INFLUENCE OF ELECTRIC FIELD ON FORMATION OF AMORPHOUS $TlIn_{1-x}Sn_xTe_2$ THIN FILMS

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The effect of electric field on the formation of amorphous $TlIn_{1-x}Sn_xTe_2$ films (x=0.02÷0.09) with a thickness of 30 nm, obtained in a constant electric field of E=3000 V•cm^{-1}intensity, in high vacuum by thermal deposition on substrates from fresh cleavages of KCl, KJ and celluloid, located at a temperature below T=213K, was studied by high-energy electron diffraction method. After the cooling of the steel table on which the substrates with the amorphous film were located ceased, the samples obtained for the study were brought to room temperature in a vacuum at a rate of 2 K/min. To prevent oxidation, the $TlIn_{1-x}Sn_xTe_2$ films were placed in a carbon capsule of 2÷4 nm thick. It was found that a constant electric field affects the interatomic distances, coordination numbers, and stabilization time of this amorphous phase.

Keywords: vacuum, electric field, electron diffraction, structure, amorphous film.
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INTRODUCTION

Solid solutions based on the compound are currently recognized as the most promising materials in the field of optoelectronics [1-5]. In the compounds included in the specified group, it is possible to smoothly change the width of the forbidden zone. Therefore, the study of the processes of formation of films of amorphous structure and prediction of their properties are of undoubted scientific and practical interest. It is known that there is a correlation between the physical properties and structure of these compounds [6-8]. Changes in the technological process of film obtaining affect the short-range order of atoms [6, 9].

We have studied the effect of a constant electric field on the short-range order of the $TlIn_{1-x}Sn_xTe_2$ solid solution, corresponding to the symmetry group and crystallizing in a structure with a tetragonal lattice [10].

EXPERIMENTAL PART

Thin amorphous films are obtained by different methods, one of which is thermal evaporation from tungsten or tantalum furnaces in a vacuum setup. By using this method, the studied nanoscale films were obtained in the VUP-5 setup. The films with a short-range atomic structure were studied by one of the most effective and at the same time accessible methods - the method of high-energy electron diffraction in the EMR-102 vacuum setup using an energy filter to filter out inelastically scattered electrons. Note that it is necessary to take into account incoherent scattering in the case of studying amorphous substances. To obtain films with a uniform distribution of atoms on the substrate surface, the value of the separation coefficient of the substance was taken into account when varying the conditions for the formation of $TlIn_{1-x}Sn_xTe_2$ nanoscale films (x = 0.02 ÷ 0.09). The distribution of the condensate composition due to coordinates on the condensation plane was determined using the formula:

$$q = \frac{Q}{4\pi h^2}\frac{1}{(1+\alpha)^{3/2}}$$

here q – is the amount of substance per unit surface area of the substrate; Q – is the amount of evaporated substance; h – is the distance from the evaporation source to arbitrary point along the condensate plane; the coefficient $\alpha = x/h$, where x is the distance from the point located directly under the evaporator to arbitrary point on the substrate surface. The film thickness was calculated using the formula

$$H = \frac{q}{\rho}$$

where ρ – is the density of the substance in g/cm3. In addition, the film thickness was monitored using a Spekor-250 spectrometer.

The atomic radial distribution function (ARDF) we used plays a significant role in identifying the structural characteristics of the short-range atomic order of amorphous films [11];

$$4\pi r^2\sum_m K_m U_m(r) = 4\pi r^2 U_0\sum_m K_m + \frac{2r}{\pi}\int_0^\infty si(s)\sin srds\,,$$

here K_m – is the effective scattering power of an atom in the substance under study, $U_m(r)$ – is the atomic density distribution function, U_0 – is the average density of atoms in a given volume. This function

