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Low Pressure Synchrotron X-ray Powder Diffraction of Cu_{5-x}M_xSbO₆ (M = Cr, Mn, W)

The large crystallographic and chemical diversity of copper-based metal oxides is one of their highlighting features and cause for pursuit into copper based material research. An interesting feature seen in copper based metal oxides is the coexistence of different copper oxidation states, in different crystallographic positions, within the same compound [1-3]. This can lead to a mixture of magnetically active Cu2+ and magnetically inactive Cu1+ within the same compound, with different structural motifs. One interesting compound that demonstrates this coexistence of mixed copper oxidation states is Cu5SbO6, which crystallises in a modified delafossite structure type (CuFeO2) [4]. Here, the magnetically active brucite-like CuO2 layer was diluted in an ordered fashion with non-magnetic Sb5+. These layers were separated by linearly coordinated, magnetically inactive Cu1+. Rietveld refinements on a range of preparation temperatures revealed a low-temperature (LT) and high-temperature modification (HT) phase transition. This is related to an ordering (HT)/disordering (LT) effect of the Sb5+/Cu2+ brucite-like layers between the Cu1+ ions. Substituting the Cu2+ or Sb5+ in the layers with other transition metals (Cr, Mn, W) could present interesting changes to the properties of the material, and potentially influence the ordered/disordered stacking of the layers.
By using solid-state Raman spectroscopy, we could show that this structure displayed a pressure-induced phase transition at room temperature for the ordered modification, which was not observed for the disordered modification. Lowering the pressure from ambient down to 20 mbar showed phonon modes at about 700 cm-1 and 550 cm-1 disappeared almost completely. Neutron powder diffraction experiments were conducted at atmospheric and low pressure on both ordered and disordered modifications. On analysis of the neutron diffraction patterns, we could show a very small shift in the reflections, and thus changes in the unit cell parameters, for the ordered modification, while these shifts were not observed for the disordered modification. These shifts should also be observed in synchrotron powder diffraction patterns. Therefore, we investigated the nature of this phase transition with variable pressure synchrotron X-ray powder diffraction.

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