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Dissipation of Current Carriers in Lead Telluride Films

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ABSTRACT
The mechanisms of current carrier scattering in polycrystalline lead telluride (PbTe) films deposited on glass substrates in the temperature range 77-300 K have been studied. The main attention is paid to scattering at the grain-to-grain limits, which is the dominant mechanism affecting the mobility of current carriers. In this work, a mathematical expression is obtained for calculating the mobility of current carriers in thin films, considering scattering on the surface and intergrain limits, which makes it possible to evaluate the influence of these mechanisms on the mobility of current carriers. The dependence of current carrier mobility in PbTe films on thickness and temperature has been studied. It has been established that the dominant scattering mechanism is scattering at grain boundaries. The activation energy of electrical conductivity was estimated, which is approximately 0.04-0.07 eV.

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Introduction
Lead telluride films are known for their unique properties, which make them promising materials for various devices, in particular, detectors and infrared radiation sources. The mechanisms of current carrier scattering have an important influence on the operational characteristics of device structures based on them [1, 2]. Such research can help improve the understanding and optimization of these processes, which in turn can lead to further improvements in their efficiency and reliability.

Works are devoted to consideration of the mechanisms of current carrier transport in polycrystalline films grown on glass substrates [1-9]. Thus, in particular, the authors of studied the mobility of carriers in polycrystalline PbTe films with a thickness of 0.1-1 microns [3]. The dominant role of surface mobility was determined, and the significant influence of grain boundaries was confirmed. Works are devoted to the issues of the mechanism of passage of current carriers through grain boundaries [2-4]. It has been established that the passage of current carriers through barriers at grain boundaries is associated with thermionic emission. In works, post-condensation processes in polycrystalline films during their aging and annealing in vacuum were considered [5-8]. It is shown that the electrical parameters of the films can change due to fragmentation or enlargement of crystallites.

Thus, many studies confirm that the structure and size of grains, as well as the growth and processing conditions of polycrystalline films have a significant impact on the mechanisms of carrier transport.

In this work, the dependence of the mechanisms of current carrier scattering in thin polycrystalline PbTe films on their thickness in the range from 2.5 to 7.7 μm at temperatures from 77 to 300 K was studied. In addition, the influence of temperature changes on the behavior of current carriers was analyzed and the key factors were identified factors influencing carrier scattering efficiency in the specified temperature range.

Elements of the Theory
In thin films, various mechanisms of current carrier scattering occur, such as scattering by the crystal lattice in the film bulk, surface, and growth defects [9, 10]. If we assume that each of these scattering mechanisms is independent, then the experimentally determined effective mobility μe can be described as follows [11]:

$$\frac{1}{\mu_e} = \frac{1}{\mu_L} + \frac{1}{\mu_s} + \frac{1}{\mu_z} \qquad (1)$$

where μ_L is the bulk mobility (on the lattice), μ_s is the surface mobility, μ_z is the mobility due to the influence of intergranular limits.

For completely diffuse scattering on a surface, according to [12]

$$\frac{1}{\mu_e} = \frac{1}{\mu_b}\left(1 + \frac{\lambda}{d}\right) \qquad (2)$$

where

$$\frac{1}{\mu_b} = \frac{1}{\mu_L} + \frac{1}{\mu_z} \qquad (3)$$

From equations (1) and (2), we obtain that the surface mobility will be equal to

$$\frac{1}{\mu_s} = \frac{1}{\mu_e} \cdot \frac{1}{1 + \frac{d}{\lambda}} \qquad (4)$$

where λ = 0.2 μm is the average length of the free run [12]. According to equations (1) and (4), scattering at grain boundaries will be equal to:

$$\frac{1}{\mu_z} = \frac{1}{\mu_e} - \left(\frac{1}{\mu_L} + \frac{1}{\mu_s}\right) = \frac{1}{\mu_e} \cdot \frac{1}{1 + \frac{\lambda}{d}} - \frac{1}{\mu_L} \qquad (5)$$

On the other hand, if the predominant scattering mechanism is scattering at grain boundaries, then the effective mobility μ_z can be determined according to [13]

$$\mu_z = \mu_0 e^{-\frac{\Delta E}{kT}} \qquad (6)$$

where ΔE is the activation energy, μ_0 is a constant depending on the growth parameters. In this case, the main contribution to the overall mobility of current carriers is made by barriers at the boundaries between grains.

