THE STRUCTURE OF THE SHORT-RANGE ORDER OF THE AMORPHOUS $TlInSe_2$

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The short-range order in thin amorphous $TlInSe_2$ films has been investigated. The curves of radial distribution of atoms in the amorphous $TlInSe_2$ films are constructed on the base of the integral analysis of the fast electrons scattering intensity and the parameters of the short-range order: the radii of the coordination spheres and numbers of the nearest neighbor have been determined.

According to data [1,2] in the Tl-In-Se system the triple $TlInSe_2$ compound having the effective photo and strain sensitive semiconductive properties, has been revealed. Electron diffraction research [3] of the phase content of the $TlInSe_2$ films, obtained by the simultaneous and consequent vacuum settling of Tl, In, Se at room temperature, shows the formation of the $TlInSe_2$ compound with the structure of TlSe type, the Tl-In-Se films are amorphous irrespective to the order of the components settling.

Fig. 1. Electron diffraction photograph from amorphous $TlInSe_2$ films.

The purpose of the present paper is to determine the short-range order parameters of amorphous $TlInSe_2$, obtained from the vapor phase. The amorphous $TlInSe_2$ films of the thickness ~200Å have been obtained by the evaporation in the vacuum from the tugsten furnace on the NaCl substrate and celluloid at room temperature, the settling velocity was ~20Å/Sec. The obtained amorphous films are characterized by the diffraction figures (fig.1), on which the diffusion lines corresponding to $S=4\pi\cdot\sin\theta/\lambda=2{,}00$Å; 3,39Å and 5,04Å are well seen. These data coincide with the data, obtained before [3]. The subsequent crystallization of these films at ~170ºC leads to the $TlInSe_2$ crystal formation with the known parameters of the tetragonal lattice $a=8{,}075$Å, $c=6{,}847$Å [4].

The curve of the experimental intensity has been obtained on the PC, conjugated to the electronograph *ER*-102. The curve of the radial distribution of atoms (*CRDA*) of amorphous $TlInSe_2$, is presented on fig.2. The curve contains three, obviously expressed maximums at $r_1=2{,}70$Å, $r_2=3{,}68$Å and $r_3=4{,}25$Å. The areas under the corresponding maximums are equal to $\Delta=28{,}4$, $\Delta=31{,}2$ and $\Delta=67{,}6$, respectively.

The distance $r_1=2{,}70$Å may be interpreted as average from the distance between In-Se and Tl-Se atoms, the tetrahedral covalent radii are, according to [6], equal to 1,47Å for thallium, 1,17Å for selenium and 1,44Å for indium. The calculation of the area value under the first peak gives the value Δ=25,9, what coincides with the corresponding experimental data of the interatomic distance in $TlInSe_2$.

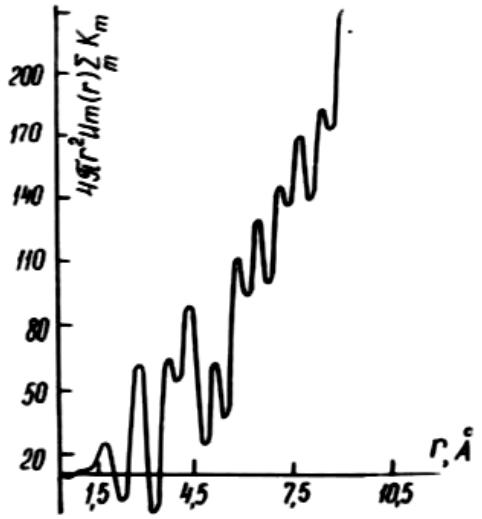

Fig. 2. The curve of the radial distribution of atoms in amorphous $TlInSe_2$ films.

