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Distribution of own defects in monocrystal epitaxial films PbTe

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Was shown, that dimensional effects in the monocrystal PbTe n-type films which has been grown on mica substrates by the method of a hot wall, connected with distributions of dopands and the centres of dispersion of free charge carriers. Approximation of experimental effective dependences of conductivity $\sigma(d)$ and product of Hall coefficient and square of conductivity $R(d)\sigma^2(d)$ from a thickness by theoretical dependences was executed.Spatial parameters of distributions of defects of growth on a boundary substrate-film and dislocations in a following layer were received. Proceeding from layered heterogeneity of the thin semiconductor PbTe films which has been grown by the method of a hot wall, were found three layers enriched free electrons to different values of concentration and two layers of the centres of dispersion connected with different types of crystal defects: interphase boundaries, dislocations, dot defects and other.

Key words: *lead chalcogenides, thin films,dimensional effects, heterogeneity*

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Inhomogeneous film structures on base of lead chalcogenides are of great interest in connection with possibility of their use for practical purposes of infrared technique [1–4] and optoelectronics [5–10], they are basic thermoelectric materials [11–14], they are used in sources of electrical power on space vehicles and in watches, are applied in refrigerating machines, in electronic, medical and scientific equipment, and even for conditioning of seats in up-market cars [11]. In works [2–4] is set dependence from thickness of properties of thin films of lead chalcogenides, that were grown by epitaxial methods,which was caused layered inhomogeneity of distribution of defects connected with boundary substrate-film. However, in this works the analysis of experimental concentration and mobility of free charge carriers was made for integral effective characteristics. Such approach gives an information about parameters of a film on the whole, but don't allow to select the influence of substrate on electrical characteristics. Evidently, that as thinner is film, the role of substrate in determining of concentration and mobility of carriers increase. However, natural is the analysis of those integral electro-physical parameters and their combinations, which at measuring, for example, conductivity or Hall coefficient, really are layered integrals of respective characteristics and their combinations. Besides, in that works main attention addressed to processes of scattering of free charge carriers, but is not noticed, that concentration of carriers can change on an order in films with different thickness. The analysis of dimensional effects in semiconductor films have to take into account dependences of dopant and acceptor centers and centers of scattering. Till now is not set identity or difference of centers of scattering and centers, that determine a concentration of free charge carriers in lead chalcogenides in region of impurity conductivity.

Therefore, at comparative studying of properties of films and bulk samples and finding-out reasons of their distinction it is necessary to take into account that a considerable role can play a change of properties with depth. The concentration of structure defects, that is caused by inconsistency of crystal structure of condensate and substrate, can decrease with keeping away from substrate. The gradient of properties take place also at opposite (free) surface. Here is possible noticeable influence of own defects, which are predefined by revaporation of condensate, segregation of one of components, adsorption and diffusion of oxygen from atmosphere, etc. This factors also influence on properties of near-surface layers of bulk samples, but in this case relative thickness of layers times less, than for films, thats why also less a degree of their influence.

It is clear, that in layered-inhomogeneity sample, values of current density and heat flow change with coordinate x on the thickness of a film. Integrating left and right parts of kinetic equations by x for effective coefficients can be written the expressions through average by thickness in such way [15] :

$$\bar{\sigma}(d) = \frac{\int_0^d \sigma(x)dx}{d} \tag{1}$$

$$\bar{R}(d)\bar{\sigma}^2(d) = \frac{\int_0^d R(x)\sigma^2(x)dx}{d} \tag{2}$$

We will express this values through distributions of concentrations of free charge carriers $n(x)$, connected with donor centers, and distributions of mobilities $\mu(x)$,connected with centers of scattering:

$$\bar{\sigma}(d) = \frac{\int_0^d en(x)\mu(x)dx}{d} \tag{3}$$

$$\bar{R}(d)\bar{\sigma}^2(d) = \frac{\int_0^d en(x)\mu^2(x)dx}{d} \tag{4}$$

With purpose of studying of distribution of electrically-active defects and centers of scattering of free charge carriers in films n-PbTe, and their separation, was improved the method, that was used in [16–18] for obtaining the distribution of radiation defects in films of lead chalcogenides and own defects in metallic films. Was obtained spatial parameters of distribution and amplitude values of concentrations of donor defects in a thick film, and similar values of characteristic for centers of scattering. Films are considered thick, if their thickness is more than value of free path for carriers of current and Debye length of shielding.