Logarithm of the expression (6)

$$\ln \mu_z = \ln \mu_0 - \frac{\Delta E}{k} \cdot \frac{1}{T}$$

makes it possible to determine the activation energy associated with the influence of grain boundaries.

Methodology of the Experiment

In thin films, various mechanisms of current carrier scattering are realized, such as scattering by the crystal lattice in the bulk of the film, surface, and growth defects [4, 14]. To study PbTe films, they were produced by the hot wall method from the vapor phase onto glass substrates, and the film growth rate was 1-3 nms^{-1}. The structure of the films was studied by electron microscopy, diffraction and optical metallography. Electrical parameters were measured by the compensation method in constant electric and magnetic fields.

To carry out measurements, we used separate films of different thicknesses, through which a current of about 0.1 mA was passed. The magnetic field was directed perpendicular to the surface of the films with an induction of 0.8 T. The measuring samples were equipped with four Hall and two current contacts, which ensured the accuracy of the measurements. Additionally, to ensure high accuracy and reproducibility of the results, experiments were carried out at different temperatures, which made it possible to study the temperature dependence of the electrical parameters of the films [15].

Taking into account the possible influence of grain boundaries on the overall mobility of current carriers, we analyzed the influence of grain size and boundaries on the electrical characteristics of the films. Using modern analytical methods, such as scanning and transmission electron microscopy, it was possible to study the morphology of the films and the relationship between structural features and electrical properties.

The resulting films were polycrystalline, with crystallite sizes of approximately 1 μm. These crystallites had a clearly formed plate-like structure, oriented predominantly by {100} planes parallel to the surface of the glass substrate. In this case, a significant misorientation of crystallites in azimuth was observed, which is confirmed by the data shown in Figure 1.

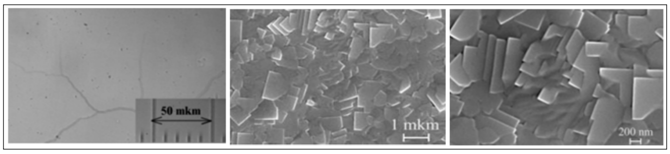


Figure 1: Microstructure of PbTe Films Deposited on Glass Substrates

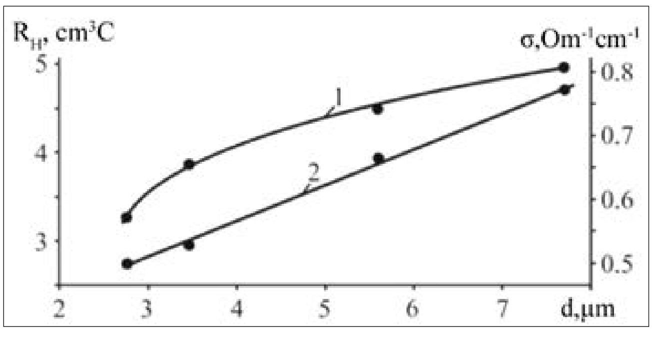
To analyze the structure of the films in more detail, additional studies were carried out using scanning electron microscopy (SEM) and X-ray diffraction (XRD). The analysis showed that lamellar crystallites have a high degree of crystallinity, and grain boundaries are clearly defined, which affects the electrical properties of the films.

The study also included studying the influence of crystallite orientation and their azimuth misorientation on the transport properties of films. It was found that high misorientation of crystallites can lead to an increase in the number of defects at grain boundaries, which in turn affects the efficiency of carrier transport [16].

