

Thermal Conductivity and Electrical Resistivity of Cadmium Arsenide (Cd_3As_2) in the Temperature Range 4.2–40 K¹

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Results on electrical resistivity and thermal conductivity measured in the temperature range 4.2–40 K are presented for single-crystal and polycrystalline samples of Cd_3As_2 . Hall effect has been studied at temperatures of 4.2, 77, and 300 K. The calculated value of the conduction electron concentration was in the range $1.87\text{--}1.95 \cdot 10^{24} \text{ m}^{-3}$. Electrical resistivity of all investigated samples was independent of temperature up to about 10 K and increased slowly at higher temperatures. The thermal conductivity shows a maximum in the region in which the lattice component of thermal conductivity dominates. The strong anisotropy of the lattice component determines the anisotropy of the total thermal conductivity. The electronic component of thermal conductivity does not exhibit any anisotropy and shows a maximum at a temperature of about 300 K.

KEY WORDS: cadmium arsenide; electrical resistivity; Hall effect; low temperatures; thermal conductivity.

1. INTRODUCTION

A permanent and very dynamic development of semiconductor electronics implies that more attention should be paid to these semiconducting compounds.

Compounds of group $\text{A}^{\text{II}}\text{B}^{\text{V}}$ belong to those binary semiconductors whose thermal and transport properties have been least studied. One of the interesting representatives of this group is cadmium arsenide, Cd_3As_2 .

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As stated earlier [1], three polymorphic phase transitions take place for the solid Cd_3As_2 at temperatures of 595, 465, and 250°C. In the high-temperature β phase, Cd_3As_2 has a cubic structure. In the low-temperature phases, it crystallizes in a tetragonal system. In all phases, Cd_3As_2 is a heavily degenerated n -type semiconductor with carrier concentrations of the order 10^{24} m^{-3} [2].

Temperature dependencies of thermal conductivity of Cd_3As_2 were presented in the literature [3–6]. In one of the papers [6] the investigations were carried out on single-crystal samples, while in the other papers [3–5] the samples were of polycrystalline structure. Separation of the lattice and electronic thermal conductivity components was also performed [3, 5, 6]. It was stated that at low temperatures (below 20 K) the lattice thermal conductivity component prevails. With increasing temperature, the contribution of the electronic component becomes more pronounced. Electrical resistivity data for single-crystal samples of Cd_3As_2 were presented in the literature [7–9]. In one of the papers [7] an anisotropy of electrical resistivity at temperatures of 4.2, 77, and 300 K observed. In contrast, in another paper [9] the anisotropy was not observed. In the present paper, the results of thermal conductivity and electrical resistivity measurements for three single-crystal samples (with different crystallographic directions) and one polycrystalline sample are presented. All samples were in the α phase.

2. EXPERIMENTAL RESULTS

2.1. Samples and Method of Measurement

Two large Cd_3As_2 single crystals were prepared by the sublimation method and one large single crystal was obtained by the Pippert-Polich method. From these single crystals samples with dimensions of $1 \times 1.5 \times 10$ – 12 mm^3 were cut. The samples were oriented in directions as follows: II, 111; III, 110; and IV, with 10° deflection from the 110 direction. Sample I was polycrystalline. For all samples, the Hall effect at temperatures of 4.2, 77, and 300 K was investigated. The value of the Hall constant did not change at these temperatures in any of the measured samples. Obtained values of the Hall constant, R_H , electron concentration, n , residual resistivity, ρ_0 , and mobility, μ , at a temperature of 4.2 K are presented in Table I.

Thermal conductivity was measured by a steady-state axial heat flow method. The temperature drop along the sample was measured with Cryo-Cal germanium thermometers.

The electrical resistivity was measured by a potentiometric method. The

Table I. Electrical Parameters of Cd_3As_2 Samples at 4.2 K

Sample	R_H	$10^{-24} n$ (m^{-3})	$10^6 \rho_{4.2}$ ($\Omega \cdot m$)	$10^{-4} \mu_{4.2}$ ($A \cdot s^2 \cdot kg^{-1}$)
I (polycrystalline)	3.20	1.95	1.53	2.1
II (111)	3.33	1.87	0.44	7.6
III (110)	3.24	1.93	0.41	7.8
IV (10° deflection from 116)	3.31	1.89	0.47	7.0

temperature variation of the sample during the measurements was less than 1 mK.