Films of stoichiometric composition were grown in vacuum chamber by the method of hot wall on mica substrates [4]. Temperatures of evaporator and substrate were controlled by thermocouples and supported constant in process of vapor deposition of material up to ± 1°C. The thickness of films were changed in range 0.05-10 micron and measured by microinterferometer with accuracy 0.02 micron. In accordance with X-ray and electron-microscopic examinations films had block monocrystal structure with sizes of blocks 5-10 micron with angular orientation less than 1° in plane (111), parallelly to surface of substrate. Thus size of blocks almost didn't depend from thickness of films. Grown films had conductivity n-type with minimal carriers concentration 6×10^{16} cm^{-3}. Measurements were carried out at temperatures from nitric to room under magnetic field 1.6 T. The dependence of specific conductivity and Hall coefficient from thickness of a film is shown on Figure.1.

Considering the models for approximation experimental data, which are the solutions of several diffusion equations with centers, which determine the concentration of free charge carriers of infinite and finite power that are localized in dot, with accordance to Fisher's ratio test was selected optimal. According to this model local concentrations of donor defect states were presented by sum of two normal distributions against uniform:

$$N_d(x) = N_1 exp(\frac{-(x-d_1)^2}{2{b_1}^2}) + N_2 exp(\frac{-(x-d_2)^2}{2{b_2}^2}) + N_3, \tag{5}$$

and local concentrations of centers of scattering — by one normal distribution of defects of first sort against uniform of defects of second sort:

$$N_S(x) = N_4 exp(\frac{-(x-d_3)^2}{2{b_3}^2}) + N_5. \tag{6}$$

Fairness of this assumption is confirmed by results.

At the specified temperatures of measurement defect states are completely ionized, thats why the concentration of free charge carriers is equal to their concentration $n(x) = N_d(x)$. The mobility

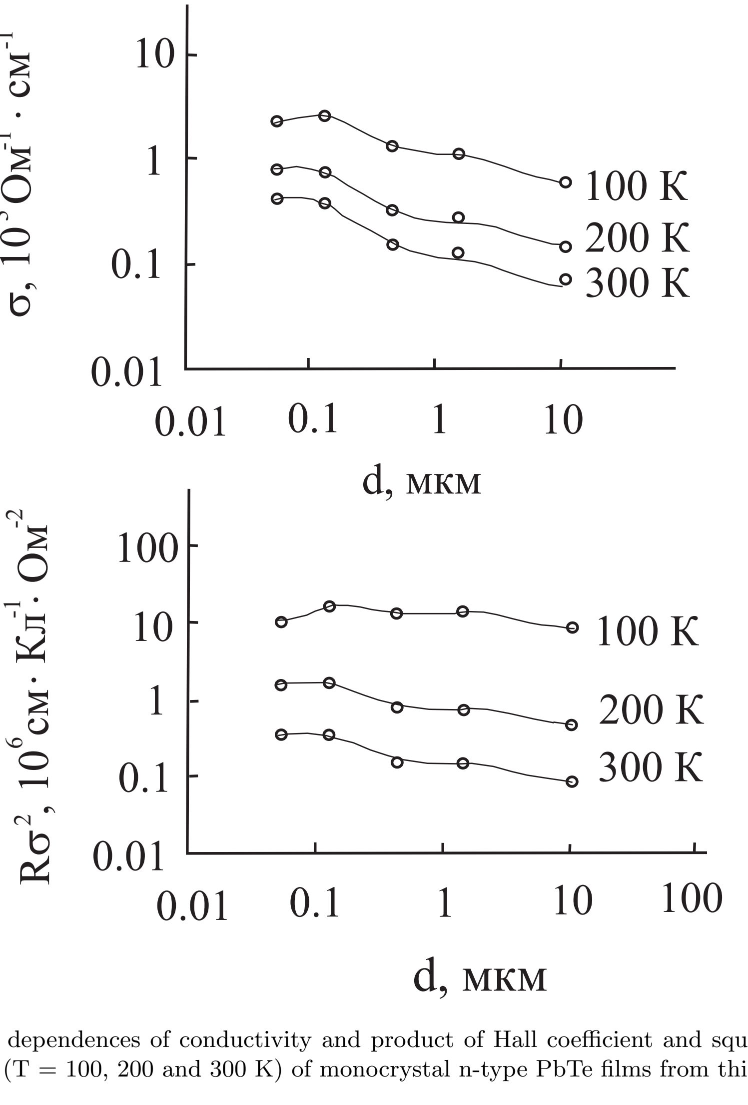

Figure 1. The dependences of conductivity and product of Hall coefficient and square of conductivity $R\sigma^2$ (T = 100, 200 and 300 K) of monocrystal n-type PbTe films from thickness.