The second coordination sphere with $r_2=3{,}68$Å may be interpreted as average of the distances In-Se and Tl-Se. There are Tl-Se distances approximately equal to r_2 in the crystal lattice of $TlInSe_2$. These distances are more than the sum of the octahedral covalent radii of Tl(In) and selenium atoms, as the sum in the case of Tl-Se is equal to 1,73Å+1,40Å=3,13Å and In-Se1,53Å+1,40Å=2,93Å. The calculation of the area value under the second peak of $TlInSe_2$, *CRDA* gives the value Δ-39,0. It is possible to explain by the fact, that obviously, in the second coordination sphere the Tl-Se distance is more possible, than that of In-Se. The distance $r_3=4{,}25$Å corresponds to the distance between same-named atoms Se-Se, Tl-Tl, In-In.

There are the same distances in the crystal lattice $TlInSe_2$, in consequence of what unlike the double structural and crystallochemical analog of the $A^2B^4C^5_2$ semiconductors, in which atoms of the IV group have undeformed tetrahedral anions [6], in compounds $A^3B^3C^6_2$, whose representative is $TlInSe_2$, analogous tetrahedrons of which are deformed. Beside the tetrahedrons deformation the specific deformation of octahedrons is observed in amorphous films $TlInSe_2$.

Possibly, it is connected to the fact, that in amorphous films $TlInSe_2$ the connection between particles is provided not only by the electrostatistic attraction of the opposite ions, but by the combination with the intermediate valence.

It has been shown by the research of the amorphous phases of the compound Ti-Se and Tl-S, that in amorphous phases of the compounds with the TlSe structure $n_{Se,\ Se}$=6, and $n_{Tl,\ Tl}$=4. It is possible to assume, that $n_{In,\ In}$ is equal to 4. Then the calculation of the area value under the corresponding peak gives the value Δ=67,3, what almost coincides with Δ_3=67,6.

Thus, it is possible to make a conclusion:

- The short-range order in the amorphous and crystal phases of $TlInSe_2$ are close and the structural elements of the crystal phase are conserved in amorphous films.

[1] *G.D. Huseynov, G.B. Abdullayev, E.M. Gojayev, et.al.* Constitutional diagram and physical properties of TlSe-InSe pseudo-binary system. Mater. Res. Bull. 1972, v.7, №12, p.1497-1503.

[2] *M.B. Babanli, A.N. Mamedov, A.A. Kuliyev.* Jurnal "Fiz. Khimiya" 1976, v.50, №7, p. 1888-1889.

[3] *D.I.Ismayilov,F.I. Aliyev, R.M.Sultanov, R.B.Shafi-zade.* Neorganicheskiye materiali, 1999, v.27, №3, p. 474-476

[4] *D. Muller, G. Eulenberger, H. Hahn*. Z. Anorg. allgem.chem., 1973, Bd 398, S. 207-220

[5] *B.K. Vainshtein, V.M. Fridkin, V.L. Inderbom.* Sovremennaya kristallographiya M. Nauka, 1979, v.2, p. 359

[6] *N.A. Goryunova, Y.A. Valov*. Poluprovodniki $A^{II}B^{IV}C_2^{V}$. M. Sov.radio.1974, p.376.

[7] *D.I. Ismayilov, M.F. Aliyeva*. Fizika, 1996, v.2, №2, p.43-45.

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AMORF $TlInSe_2$ TƏBƏQƏLƏRİNDƏ YAXIN NİZAM QURULUŞU

$TlInSe_2$ nazik amorf təbəqələrinin yaxın nizam quruluşu tədqiq edilmişdir. Sürətli elektronların səpilmə intensivliklərinin inteqral analizi əsasında atomların radial paylanma əyriləri qurularaq yaxın nizam parametrləri koordinasiya sferalarının radiusları və yaxın qonşuluqdakı atomların sayı - koordinasiya ədədləri təyin olunmuşdur.

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СТРУКТУРА БЛИЖНЕГО ПОРЯДКА АМОРФНЫХ ПЛЕНОК $TlInSe_2$

Исследован ближний порядок в тонких аморфных пленках состава $TlInSe_2$. На основе интегрального анализа интенсивности рассеяния быстрых электронов построены кривые радиального распределения атомов в аморфных пленках соединения $TlInSe_2$ и определены параметры ближнего порядка: радиусы координационных сфер и числа ближайщих соседей.

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