C6-12-P07

Thermoelectric Properties of $MnSi_{\sim 1.73}$ Produced by Cold Pressing and Sintering

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It is well known that $MnSi_{\sim 1.73}$ is a p-type thermoelectric semiconductor with high heat resistance and high anti-oxidation properties. Dimensionless figure of merit of the material is 0.4, which is two times greater than that of a p-type $FeSi_2$. Practical use of $MnSi_{\sim 1.73}$, however, has been limited, as the sintered body can be produced only by the costly hot-pressing technique. The authors have already reported a low cost process to produce the $FeSi_2$ with higher relative density than 90% by using the cold-pressing and sintering. Recently, $MnSi_{\sim 1.73}$ sintered bodies with higher relative density than 90% have successfully been produced by that technique in our laboratory. The figure of merit of the material at room temperature is comparable to that of sintered bodies produced by the conventional hot-pressing technique.

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Crystal structure, electric and magnetic properties in Na_xCoO_2

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Recent discovery of large thermoelectric power in single crystal Na_xCoO_2 has stimulated broad interest in application of p-type thermoelectric devices. In this study, we investigated crystal structure, electric and magnetic properties in polycrystalline samples of Na_xCoO_2. The crystal structures were analyzed using a Rietveld analysis program RIETAN-2000 based upon the x-ray and neutron diffraction patterns. The electron density distributions at room temperature were visualized by an elaborate method, which is a combination of the maximum entropy method (MEM) and the Rietveld refinement. The four-probe dc resistivity and magnetic susceptibility were measured using a home made device and a SQUID magnetometer (MPMS) as a function of temperature, respectively. Recently, an anomaly temperature was reported in the temperature dependence of resistivity for x = 0.55, 0.65 and 0.75 samples by Motohashi *et al.* In particular, x = 0.75 was confirmed the existence of the first-order phase transition. In contrast, we found the change of crystal structure between x = 0.79 and 0.85 samples at room temperature. This means that the crystal structures of x = 0.85 or x > 0.85 samples at room temperature are in the low temperature phase which was revealed by Tojo *et al.*

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Thermoeletcric Properties of $Y_2Mo_2O_7$-Based Pyrochlore Solid-Solutions

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The effects of the composition of $Y_{2-x}M_xMo_{2-y}M'_yO_7$ (M = La, Ca, M' = Ti) on the Seebeck constant and the electrical conductivity were investigated for pyrochlore-type solid solutions. The substitution of La^{3+} for Y^{3+} increased the electrical conductivity, which was attributed to the enlargement of the lattice constant. A part of Y^{3+} was substituted with Ca^{2+}, and a part of Mo^{4+} was substituted with Ti^{4+} in the hope that a decrease in the carrier concentration should increase the Seebeck coefficient. The substitution of Ca2+ increased both Seebeck doefficient and the electrical conductivity. The substitution of Ti^{4+} increased the Seebeck coefficient but too much substitution deteriorates the electrical conductivity. The highest power factor obtained was $2.3x10^{-5}$W/Km for $Y_{1.8}Ca_{0.2}Mo_2O_7$ at 500-550K.

C6-12-P10

Negative Thermopower Induced by Spin-Entropy Backflow

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Since in 1997 the high thermoelectric performance was discovered in the layered Co oxide $NaCo_2O_4$, the strongly correlated electron systems are studied extensively as a possible candidate for thermoelectric materials. $NaCo_2O_4$ is a p-type thermoelectric oxide and there are no n-type thermoelectric oxides comparable with $NaCo_2O_4$. Therefore we tried to make an n-type thermoelectric oxide in the strongly correlated electron systems. In this system, the thermopower in high-temperature limit is expressed as $Q = -k_B/e \cdot \ln \{(g_a/g_b) \cdot y/(1-y)\}$ by Koshibae *et al.* where g_a, g_b represents the degeneracy of the a and b ions, respectively and y represents the concentration of b ion. We can obtain a negative thermopower through the term of $-k_B/e \cdot \ln (g_a/g_b)$ in a hole-doped system if $g_a > g_b$. We synthesized $Ca(Mn_{3-x}Cu_x)Mn_4O_{12}$ in which a hole is doped by the substitution Cu for Mn. For x=1, Mn^{3+}:Mn^{4+}=1:1 is realized, where $-k_B/e \cdot \ln (g_a/g_b)$ is expected to be –79 V/K. The thermopower is observed to be –32 V/K at 955 K, which is qualitatively consistent with the theoretical prediction. This negative thermopower is caused by a mechanism that the net spin entropy flows along the opposite direction of the hole current. This "entropy-backflow" mechanism can make the thermopower of hole-doped conductor negative.