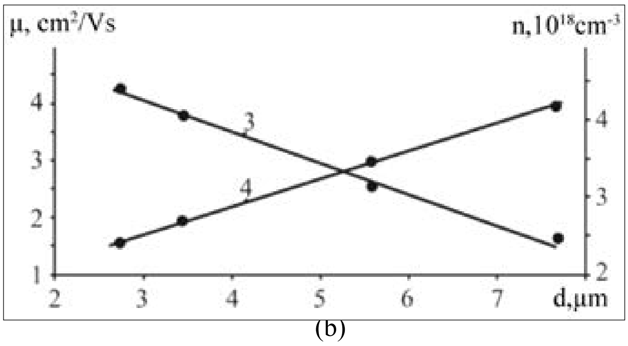
In addition, temperature measurements were made to determine the dependence of electrical parameters on temperature. These measurements showed that temperature changes can have a significant effect on the mobility of current carriers, especially at low temperatures, where the role of grain boundaries becomes dominant [16].

Research Results and their Analysis

In thin films, various mechanisms of current carrier scattering are realized, such as scattering by the crystal lattice in the bulk of the film, surface, and growth defects [4, 14]. To study PbTe films, they were produced by the hot wall method from the vapor phase onto glass substrates, and the film growth rate was 1-3 nms^{-1}. The structure of the films was studied by electron microscopy, diffraction and optical metallography. Electrical parameters were measured by the compensation method in constant electric and magnetic fields.



(a)



(b)

Figure 2: Experimental Dependences of a) Specific Electrical Conductivity (1) and Hall Constant (2)
b) Carrier Concentration (3), Hall Mobility (4) of PbTe Films on Thickness at Room Temperature

As can be seen from the graphs, with increasing film thickness, an increase is observed in the specific electrical conductivity (Figure 2a, curve 1), the value of the Hall coefficient (Figure 2a, curve 2) and the mobility of charge carriers (Figure 2b, curve 4). At the same time, the concentration of current carriers, determined using the Hall effect, decreases (Figure 2b, curve 3).

Dependency analysis Figure 2 shows that the increase in electrical conductivity and mobility of charge carriers with increasing film thickness can be associated with a decrease in the impact of surface defects and grain-to-grain limits on the transport properties of current carriers. A decrease in the carrier concentration with increasing film thickness may indicate a decrease in the number of impurities or defects acting as donors or acceptors.

In Figure 3 shows the temperature dependences of charge carrier mobility in PbTe films

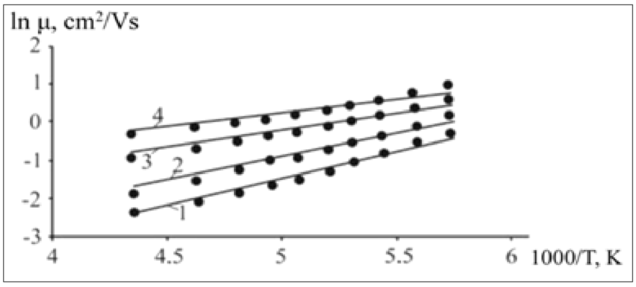


Figure 3: Temperature Dependences of Current Carrier Mobility for PbTe Films of Different Thicknesses d, μm: 1–2.7; 2–3.5; 3–5.5; 4–7.6.

Data in Figure 3 show that the mobility of charge carriers varies significantly with temperature, which indicates the complex nature of the scattering mechanisms that dominate at different temperature regimes. In particular, at low temperatures the mobility is limited by scattering at grain boundaries and defects, while with increasing temperature the main contribution comes from scattering on the crystal lattice.

A detailed analysis of the temperature dependences of mobility allows us to better understand the nature of the dominant scattering mechanisms in different temperature ranges and their influence on the electrical properties of films. This, in turn, facilitates the development of new methods for optimizing film growth and processing technology to achieve the desired electrical characteristics.