The total error of the measurement in both thermal conductivity and electrical resistivity was estimated not to exceed 7%. This large error of measurement resulted from the systematic error of detection of the distance between electrodes during electrical resistivity measurement.

2.2. Electrical Resistivity

The temperature dependence of electrical resistivity of Cd_3As_2 is shown in Fig. 1. All Cd_3As_2 samples measured in the low-temperature

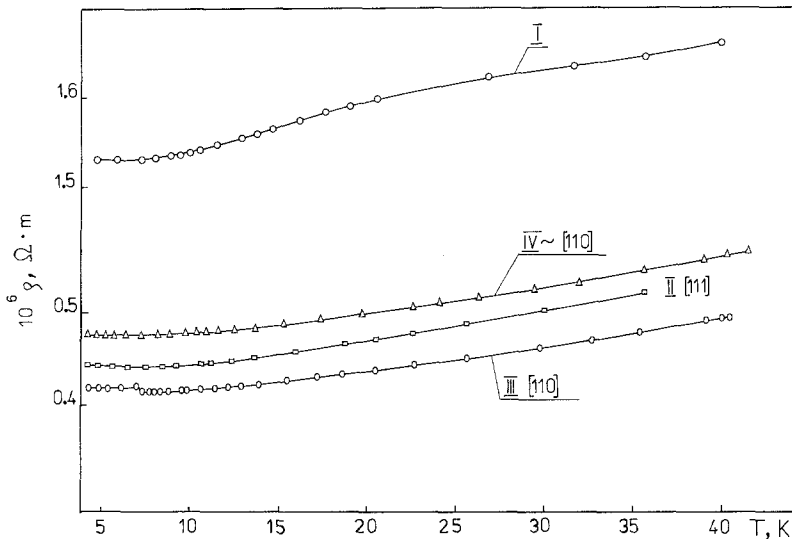


Fig. 1. The temperature dependence of the electrical resistivity, $\rho(T)$, for single-crystal and polycrystalline Cd_3As_2 . I—polycrystalline sample; II, III, and IV—single-crystal samples.

range (from 4.2 to 10 K) are characterized by a constant value of electrical resistivity. This constancy of the electrical resistivity in this temperature range is probably caused by scattering of conduction electrons, physical defects, and chemical impurity ions [9, 10]. At higher temperatures (10–40 K), the electrical resistivity of the investigated samples increases slowly. In this temperature range, electrical resistivity is probably limited by scattering of conduction electrons by optical vibrations of the crystal lattice [1], which is no longer independent of temperature.

As one could expect, the electrical resistivity of polycrystalline sample I was much higher than the values measured for single crystals. No systematic dependence of electrical resistivity on crystallographic directions was observed.

The resistivity for sample II (111) is located between the $\rho(T)$ curve for sample III and that for sample IV (Fig. 1). This fact is quite striking if one remembers that samples III and IV were those were similarly oriented.

2.3. Thermal Conductivity

The dependence of thermal conductivity on temperature for Cd_3As_2 in the temperature range 4.2–40 K is shown in Fig. 2. All of the plots show

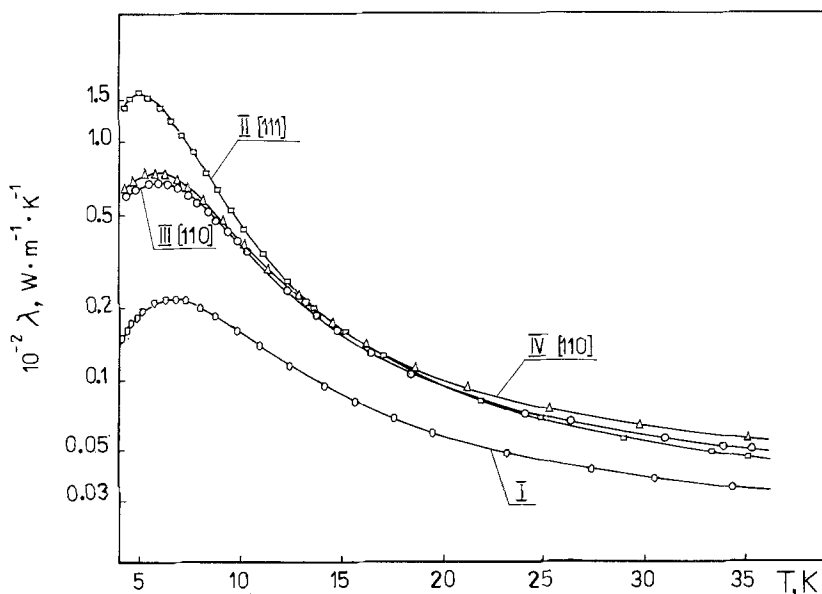


Fig. 2. The temperature dependence of the thermal conductivity coefficient, $\lambda(T)$, for single-crystal and polycrystalline Cd_3As_2 . I—polycrystalline sample; II, III, and IV—single-crystal samples.

