Single Crystal Studies of the Incommensurate Composite Structure of Rb-IV
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A number of elements have recently been shown to have a composite incommensurate high pressure phase. This phase has a so-called 'host-guest' structure type comprising a tetragonal 'host' framework with channels along the fourfold c axis. Within these channels are 1D chains of atoms that form a 'guest' structure that is incommensurate with the host. We have observed host-guest structures in the alkali and alkaline-earth metals Rb, Sr, Ba, and in the group Va elements Bi, Sb and As [1]. Among these elements Rb is unique in having a 16-atom host structure, and transition to a disordered phase comprising liquid-like guest chains [2].

The 1D guest chains in Rb-IV are more than 7 Å apart [3], and this raises the question as to the nature of the host-chain and chain-chain interactions in the ordered phase, and how this interaction weakens or vanishes at the transition to the disordered phase. The strength of the host-chain interaction can be inferred from the intensity of the hklm modulation reflections. Although these extremely weak reflections could not be detected with the powder techniques used previously to determine the structure of Rb-IV [3], they should be detectable using single crystal methods. In this talk I will present new results on the full modulated structure of Rb-IV using x-ray diffraction data collected from high quality single crystals of Rb-IV at ~18GPa.


Keywords: rubidium, incommensurate composite structure, high-pressure crystallography