MS27-2-9 Crystal structures of V_2O_5 and V_6O_{13} at high pressures: implications for the Wadsley phase family behaviour under extreme conditions
#MS27-2-9

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Abstract
The so-called *Wadsley* phases with 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 V_2O_5 and of V_6O_{13} (n=3) at ambient conditions are closely related, especially if we assume sixfold coordination of vanadium in an α-V_2O_5 with one V-O distance being longer. The crystal structures of the α-V_2O_5 (space group *Pmmn*) and α-V_6O_{13} (space group *C*2/*m*) polymorphs can be described as built of single layers and alternating layers of single and double layers of VO_6 polyhedra respectively. [8,9]
We have now studied single crystals of V_2O_5 and V_6O_{13} as a function of pressure at Petra III, DESY. Our study [10] shows a complete irreversible amorphization of the α-V_2O_5 sample above 7.3 GPa. Further investigation of the HP-HT behaviour of α-V_2O_5 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-V_2O_5 polymorph with Sb_2O_5 structure, which can be recovered at ambient conditions. High-pressure single crystal diffraction experiments α-V_6O_{13} 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.
Opposed to the ambient polymorph, the δ-V_2O_5 polymorph, which crystallizes from the amorphous material, consists of only double layers of VO_6 polyhedra. This configuration is similar to the one of a metastable VO_2(B). [11] Comparing higher stability of the hybrid single-double layered α-V_6O_{13} to the single layered structure of α-V_2O_5 which collapses under pressure, we propose that the binary oxides in the *Wadsley* series would tend to transform to the stable double-layer like configuration of the VO_2(B) type at extreme conditions. [10] This hypothesis requires further confirmation by performing HP measurements on V_6O_{13} at higher than previously attained pressures as well as closer investigation of the other members of the *Wadsley* series.

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