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specifies the probability of finding atoms oriented in space in a certain way at a certain distance from each other and allows one to determine the number of neighbors around a particular atom. $TlIn_{1-x}Sn_xTe_2$ films 30 nm thick were obtained by evaporating the synthesized substance in a vacuum of ~10^{-5} Pa. The deposition of nanothick films was performed on substrates of fresh KCl, KJ chips or celluloid-coated meshes at a temperature below T=213 K at a rate of 6 nm/s. The temperature of the steel table on which the substrates were placed was measured with a copper-constantan thermocouple. As the cooling of the substrates was stopped, the amorphous samples obtained for the study were brought to room temperature in vacuum at a rate of 2 K/min. To prevent oxidation, the $TlIn_{1-x}Sn_xTe_2$ films were placed in a carbon capsule of 2-4 nm thick. To determine the optimal conditions for their formation, a thorough study of the composition and properties of the films is required. Difficulties arose in controlling the composition and homogeneity of the original sample. The phase composition of the films under study was controlled using a Shimadzu XRD-6000 diffractometer with CuK_α radiation. Not all of the obtained samples were suitable for research, since the atomic roughness on the substrates and the stress at the film-substrate interface caused a destructive effect on the films during their separation from the substrates, which is confirmed in [12].

RESULTS AND DISCUSSION

Electron diffraction patterns were recorded for 30 nm thick $TlIn_{0.93}Sn_{0.07}Te_2$ films obtained by thermal evaporation and condensation on substrates at T_s = 211 K. temperature Interpretation of these electron diffraction patterns with three diffuse rings (Fig. 1) from the above samples yielded values of S = $4\pi\sin\theta/\lambda$=14.75, 33.14, 40.97 nm^{-1}, i.e. three maxima are observed on the electron scattering intensity curve depending on the scattering angle (Fig. 2). The $I_э(S)$ curves were obtained as dependence of intensity on the scattering angle. Further analysis of the radial distribution curve of atoms revealed the short-range order parameters of $TlIn_{0.93}Sn_{0.07}Te_2$ r_1= 0.301; r_2=0.392 and r_3=0.509 nm. The r_1 value found corresponds to the sum of the covalent radii of In-Te atoms, the r_2 value corresponds to the distances between Tl-Te ions, and the third maximum r_3 corresponds to the distances between identical atoms. The changes in r values are about 2.8%. Most likely, they are related to the influence of the electric field on the arrangement of atoms in the films. The coordination number (CN) calculated from the areas under the first coordination maximum corresponds to n_1=4 (Fig. 3).

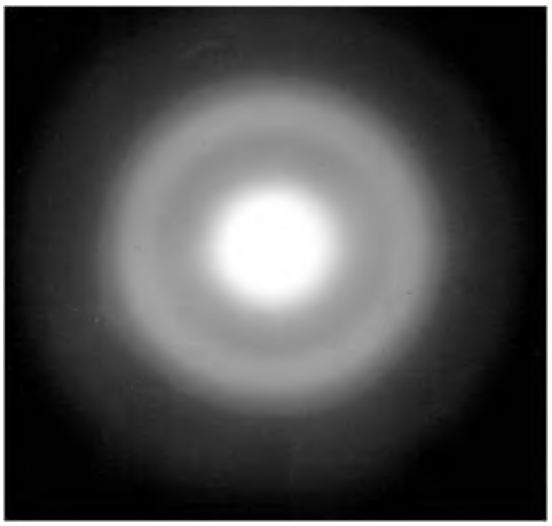

Fig. 1. Electron diffraction patterns of $TlIn_{0.93}Sn_{0.07}Te_2$ amorphous film.

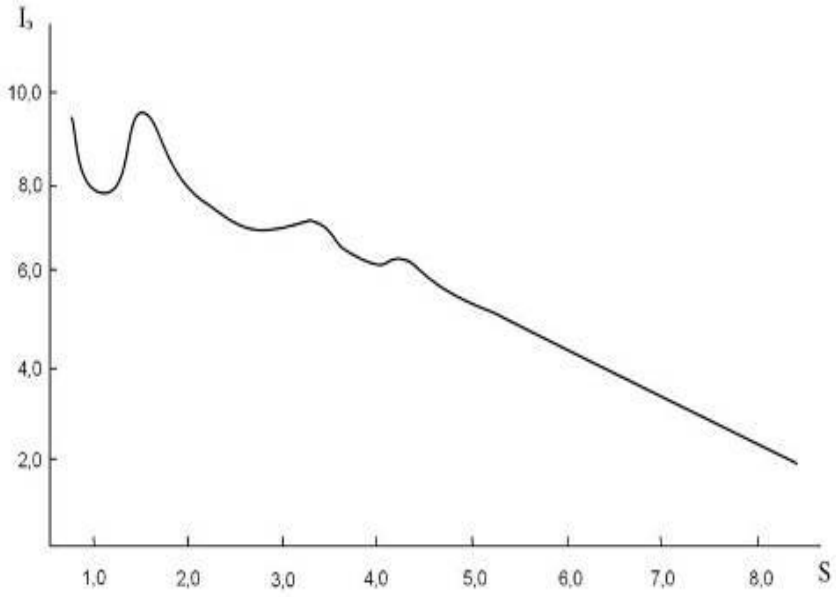

Fig. 2. Experimental intensity curve $I_e(S)$ of $TlIn_{0.93}Sn_{0.07}Te_2$ amorphous compound.

