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Transport Properties of $NaCuO_2$ Thermoelectric Material

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Abstract: ***We synthesized a thermoelectric material $NaCuO_2$ by taking analytical grade NaO and CuO in stoichiometric ratio by solid state reaction method at 1173K. Morphological and Compositional Analysis were carried by SEM and EDAX. Thermopower, Electrical and Thermal Conductivity measurements were carried from room temperature to 773K. SEM analysis showed that the sample is polycrystalline, with small but well-formed crystals. EDAX profile confirmed stoichiometry of the sample. It was observed that Thermopower increases from 175μV/K to 250μV/K with the increase of temperature from 350k to 700k. Electrical conductivity measurements revealed that conductivity varies from 10^{-3} to $6x10^{-3}$ $\Omega^{-1}cm^{-1}$ and activation energy increases from 0.17eV to 0.47eV. Thermal conductivity measurements confirmed that it is independent of temperature and found to be 7.656 w/m-k. The figure of merit found to be 1.5 at room temperature, which indicates that $NaCuO_2$ is suitable as thermoelectric material. For better understanding of the nature of $NaCuO_2$ as thermoelectric material, it is proposed to carry compositional studies, optical and dielectric studies.***

Keywords: EDAX, composition, electrical conductivity, figure of merit, oxides, SEM, thermal conductivity

1. Introduction

Thermoelectrics as a field has been attracting increasing attention in recent years. Thermoelectrics are perhaps the simplest technology for direct thermal to electric energy conversion and can be used in both refrigeration and power generation devices. The current interest is stimulated in large measure by energy applications, where efficiency is a key parameter. The efficiency of thermoelectric devices is characterized by a material-dependent figure of merit $ZT = S^2\sigma T/\kappa$, where T is the temperature, S is the Seebeck coefficient or thermopower, σ is the electrical conductivity, and κ is the thermal conductivity, including both the electronic and lattice contributions. Currently, the most widely used thermoelectric materials are conventional "heavy-metal-based" semiconductor alloys, including Bi_2Te_3 [1]-[3] and PbTe [4]-[8] with *ZT* values of 1~2. Although the high *ZT* values in these systems make them attractive as thermoelectrics, there are potential supply issues with Te and the use of Pb is unattractive in certain applications due to toxicity. It therefore remains of interest to find non-toxic thermoelectrics based on abundant elements, provided that these new materials also have high performance. Metal oxides provide one potential avenue for this. Here we discuss p-type oxides based on divalent Cu. Cupric oxide is a p-type material with indirect bandgap of 1.2eV(experimental) (9) and 1eV (theoretical) (10). Many theoretical studies using density functional theory indicate that producing n – type conductivity by doping in CuO is almost impossible, sodium doping should act as p-type dopant (11).

In particular, [4] one needs a combination of high conductivity and high thermopower and [5] one needs high conductivity and low lattice thermal conductivity. It has long been understood that optimization plays a critical role. In particular, as was emphasized long ago by Ioffe [4] the carrier concentration needs to be optimized in order to obtain the best balance between thermopower and conductivity in a given semiconductor system. With such optimization, a variety of materials with ZT ~ 1 have been discovered over the years. With this in view The present investigation was undertaken to study the dc electrical conductivity, thermopower and thermal conductivity as a function of temperature for $NaCuO_2$.

2. Objectives

- Synthesis of $NaCuO_2$ by solid state method.
- Study of Morphology and Transport properties of the prepared sample.

3. Experimental Details

3.1 Synthesis of $NaCuO_2$

Polycrystalline sample of $NaCuO_2$ was prepared by solid-state reaction method explained elsewhere. Highly pure NaO and CuO were used in the preparation of the present samples. The mixtures were calcined at 1173K for 12 hours in air. The temperature was slowly increased (10^0C/min) from room temperature to 1173K. The product was finely ground, pressed into pellets using a high pressure hydraulic press and the pellets were sintered at 1273K for 2 hours in muffle furnace

3.2 Morphology Studies

SEM and EDAX studies were carried using JEOL J. SM-35 Scanning Electron Microscope.

3.3 Transport Properties

The electrical conductivity was measured by two probe method from 300K to 700K using conductivity setup from Pushpa Scientifics, Hyderabad. Thermo emf measurements were carried using thermoelectric measurement setup from Pushpa Scientifics, Hyderabad. Thermal conductivity measurements were carried by TK04 from Thermophysical Instruments, Germany.

4. Results and Discussion

Figure 1 shows the SEM micrograph at two magnifications of the prepared sample. EDAX profile is shown in figure 2.

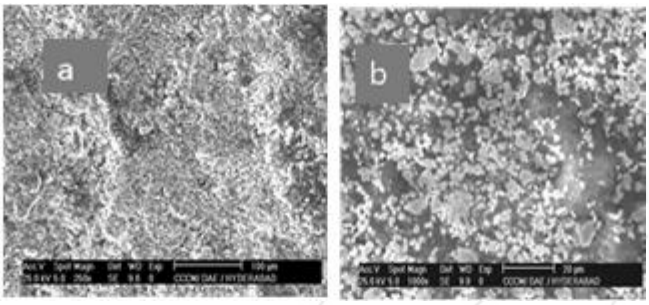

Figure 1: SEM photograph of $NaCuO_2$ a) with 250 magnification b) with 1000 magnification

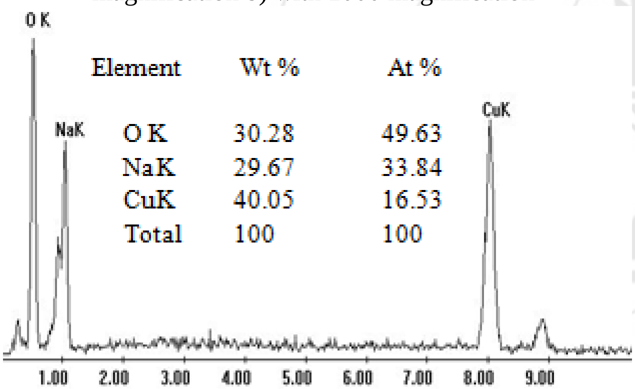

Figure 2: EDAX profile of $NaCuO_2$. Inset indicates the atomic ratios of Na, Cu and O_2.

