (2014).
[9] Foster *et al*, J. Appl. Phys **122**, 025117 (2017).