ATOM RADIAL DISTRIBUTION IN AMORPHOUS FILMS $Yb_{1-x}Sm_xAs_2Te_4$

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Electron scattering intensity curve from amorphous $Yb_{1-x}Sm_xAs_2Te_4$ films has been obtained by electron diffraction method depending on the scattering angle to S_{max}=120nm^{-1}.

Atom radial distribution curve has been plotted. The radii of coordination spheres have been determined in $Yb_{1-x}Sm_xAs_2Te_4$.

The use of complex compounds of rare-earth elements under pressure of chalcogenide saturated vapors allows obtaining by thermal spraying of the films which are perspective ones for formation of planar light guide [1].

The amorphous films of compounds of $Yb_{1-x}Sm_x$–As_2Te_3 system containing glass chalcogenides (GCh) and rare-earth elements obtained by thermal evaporation have been investigated in refs [2-3].

The atom radial distribution in amorphous films $Yb_{1-x}Sm_xAs_2Te_4$ (x=0,02%) has been studied in the present work.

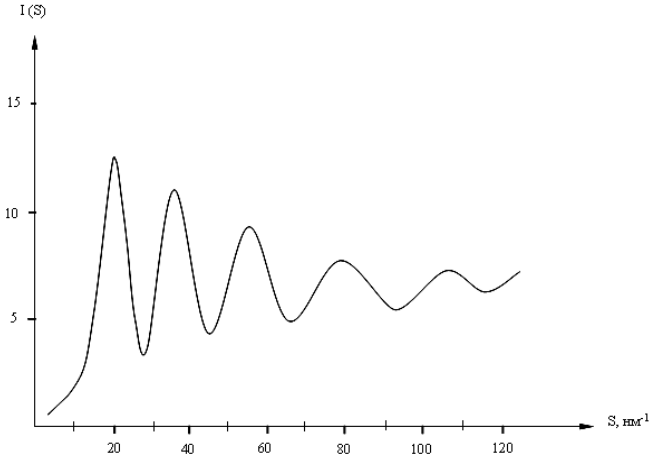

Fig.1. The intensity curves of electron scattering for $Yb_{1-x}Sm_xAs_2Te_4$ amorphous films.

The amorphous films $Yb_{1-x}Sm_xAs_2Te_4$ with thickness ~30 nm are obtained by thermal evaporation of monocrystalline $Yb_{1-x}Sm_xAs_2Te_4$ from specially made furnaces from wolfram-rhenium alloy in vacuum ~10^{-5}Pa. The dosed content of Sm impurity in compounds is 0.02%. The freshly cleaved faces of NaCl, KCl crystal and amorphous celluloid being at room temperature are used as substrates. The deposition rate of films is ~10 nm/sec. The obtained amorphous films are stable at room temperature and crystallize at temperature T=503K. $Yb_{1-x}Sm_xAs_2Te_4$ in crystalline state has rhombic lattice with parameters: a=1,148, b=1,410, c=1,410, c=0,407nm sp.gr.P_{man}.

The crystallization of amorphous films shows the identity of the compositions of amorphous and crystalline films. The structure of short range ordering in $Yb_{1-x}Sm_xAs_2Te_4$ films is studied by diffraction method of fast electrons (U_{acc}=74kV) with the use of rotating sector that allows revealing the maximums of diffraction reflection in far-angular region. The intensity curve of electron scattering the maximal value of "S" for which is equal to S_{max}=120nm^{-1} (fig.1) has been constructed after electron-diffraction pattern microphotometering. The five maximums at S_1=21,0 nm^{-1}; S_2=36,0 nm^{-1}; S_3=56,0 nm^{-1}; S_4=79,0 nm^{-1}; S_5=106,0 nm^{-1} are observed on intensity curve of electron scattering in the dependence on scattering angle.

The method of atom radial distribution is used for definition of amorphous film structures. The curves of atom radial distribution (CARD) for amorphous compounds are constructed by us on the base of known formula [4]:

$$4\pi r^2 \sum_i \sum_j c_i k_i k_j \rho_{ij}(r) = 4\pi r^2 \rho_o \left(\sum_i c_i k_i \right)^2 + \frac{2r}{\pi} \alpha \int_o^s s[\alpha(s) - 1] \sin srds \qquad (1)$$