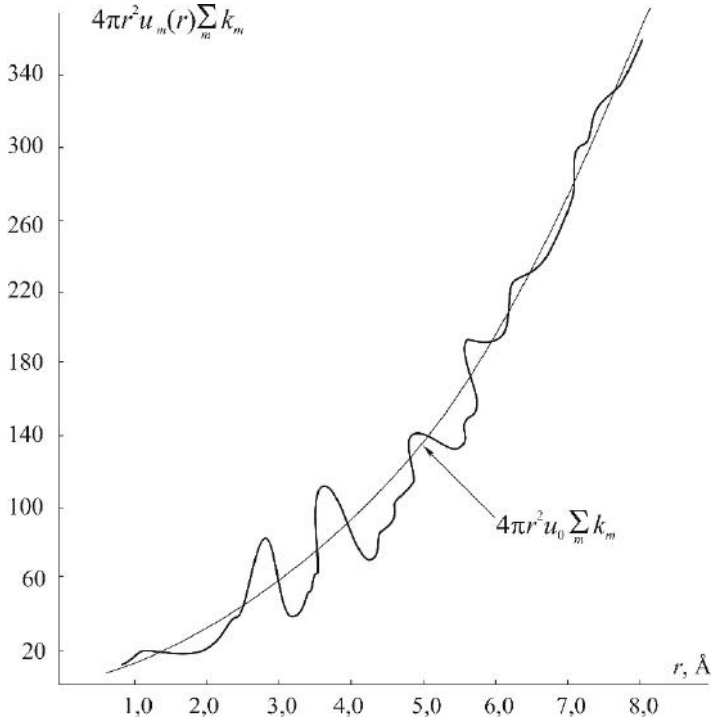

Fig. 3. Radial distribution curve of $TlIn_{0.93}Sn_{0.07}Te_2$ atoms.

For the CN calculated from the areas under the second coordination maximum, n_2=6 should be obtained, which indicates an octahedral environment of thallium atoms by tellurium ions. However, the area of the second peak of the ARDC gives an overestimated CN value, n_2=6.8. In this case, this is due to an increase in the intensity of the second main peak of the functions, which is determined by the interaction of Tl - Te and Sn atoms, taking into account the chemical bonding of the elements of the ternary compound $TlInTe_2$ ($Tl^+(In^{3+}Te_2^{2-})^-$) in an electric field. In addition, the negatively charged chains Te_2^{2-}- In^{3+}- Te_2^{2-} formed in this compound along the tetragonal axis consist of In^{3+} ions, partially Sn^{4+} and their nearest tetrahedral environment, including four Te^{2-} ions. The calculations performed allow us to assume that in the structure of $TlIn_{1-x}Sn_xTe_2$ films, the main matrix consists of tetrahedral and octahedral environments of atoms. It was found that in nanosized layers of $TlIn_{1-x}Sn_xTe_2$ compositions, which are in the amorphous state and crystallize in tetragonal syngonies, a certain fraction of the thallium atoms has an environment consisting of eight Te atoms and has a dense packing of structural units. It was found that the values of the indicated quantities depend on the chemical composition of the studied films and the degree of their doping with tin. It is interesting to note that the difference between the crystalline and amorphous states lies in a greater spread of bond lengths and valence angles in the amorphous body [11, 13]. It was determined that under the influence of an electric field and large values of "x" the reaction of the interaction of the element Sn with the compound $TlInTe_2$ leads to formation of substitution solid solutions with increased values of r of the indicated chemical compositions of $TlIn_{1-x}Sn_xTe_2$. When storing amorphous films in a vacuum of 10^{-2} Pa at room temperature in the dark, they retain their structural features for more than six months. It should also be noted that the conditions for obtaining amorphous $TlIn_{1-x}Sn_xTe_2$ films also affect their crystallization temperature [14].

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