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THERMAL CONDUCTIVITY OF SELENIUM DOPED WITH ZINC AT DIFFERENT CONCENTRATIONS IN THE SOLID AND LIQUID STATES

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We have measured the thermal conductivity in both solid and liquid states for amorphous sample of selenium doped with three different concentrations (10,1000,50000 ppm) of zinc. The measurements were taken in the temperature range from 323 to 713 K, and were carried out using the concentric cylinder method. It was found that thermal conductivity of the samples is of the phonon type. Its temperature dependence follows the relation $k_{ph} \propto T^{-1}$, and can be explained by the influence of thermal effects on the atomic structure.

KEY WORDS: Amorphous and liquid structure doped selenium.

INTRODUCTION

The thermal conductivity of amorphous semiconductors has attracted a great deal of interest in the last years. Several trials have been made to investigate the phonon processes in such materials and their changes at the phase transition point^{1–3}. The thermal conductivity of “Selenium doped with Indium and Iodine” and “Selenium doped with Lead, Sulphur and Thalium” have been measured both in the solid and liquid states^{4,5}.

The aim of the present contribution is to study the thermal conductivity of selenium doped with different concentrations of zinc. The melting point is about 556 K for the three samples. X-ray diffraction for the three samples were carried out. They showed that the three samples are in the amorphous form.

1 EXPERIMENTAL DETAILS

The samples were prepared from highly pure elements (99.999%), where pure selenium was doped with various concentrations of zinc: 10, 1000, 50000 ppm (wt%). Table 1 shows the concentration of zinc additives in atomic percent.

The synthesis of the samples was carried out under high vacuum, (10^{-3} Pa) in silica tubes at 723 K for more than 6 h with frequent rocking to insure the

Table 1 Concentration of Zn additives in the prepared samples (atomic percent) $\text{Se}_{1-x}\text{Zn}_x$ Samples.

Sample	Zn (atomic percent)	Zn (weight percent)
Sample 1	0.0011	10 ppm
Sample 2	0.112	1000 ppm
Sample 3	5.69	50000 ppm

homogenization of the melt. The tubes were then quenched in ice to obtain the samples in the amorphous state. The solid materials were then heated in an inert atmosphere until melting, then transferred to the measuring cell.

The thermal conductivity measurements were carried out using the concentric cylinder method⁶ under steady state thermal conditions, where the material is placed in the cylindrical gap between two concentric graphite cylinders kept in nitrogen atmosphere⁷.

The thermal conductivity was calculated using the formula:

$$k = Q \ln \frac{d_2}{d_1} [2\pi L (t_1 - t_2)]^{-1} \quad (1)$$

where d_1 and d_2 are the diameters of the inner and outer cylinders, t_1 and t_2 are the temperatures at the two sides of the sample, L is the length of the cylinder, and Q is the quantity of the heat generated and is given by:

$$Q = m(\Delta T / \Delta t) s,$$

where m is the mass of external cylinder, $(\Delta T / \Delta t)$ is the temperature gradient, and s is the specific heat of graphite.

Measurements were carried out over a wide range of temperatures below and above the melting point.

2 RESULTS AND DISCUSSION

It is usually convenient to analyze the thermal conductivity k in terms of four contributions:

$$k = k_e + k_{ph} + k_{am} + k_r$$

where k_e is the electron component, k_{ph} is the phonon component, k_{am} is the ambipolar component, and k_r is the radiation component, which is assumed to be zero in this case. Cutler⁸ has pointed out that: $k_e = W_0 \sigma T$,

Where W_0 is the constant $\pi^2 k^2 / 3e^2$ which is equal to $2.45 \times 10^{-8} \text{ V}^2 / \text{deg}^2$. We can claim that the contribution of k_e is relatively small, and its increase with temperature is insufficient to have a noticeable effect on k .