Formation of particles is clearly seen from the two SEM micrographs. It is observed from these micrographs that the particles are well dispersed, dense and uniform. Average grain size found to be 0.6µm. The EDAX profile indicates that the compound is stoichiometric. It is also evident that the grains are random in shape, size and orientation. SEM analysis showed that the sample is polycrystalline, with small but well-formed crystals.

Temperature variation of Conductivity (σ) of $NaCuO_2$ is depicted in Figure 3. The inset depicts the temperature variation of ln σ from which activation energy was calculated. Temperature dependence of Thermopower (Seebeck Coefficient) S and Charge Carrier density (n) is illustrated in figure 4 and figure 5 respectively. It was found that conductivity increases with temperature from 10^{-3} to $6x10^{-3}\,\Omega^{-1}.cm^{-1}$.

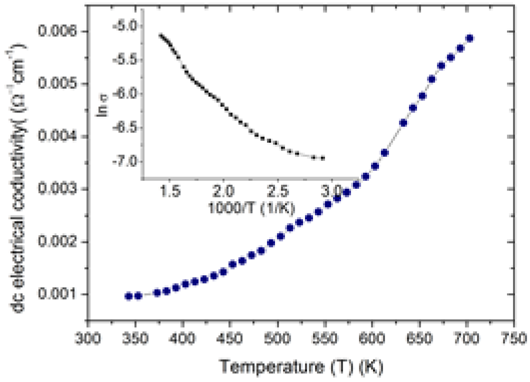

Figure 3: Temperature variation of conductivity (σ) of $NaCuO_2$. Inset shows lnσ v/s 1000/T.

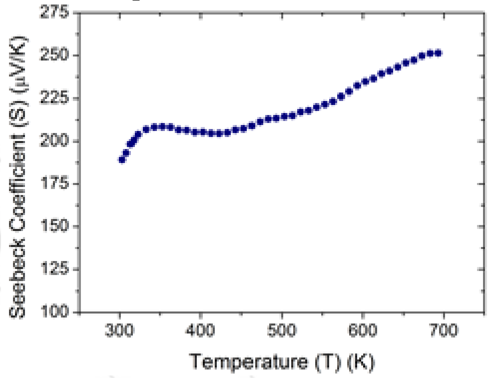

Figure 4: Temperature variation of Thermopower (S) of $NaCuO_2$

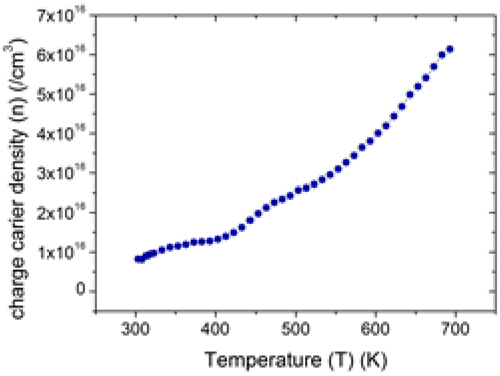

Figure 5: SEM photograph of $NaCuO_2$ a) with 250 magnification b) with 1000 magnification.

P J M Isherwood etal [14] found that Sodium-doped films showed resistivities four orders of magnitude lower than pure CuO, demonstrating that sodium is an effective dopant for CuO. They observed that addition of oxygen to the deposition environment reduces the resistivity at an oxygen partial pressure of $6.2x10^{-2}$ Pa and further increase in oxygen partial pressure causes a slight increase in resistivity. Density functional theory modelling of CuO has shown both of Oxygen and Na addition to be shallow acceptor states, meaning that they both contribute to an increased charge carrier concentration. This is evident from the increase in charge carrier density with temperature as shown in figure 5. The activation energy was found to increase from 0.1eV to 0.47eVas temperature increases. From figure 4 it is clear that Thermopower increased from 175 to 250µV/K with temperature. Positive thermopower confirms that the charge carriers are holes and the sample has p-type conductivity.

From figure 5 it is evident that the charge density increased from $1x10^{16}$ to $7x10^{16}$ /cc. The low resistivity and high thermopower of this material may be due to the interaction of lattice with the charge carriers. Estimation of mobility and compositional studies throw light on the effect of Na doping on CuO. From thermal conductivity measurements it was observed that it is independent of temperature and found to be 7.656 W/m-K. The figure of merit of NaCuO2 as estimated using the equation 1 and found to be 1.5.

$$ZT = \frac{S^2 \sigma T}{k} \quad (1)$$

Where ZT is the figure of the sample. 'S' is Thermopower, 'σ' is Electrical Conductivity, 'T' is absolute Temperature and 'k' Thermal Conductivity.

5. Conclusions

Stoichiometric $NaCuO_2$ as prepared by solid state method and carried surface morphology, electrical conductivity, thermal conductivity and thermopower studies. Morphology studies confirmed the formation of Stoichiometric and polycrystalline $NaCuO_2$. Thermal conductivity, Electrical Conductivity and Thermopower measurements revealed that it has good capability as thermoelectric material with figure of merit of 1.5. For better understanding of the nature of NaCuO2 as thermoelectric material it is proposed to carry compositional studies, optical and dielectric studies.

6. Acknowledgements

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