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Thermoelectric Properties of Cu-Filled Chevrel-Phase Sulfides

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Abstract –Cu-filled Chevrel-phase sulfides $Cu_xMo_6S_8$ have been prepared by reacting appropriate amounts of Cu, Mo, and MoS_2 powders and subjecting the resulting product to pressure-assisted sintering. The Seebeck coefficient, electrical resistivity, and thermal conductivity measurements have been made on the sintered samples in compositional range $2.0 \le x \le 4.0$ between 300 and 950 K. The sintered samples had a large positive Seebeck coefficient, low electrical resistivity, and low thermal conductivity. The thermoelectric properties can be improved with an increase in the Cu content. The highest dimensionless thermoelectric figure of merit *ZT* of 0.4 was found in $Cu_{4.0}Mo_6S_8$ at 950 K.

Ternary molybdenum chalcogenides with the general formula $M_xMo_6X_8$ (M = metal, X = S, Se, Te), called Chevrel phases [1], have received considerable attention as potential high-temperature thermoelectric materials. The host structure of a Chevrel phase consists of a stacking of Mo_6X_8 clusters. The M atoms fill the space between the Mo_6X_8 clusters. Caillat *et al.* [2] reported dimensionless thermoelectric figure of merit *ZT* in excess of 0.6 at 1150 K in $Cu_{1.38}Fe_{0.66}Mo_6Se_8$. Since Chevrel-phase chalcogenides have similarity in the electrical and thermal properties, the Chevrel-phase sulfides are also expected to have excellent high-temperature thermoelectric properties. Therefore, the purpose of this study was to investigate the thermoelectric properties of $Cu_xMo_6S_8$ to determine their potential as high-temperature thermoelectric materials. In this presentation, we report the effect of Cu content on their thermoelectric properties.

The samples were prepared by mixing and reacting appropriate amounts of Cu, Mo, and MoS_2 powders at 1273–1523 K for 8 h in vacuum. The resulting powders were then consolidated by pressure-assisted sintering. The sintering was conducted at 1223–1473 K for 1h under a uniaxial pressure of 30 MPa in vacuum. The density of all the sintered samples was greater than 95% of the theoretical density. The Seebeck coefficient, electrical resistivity, and thermal conductivity of the sintered samples have been measured over the temperature range from 300 and 950 K.

X-ray analysis showed that all the sintered samples consisted entirely of the hexagonal Chevrel phase. The value of the lattice parameters *a* and *c* increased with the Cu content. The thermoelectric properties vary with Cu content as shown in Fig. 1. All the sintered samples have a positive Seebeck coefficient. Moreover, they show metal-like behavior: the Seebeck coefficient and the electrical resistivity increase linearly with temperature. The thermal conductivity is low, ranging from 1.3 to 3.9 W K^{-1} m^{-1}. An important finding here is that the chemical composition has a marked effect on the thermoelectric properties. As Cu content increases, the Seebeck coefficient and electrical resistivity increase while the thermal conductivity decreases. As a result, the *ZT* value increases with the Cu content. The highest *ZT* of 0.4 was found in $Cu_{4.0}Mo_6S_8$ at 950 K.

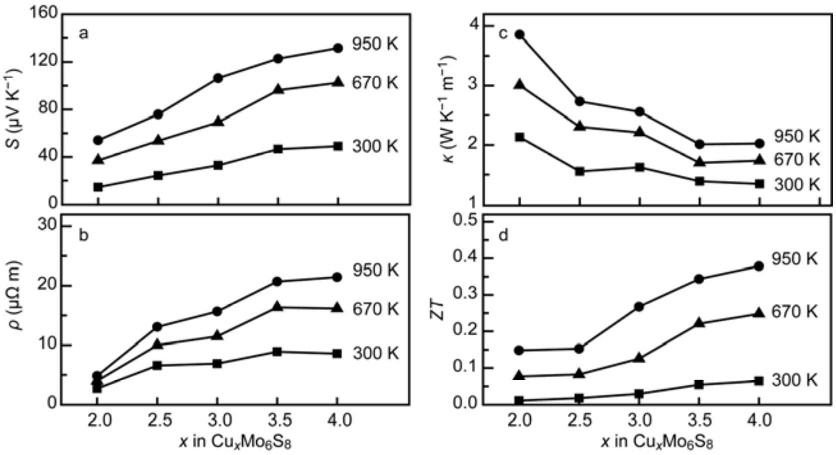

Figure 1: **a)** Seebeck coefficient *S*, **b)** electrical resistivity *ρ*, **c)** thermal conductivity *κ*, and **d)** dimensionless thermoelectric figure of merit *ZT* versus Cu content for $Cu_xMo_6S_8$ at 300, 670, and 950 K.

[1] R. Chevrel, M. Sergent and J. Prigent: J. Solid State Chem. 3 (1971) 515 – 519.
[2] T. Caillat, J.-P. Fleurial and G.J. Snyder: Solid State Sci. 1 (1999) 535 – 544.