In order to clarify the dominant mechanism of charge carrier scattering, the temperature dependence of the mobility μ(T) was analyzed. It is known that the temperature dependence of mobility for films of thickness d can be expressed using the following equation [17]:

$$\mu = \mu_0 T^{-n(d)} \quad (7)$$

where μ_0 is a constant value depending on the material and structure of the film; n(d) is an indicator that determines the dominant scattering mechanism in films for a given thickness.

Studies have shown that at low temperatures (77-150 K) the value of n is close to 1, which indicates the predominance of scattering at grain boundaries and defects. As the temperature increases to 300 K, the value of n approaches 1.5-2, which indicates an increase in the influence of phonon scattering on the crystal lattice.

For high-quality lead chalcogenide films, the value of n is approximately 2.5, which is associated with scattering by long-wave acoustic phonons, taking into account the temperature dependence of the effective mass of charge carriers [18]. In the case of surface scattering, the value of n is approximately 0.5, while large values of n are associated with scattering from growth defects [14, 19].

For PbTe thin films under different growth and processing conditions, different dominant scattering mechanisms can be observed. Thus, as the film thickness decreases, the effect of surface scattering increases, which leads to a decrease in the value of n to 0.5. This is confirmed by an increase in the concentration of defects and irregularities on the film surface, which create additional potential barriers for charge carriers.

In addition, the values of n greater than 2.5 indicate the presence of a significant number of growth defects such as dislocations, vacancies and intergranular boundaries. These defects create additional scattering mechanisms, which have a significant impact on the transport properties of charge carriers [18, 19].

For the films studied, the values of n were found to be in the range of approximately 0.7–1.4. This indicates the predominance of charge carrier scattering at the grain boundaries of the film thicknesses under study. This was confirmed by relatively thick dependences of the current carrier mobilities, calculated from scattering at grain boundaries, on those measured experimentally. It was found that the data differ insignificantly, which once again confirms the dominance of scattering at grain boundaries.

Note that the thickness (see Figure 4) dependences of the carrier mobilities of PbTe films, calculated by scattering at grain boundaries, differ slightly from the experimental ones. This further confirms the dominance of current carrier scattering at grain boundaries.

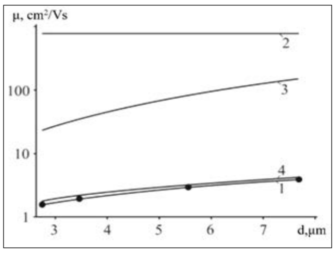


Figure 4: Dependences of the mobility of current carriers on the thickness of PbTe films at room temperature: 1 – experiment (μ_{exp}), 2 – bulk crystal (μ_L), 3 – surface mobility (μ_s), 4 – scattering at the grain boundaries (μ_z).

The activation energy, calculated from the temperature dependence of the Hall mobility using formula (6), is approximately 0.04-0.07 eV. This value also indicates the important role of grain boundaries in the transport of current carriers, since it reflects the energy required for the passage of carriers through the barriers formed between crystallites.

These results confirm that to optimize the electrical properties of PbTe films, it is necessary to pay special attention to controlling the conditions for the formation of grain boundaries and avoiding defects that can form on the surface and the film itself.

Conclusion

- In the work, a mathematical expression was obtained for calculating the mobility of current carriers in thin films in which scattering occurs on the surface and grain boundaries. This expression allows us to take into account the influence of these two scattering mechanisms on the mobility of current carriers in films.
- The dependence of the carrier mobility of PbTe films grown on glass substrates on their thickness and temperature was studied. It has been experimentally established how the mobility changes under different conditions for producing such films.
- It was discovered that the dominant mechanism affecting the mobility of current carriers is scattering at grain boundaries.
- An assessment was made of the activation energy of electrical conductivity, which is associated with the scattering of carriers at grain boundaries. This estimate allows us to understand how much energy is needed for charge carriers to pass through barriers formed at the boundaries between film crystallites.

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