	Experiment title: Strucutral modifications and magneto-striction in the 1-dimensional charge ordered phase of Yb_4As_3	Experiment number: HE 1171
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Report:

Electronic charge localization leading to metal-insulator type of phase transitions has attracted great interest in the past. A particular interesting material is Yb_4As_3, where a first order charge order transition is observed at approximately 290K. The charge order in Yb_4As_3 leads to a structural phase transition from cubic ($I\bar{4}3d$) at ambient temperatures to hexagonal; R3c symmetry below T_{CO}. At ambient temperatures, chemical considerations assuming As^{3-} lead to an intermediate valence of Yb of 2.25. In this work we have performed a detailed structural investigation of Yb_4As_3 with high-resolution powder diffraction. The information on the temperature dependence of the inter-atomic positions has been used to calculate the bond lengths and bond valence sums.

The temperature dependence of the lattice constants a and c are continuously increase at low temperatures but there is a significant change in the behavior at approximately 250K. Around this temperature, the lattice constant a exhibits a turnover and decreases again for increasing temperatures, whereas c starts to

increase even stronger so that the temperature dependence of the unit cell volume is roughly linear. The local structure of the Yb along the [111] direction is shown in Fig. 1. There is a threefold symmetry along the [111] direction, but no longer along the former body diagonals of the cube [-1 1 1], [1 –1 1], and [1 1 –1] as the Yb(2) ions do no longer have any site symmetry. There are six As neighbors to Yb(1) for which three of them with equal distance build a triangle around the [111] directions. Those two triangles are rotated to each other by an irregular angle of 38.5°, which is an important structural behavior significantly affecting the one-dimensional magnetic properties of the material. There are two times three equal Yb(1)-As bonds. For the other former body diagonals of the cube, the Yb(2) ions have six different Yb(2)-As(1-6) bond lengths, but again three of them have a similar size. Its temperature dependence is shown in figure 2. The average bond length of each triple are both longer by 0.09 Å between the Yb(2)-As compared to those of the Yb(1)-As, indicating the different valence states of the Yb ions.

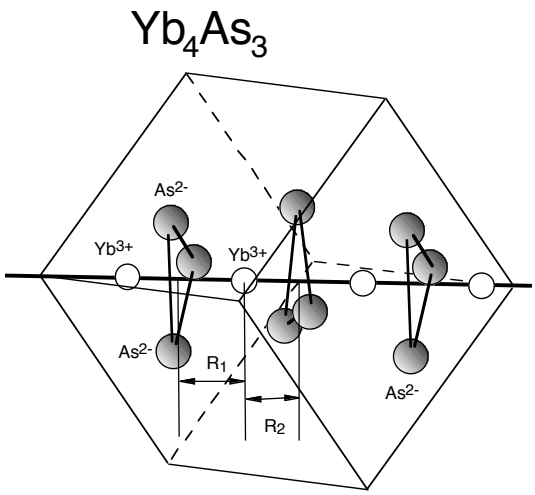

Fig. 1 Local structure along the body diagonal of the Yb^{3+} chain.

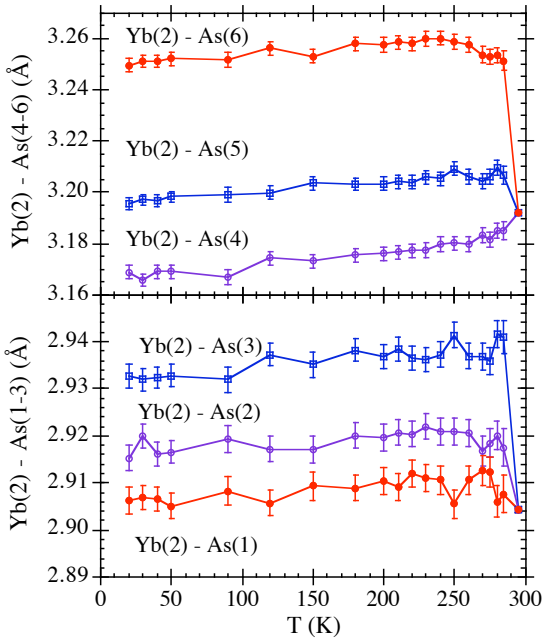

Fig. 2 Yb-As bond lengths of the divalent Yb ions