

Structural study of the Wadsley-type vanadium oxides V₂O₅ and V₆O₁₃ at extreme conditions

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The so-called Wadsley phases with the general formula V_nO_{2n+1} form a homologous series of compounds [1]–[3]. They have arisen much interest due to the observed metal-insulator transitions and their potential application as battery materials. [4]–[7] The crystal structures of the parent compound V₂O₅ and of V₆O₁₃ ($n=3$) at ambient conditions are closely related.

We have now studied single crystals of V₂O₅ and V₆O₁₃ as a function of pressure at Petra III, DESY. Our study [8] shows a complete irreversible amorphization of the α -V₂O₅ sample above 7.3 GPa. Further investigation of the HP-HT behaviour of α -V₂O₅ was performed at the large volume press at ID06 at the ESRF, where we followed the evolution of the sample with *in-situ* synchrotron radiation. Heating of the amorphous phase led to the formation of the δ -V₂O₅ polymorph with Sb₂O₅ structure, which can be recovered at ambient conditions. High-pressure single-crystal diffraction experiments α -V₆O₁₃ show an anomalous behaviour between 2 and 3 GPa, yet the ambient pressure polymorph seems to be stable up to the highest pressures reached in the experiment.

Furthermore, we performed low-temperature single-crystal X-ray diffraction experiments on α -V₆O₁₃. Our data allow for a conclusive determination of the crystal structure below the metal-to-insulator transition, especially as this structure has long been disputed [9], [10]. Additionally, we have detected a structural phase transition associated with antiferromagnetic (AFM) ordering at 55 K.

References

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