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Structure-related thermoelectric properties of $SrNbO_{3.4}$

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Introduction

Low-dimensional materials has a potential to be good thermoelectrics owing to their reduced thermal conductivity by phonon scattering and the enhanced thermopower by steep change in density of states at the Fermi level. We have studied quasi-one-dimensional (Q1D) Hollandite $Ba_{1.2}Rh_8O_{16}$ and found large power factor of 30 $\mu W/cmK^2$ at 75 K comparing with that seen in Na_xCoO_2 at 300 K [1].

$SrNbO_{3.4}$ with $Nb^{4.8+}$ ($4d^{0.2}$) is known to be a good Q1D conductor [2]. $SrNbO_{3.4}$ (n=5) belongs to homologous series of $Sr_nNb_nO_{3n+2}$, and is derived from the three-dimensional network of $SrNbO_3$ perovskite structure by separating the NbO_6 octahedra parallel to the (110) planes and introducing additional oxygen. (see the inset of Fig. 1) We have grown single crystals of $SrNbO_{3.4}$ and investigated structure-related thermoelectric properties performing synchrotron x-ray diffraction measurement.

Experiments

High-quality single crytals of $SrNbO_{3.4}$ were grown by a traveling solvent floating zone method with a growth velocity of 10 mm/h in a mixed gas flow of Ar(97%) and H_2(3%) with 0.2 l/min. Large single crystals with a typical dimension of 5mm*5mm*1mm were successfully grown. Synchrotron powder x-ray diffraction measurements with wavelength of 0.7749 Å were carried out at the BL-8A at the Photon Factory, KEK, controlling the temperature from 80 to 300 K, and the structural refinements were performed by Rietveld analysis (RIETAN-FP).

The resistivity was measured by a four-probe method in a liquid He cryostat. Gold wires were carefully attached to the sample using silver paste (DuPont4922) as electrodes. The thermopower was measured using a steady-state technique in a liquid He cryostat with copper-constantan thermocouple to detect a small temperature gradient of about 1 K/cm.

Results and Discussion

As shown in Fig. 1, synchrotron x-ray diffraction pattern of ground single crystal was well fitted by orthorhombic symmetry ($Pnnm$, Int. Tables: A-58-1) with lattice parameters of a=3.988 Å, b=5.676 Å, and c=32.467 Å.

Fig. 2(a) shows the temperature dependence of the resistivity. The magnitude is found to be 7, 110, and 840 mΩcm for the *a*, *b*, and *c* axes, respectively showing the anisotropy of ~15 in the *ab* plane. The thermopower along *b* axis is -150 μV/K, which is one order of magnitude larger than those of -15 and -25 μV/K along *a* and *c* axes. In particular, the anisotropy in the thermopower appears at around 100 K, which relates to change of activation energy of the resistivity shown in Fig. 2(a). We observed a small modification of NbO_6 octahedra at around 100 K, which causes a dimensional crossover from higher-dimensional to quasi-one-dimensional electronic structure in $SrNbO_{3.4}$ [3].

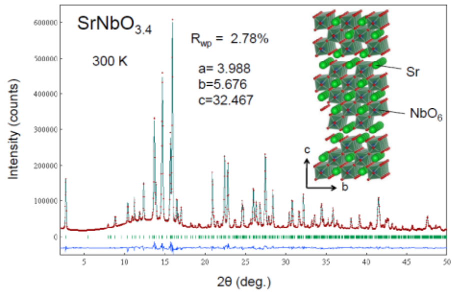

Fig. 1: X-ray powder diffraction pattern of $SrNbO_{3.4}$ at 300 K

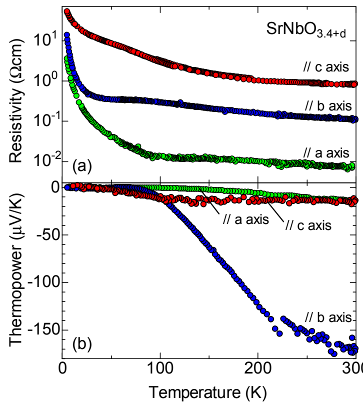

Fig. 2: (a) Resistivity and (b) thermopower of $SrNbO_{3.4}$

References

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