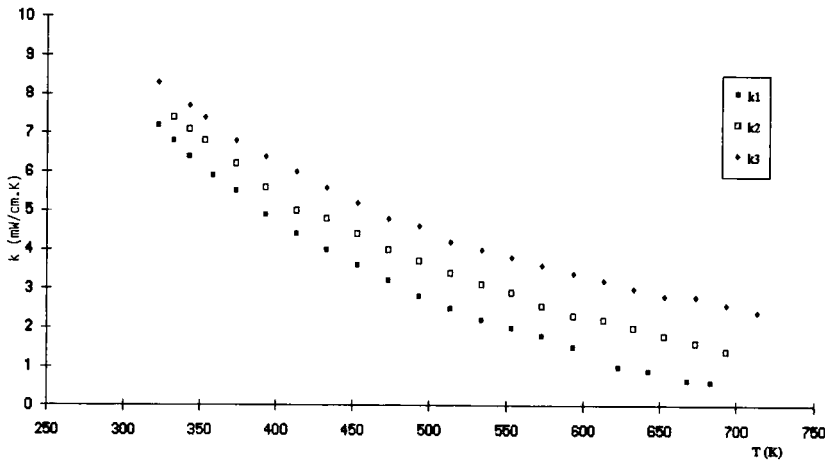


Figure 1 Temperature dependence of the thermal conductivity of Se doped with Zn at different concentrations in the solid and liquid states.

Magomedov *et al.*,⁹ have mentioned that the temperature dependence of the phonon thermal conductivity k_{ph} limited by umklapp processes could be considered as

$$k_{ph} = B T_{mp}^{3/2} \rho^{2/3} / A^{7/6} T,$$

where B is a coefficient ($B = 13$ for covalent crystals and 1.5 for ionic crystals), T_{mp} is the melting point, ρ is the density of the sample, A is the average atomic weight, and T is the temperature.

Cutler⁸ stated that:

$$k_{am} = \frac{\sigma_h \sigma_e}{\sigma_h + \sigma_e} (S_h - S_e)^2 T,$$

where σ is the electrical conductivity and S is the thermoelectric power, for holes (h) and electrons (e), respectively.

Figure 1 show the thermal conductivity k for selenium doped with zinc at different concentrations. According to the previous analysis of the thermal conductivity components, the decrease of k could be attributed to a decrease of k_{ph} . The abrupt decrease before the melting point in both samples is due to the decrease of density on melting, and the subsequent increase of the distance between molecules which leads to a weakening of the bonds between molecules and an increase in the degree of disorder.

We can thus conclude that the conduction due to electrons, σ_e is nearly zero, and therefore k_{am} , which is the ambipolar component of thermal conductivity, can be neglected. This explains why there is no slight increase in k after the melting point.

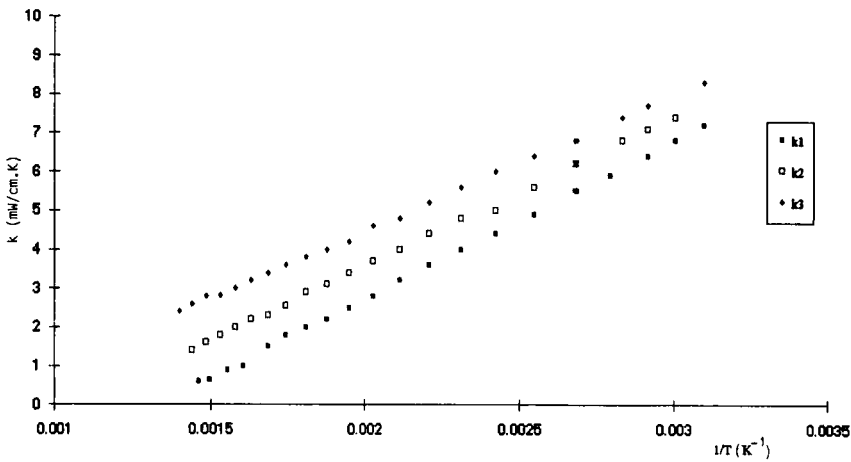


Figure 2 The thermal conductivity versus $1/T$ for Se doped with Zn at different concentrations in the solid and liquid states.

Similar behaviour has been observed by Magomedov *et al.*,¹⁰ for the compound TlSbSe_2 .

Figure 2 shows the variation of k with $1/T$. It is clear from the figure that the relation between k and $1/T$ is a linear relation for the three samples. This means that $k \propto 1/T$ and this is in agreement with the Magomedov formula⁹.

3 CONCLUSIONS

The thermal conductivity k of $\text{Se}_{1-x}\text{Zn}_x$ ($x = 0.000011, 0.00112, 0.0569$) varies with temperature as T^{-1} indicating that the thermal conductivity is of phonon type, and the temperature dependence of k can be explained by the influence of thermal effects on the atomic structure. The thermal conductivity k for the three samples is proportional with $1/T$.

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