well-defected maxima. The highest value of thermal conductivity in the region of maximum is shown by sample II, with crystallographic direction 111. Samples III and IV, with similar orientations, show nearly identical $\lambda(T)$ dependences, the value of λ for the latter being slightly higher. The lowest values of λ in the entire temperature range are exhibited by the strongly defected polycrystalline sample I. As can be seen in Fig. 2, the temperature at which the maximum of the $\lambda(T)$ curve appears, T_{\max} , depends on the value of λ_{\max} ; that is, the higher the value of λ_{\max} , the lower the temperature T_{\max} . The dependence of T_{\max} on λ_{\max} is analogous to that of metal and dielectric polycrystalline samples and contrary to that of anisotropic single-crystal metals.

The comparison of λ_{\max} values with ρ_0 for single-crystal Cd_3As_2 samples does not lead to any straightforward functional relation of these quantities.

The total thermal conductivity coefficient for semiconducting compounds may be written as follows:

$$\lambda_t = \lambda_e + \lambda_l + \lambda_b + \lambda_p + \lambda_{\text{exc}} \quad (1)$$

where λ_t is the total thermal conductivity and λ_e , λ_l , λ_b , λ_p , and λ_{exc} are the electronic, lattice, bipolar, photon, and excitation components of thermal conductivity, respectively.

In the temperature range 4.2–40 K for Cd_3As_2 the lattice and electronic components dominate, i.e.,

$$\lambda_t = \lambda_e + \lambda_l \quad (2)$$

On the bases of the literature data [3, 5], where the Lorentz function $L(T)/L_0$ was evaluated, we have separated the electron and lattice components of thermal conductivity.

The electronic component of thermal conductivity can be written in the following form:

$$\lambda_e = \frac{L(Y)T}{\rho(T)} \quad (3)$$

and the lattice component as

$$\lambda_l = \lambda_t - \frac{L(T)T}{\rho(T)} \quad (4)$$

The temperature dependence of the electronic thermal conductivity component $\lambda_e(T)$ is presented in Fig. 3.

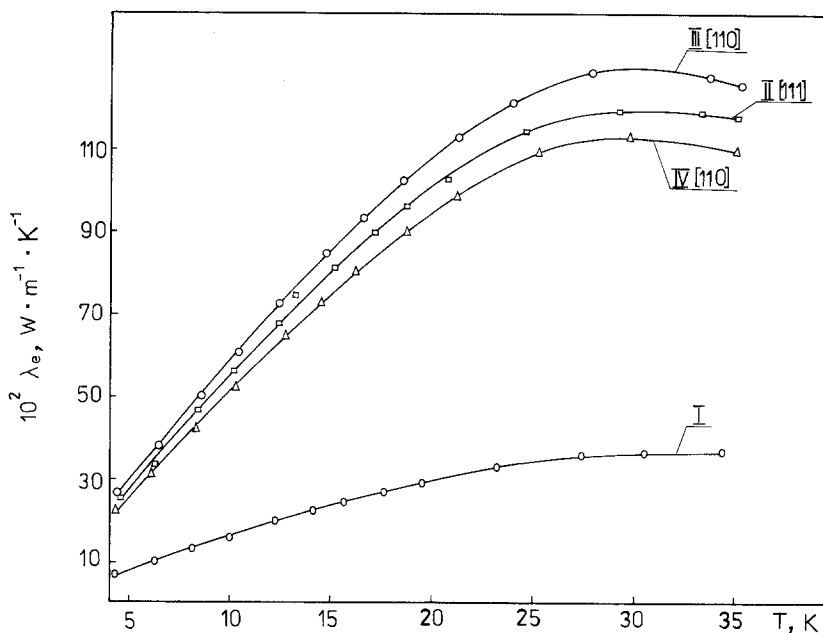


Fig. 3. The temperature dependence of the electronic component of thermal conductivity, $\lambda_e(T)$, for single-crystal and polycrystalline Cd_3As_2 . I—polycrystalline sample; II, III, and IV—single-crystal samples.