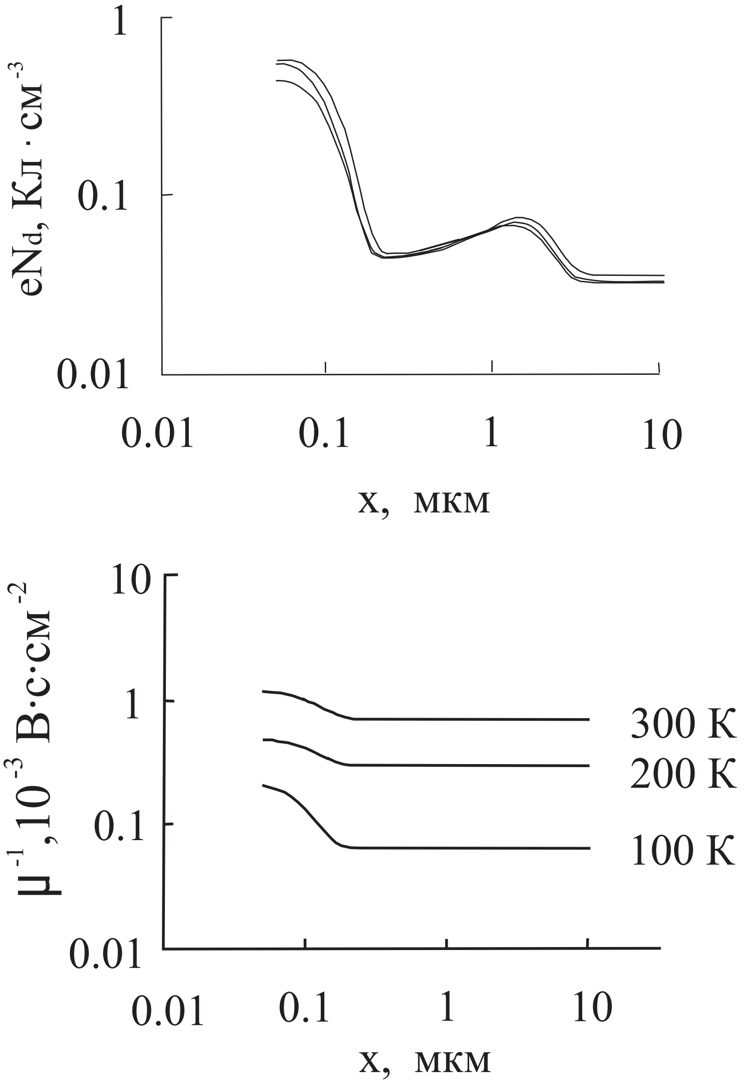

Figure 2. The distributions of concentration of charges of donor centers eN_d and reverce mobility μ^{-1} (T = 100, 200 and 300 K) in monocrystal film n-PbTe from normal coordinate to surface of a film ($x = 0$ respond substrate-film interface).

of free charge carriers is inversely proportional to concentration of centers of scattering $\mu_i(x) = \frac{k_i}{N_i(x)}$, where k_i - is a coefficient of proportion, or

$$\mu^{-1}(x) = \mu_1^{-1} exp(\frac{-(x-d_3)^2}{2b_3^2}) + \mu_2^{-1} \tag{7}$$

The parameters of approximation are presented in the Table 1.

Table 1. The parameters of model dependences, which approximate experimental data.

T, K	100	200	300
eN_1, C/cm^3	0.53	0.41	0.52
d_1,micron	0.056	0.048	0.047
b_1,micron	0.050	0.048	0.047
eN_2,C/cm^3	0.035	0.038	0.037
d_2,micron	1.27	1.48	1.40
b_2,micron	0.77	0.74	0.71
eN_3,C/cm^3	0.033	0.036	0.034
μ_1^{-1},10^{-3}V×s×cm^{-2}	0.15	0.20	0.49
d_3,micron	0.033	0.033	0.031
b_3,micron	0.052	0.062	0.068
μ_2^{-1},10^{-3}V×s×cm^{-2}	0.068	0.30	0.70

The concentration of donor states near the substrate more 10 times bigger then concentration in intermediate layer and in ~ 20 times — uniformly distributed on thickness of a film dot defects. The amplitude value of distribution of near-surface centers of scattering with temperature change another than phonon, that point on their different nature: $\mu_1^{-1} \sim \mathrm{T}^{1/2}$, and $\mu_2^{-1} \sim \mathrm{T}^{3/2}$. In accordance with data presented in [1], first mechanism is the scattering on a surface of a film or dislocations, and second is phonon scattering.

The creation of non-uniform distribution of various-sort defects is one of ways of increasing of thermoelectric quality factor of materials and can promote formation of superlattices, properties of which used for designing new functional elements of semiconductor devices of micro- and optoelectronics.

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