Here $\rho_{ij}(r)$ is partial function of radial distribution of atomic density of j-type atoms round i-type ones, α is normalizing constant, α (s) is structural factor, $S=4\pi\sin\theta/\lambda$, where θ is scattering angle. The "c" coefficients in formula (1) take into consideration the relative content of element atoms including in chemical formula of investigated compound. The relative atom scattering abilities of each chemical element "k" are defined by the formula:

$$k_i = \frac{k(s)}{\sqrt{\sum_{i=1}^{3} c_i f_i^2(s)}} \qquad (2)$$

where f_1(s) is atom scattering factor of i-type element. The average atomic density ρ_0 of investigated amorphous films is calculated by the following formula:

$$\rho_0 = \frac{\rho N_A}{\sum_I c_i A_I} \qquad (3)$$

where ρ is density of crystalline substance in g/sm^3, A_i are element atomic masses including into chemical formula, N_A is Avogadro constant which is equal to $6\cdot10^{23}$mol^{-1}. The normalizing constant "α" for transition from relative intensity units to absolute ones defined by us on average atomic density is equal to α=0,09 for $Yb_{1-x}Sm_xAs_2Te_4$. The average atomic density ρ_0 calculated on (3) is equal to ρ_0=0,426nm^{-1}. K_{Yb}=1,319; K_{As}=0,714; K_{Te}=1,031 are obtained for scattering abilities of ytterbium, arsenic and tellurium. CARD (fig.2) is calculated and constructed on the base of obtained experimental intensity on formula (1). The radii of first and second coordination spheres which are equal to 0,245nm and 0,372nm correspondingly are defined from CARD. The radius decrease of coordination spheres in $Yb_{1-x}Sm_xAs_2Te_4$ in comparison with amorphous $YbAs_2Te_4$ is connected with impurity influence of Sm atoms [5]. The first coordination maximum on CARD of amorphous $Yb_{1-x}Sm_xAs_2Te_4$ corresponds to As – Te distance, but atoms of tellurium and arsenic are connected with each other by the covalent bond. It follows from the fact that sum of covalent radii of arsenic and tellurium is equal to $r_{As}^{cov}+r_{Te}^{cov}$ =0,121nm+0,117nm = 0,238nm that is close to the radius value of first coordination sphere (r_1=0,245). The Yb^{2+} ions in the structure of amorphous $Yb_{1-x}Sm_xAs_2Te_4$ are in the second coordination sphere of arsenic atoms and are nearest neighbors of tellurium atoms. The sum of radii of first coordination sphere and Yb^{2+} ion ($r_1 + r_{Yb}$ =0,245 + 0,107 = 0,352 nm) evidences about this fact that is close to the radius value of second coordination sphere r_2=0,352 nm).

Thus, it is established that the obtained films are amorphous ones at vacuum deposition of monocrystalline $Yb_{1-x}Sm_xAs_2Te_4$ on NaCl, KCl substrates and on amorphous celluloid being at room temperature.

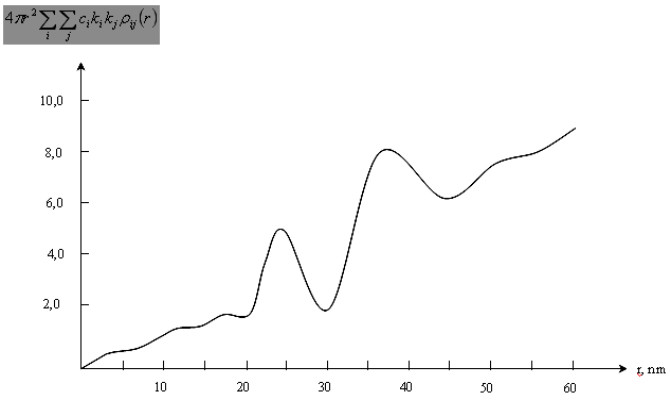

Fig.2. The curve of atom radial distribution $Yb_{1-x}Sm_xAs_2Te_4$.

It is shown that impurities of Sm atoms influence on radius values of coordination spheres of $YbAs_2Te_4$, i.e. I and II radii of coordination spheres of $Yb_{1-x}Sm_xAs_2Te_4$ decrease in comparison with $YbAs_2Te_4$.

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[4] *A.F. Skrishevsky*. Strukturniy analiz jidkostey i amorfnikh tel. M.: Visshaya shkola, 1980. s. 328. (in Russian)

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$Yb_{1-x}Sm_xAs_2Te_4$ NAZİK TƏBƏQƏLƏRİNDƏ ATOMLARIN RADİAL PAYLANMASI

$Yb_{1-x}Sm_xAs_2Te_4$ nazik təbəqələrindən elektronların səpilməsinin intensivlik əyriləri səpilmə bucağından (C_{max}=120 нм$^{-1}$) asılı olaraq alınmışdır. $Yb_{1-x}Sm_xAs_2Te_4$ nazik təbəqələrində atomların radial paylanma əyrisi qurulmuş və koordinasiya sferalarının radiusları təyin edilmişdir.

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РАДИАЛЬНОЕ РАСПРЕДЕЛЕНИЕ АТОМОВ В АМОРФНЫХ ПЛЕНКАХ $Yb_{1-x}Sm_xAs_2Te_4$

Получена кривая интенсивности рассеяния электронов в зависимости от угла рассеяния до S_{max}=120нм$^{-1}$ для аморфных пленок $Yb_{1-x}Sm_xAs_2Te_4$.
Построена кривая радиального распределения атомов. Определены радиусы координационных сфер в $Yb_{1-x}Sm_xAs_2Te_4$.

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