The $\lambda(T)$ plots show maxima occurring at a temperature about 30 K and their shapes are similar to the $\lambda(T)$ plots for metals. The polycrystalline strongly defected sample is characterized by the lowest values of thermal conductivity and rather flat maximum in the $\lambda(T)$ plot.

We did not succeed in deriving the $\lambda_e(T)$ dependence within the framework of Wilson's theory. The reason for this failure may lie in that we used in our analysis the Lorenz function derived on the basis of the one-band model [3, 5]. In Cd_3As_2 there is a possibility that two groups of conductivity electrons exist. Taking this into account one may find that a correction in the $L(T)$ dependence derived earlier is necessary, and this in turn would imply changes in the $\lambda(T)$ dependence. Unfortunately, such a correction has not been made up to the present day. The temperature dependence of the lattice component of thermal conductivity is plotted in Fig. 4. When comparing Figs. 4 and Fig. 3, one may see that in the region of λ_{max} lattice component λ_l dominates in the total thermal conductivity. This implies that the large anisotropy of the total thermal conductivity of Cd_3As_2 results mainly from the anisotropy of the lattice component.

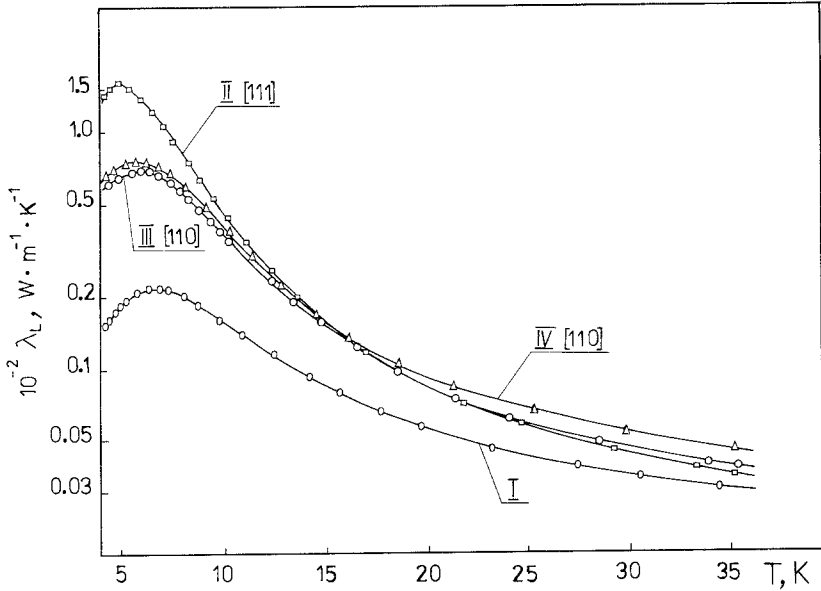


Fig. 4. The temperature dependence of the lattice component of thermal conductivity, $\lambda_l(T)$, for single-crystal and polycrystalline Cd_3As_2 . I—polycrystalline sample; II, III, and IV—single-crystal samples.

3. SUMMARY

The dependence of electrical resistivity on temperature in the low-temperature range (4.2–40 K) for single-crystal and polycrystalline Cd_3As_2 is similar to typical analogous plots for metallic samples. Up to about 10 K, Cd_3As_2 samples were characterized by a constant value of electrical resistivity which depended on the degree of structural disorder, on the conductivity electron concentration, and only slightly on the crystallographic orientation. We did not observe any meaningful anisotropy of electrical resistivity in our Cd_3As_2 samples. Thermal conductivity coefficients of Cd_3As_2 samples showed maxima, the positions of which depended on the structural disorder and crystallographic orientation.

Separation of the electronic and lattice components of λ showed that the lattice component dominated in the region of the maximum of the $\lambda(T)$ plot, and moreover, the lattice component was characterized by a strong anisotropy.

The electronic component of thermal conductivity showed a maximum at a temperature of about 30 K .

It was not possible to find any functional dependence for the electronic component of thermal conductivity in the framework of Wilson's theory with the present states of knowledge of electronic processes in Cd_3As_2 .

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