Partially-disordered structure of quasi one-dimensional conductor Tb_3RuO_7

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Introduction

A series of Ln_3RuO_7 crystals composed of trivalent lanthanide and pentavalent transition metal Ru oxides is structurally characterized by the presence of infinite single chains of corner-linked RuO_6 octahedra embedded in the matrix of Mn and O atoms. The series shows a polymorphism. Single crystals of Tb_3RuO_7 were grown by the flux method and the structure was investigated at room temperature by the single-crystal synchrotron X-ray diffraction.

Experimental

Reagent powders of Tb_4O_7, RuO_2 and $SrCl_2$ were mixed together in the molar ratio of 7.5:10:90 and put into a platinum crucible of $25cm^3$ and heated at 1373K in air for 10 hrs. The sample was then cooled at 5K/hr to 973K followed by a discharge in ambient conditions. The sample batch was washed by warm water to dissolve flux. Single-crystal diffraction data were collected using synchrotron X-rays of 0.6886Å at the Photon Factory Tsukuba.

Results and Discussion

Presence of residual electrons near the Tb5 atom position in the figure suggested a positional disorder of the atom. Similar topography was obtained for Tb6. The least-squares refinement, assuming split atom models for Tb5 and Tb6, yielded a final R_F value of 0.018 for 7559 independent reflections. Eight and six percents of Tb atoms are slightly displaced from the regular Tb5 and Tb6 positions by 0.323(5) and 0.395(6)Å, respectively.

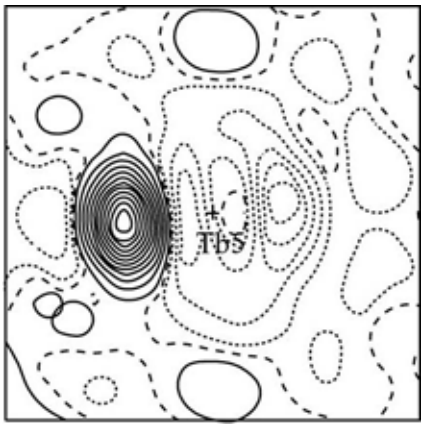

FIGURE: The difference Fourier map of Tb_3RuO_7 assuming a single atom model for Tb5 (2.0 e/Å^{-3} contour intervals, 2.1x2.1 Å^2 section perpendicular to *a*).

Biographical Sketch

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