THE INFLUENCE OF Sm IMPURITIES ON ATOMIC SPACINGS IN AMORPHOUS NANOTHICKNESS FILMS OF $Yb_3As_4Se_9$ COMPOUNDS

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The curve of electron scattering intensity in the dependence on scattering angle up to S_{max}=210nm^{-1} for thin amorphous films $Yb_{3(1-x)}Sm_xAs_4Se_9$ (x=0,2 at.%) is obtained. The curve of atom radial distribution is constructed. The radiuses of coordination spheres and partial coordination numbers in $Yb_{3(1-x)}Sm_xAs_4Se_9$ are defined. It is shown, that Sm atom impurities influence on atomic spacings in $Yb_3As_4Se_9$.

The structure of short range order in thin amorphous films $Yb_3As_4Se_9$ has been earlier studied by us and atomic spacings and atom coordination number in the amorphous film of above mentioned compounds have been defined [1]. The given work is dedicated to study of Sm impurity influence on atomic spacings in amorphous films $Yb_3As_4Se_9$.

The amorphous films of thickness ~35 nm are obtained at evaporation of monocrystalline $Yb_{3(1-x)}Sm_xAs_4Se_9$ (x=0.2ат.%) and further precipitation with velocity ~10 nm/s on NaCl, KCl substrates and amorphous celluloid, being at room temperature. The dosing content of Sm impurity in $Yb_3As_4Se_9$ is 0.2 at%. The pressure of residual gases in coating chamber is ~10^{-4} Pa. Further crystallization of obtained amorphous films shows the composition identity of amorphous and crystalline films. The thin films are investigated with the help of diffraction method of high-speed electrons on vertical electron diffractometer by EMR–102 brand at accelerating voltage 75 kV.

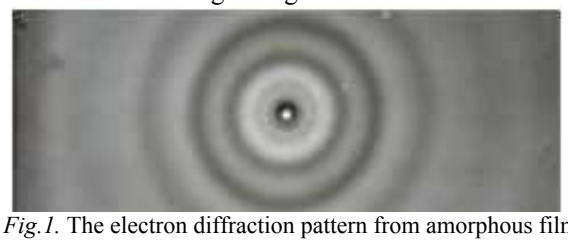

Fig.1. The electron diffraction pattern from amorphous films $Yb_{3(1-x)}Sm_xAs_4Se_9$.

The electron diffraction patterns from amorphous films are obtained by the method of alternating exposure that allows taking into consideration the far-angular electron scattering, consisting the valuable information about atomic spacings and coordination numbers. This allows increasing the reliability of obtained atomic spacings and coordination numbers in studied amorphous films. The electron diffraction patterns from amorphous films $Yb_{3(1-x)}Sm_xAs_4Se_9$ are obtained with the help of rotating sector for Ge with further correction on given substance [2] (fig.1). The intensity curve, the maximum "s" value for which is equal S_{max} =210 nm^{-1} has been constructed after microphotometry. The 8 maximums at S: S_1 =22,5; S_2 =37,0; S_3 =57,0; S_4 =85,0; S_5 =109,5; S_6 =136,0; S_7 =163,0; S_8 =192,0 nm are observed on the curve of high-speed electron scattering intensity (fig.2).

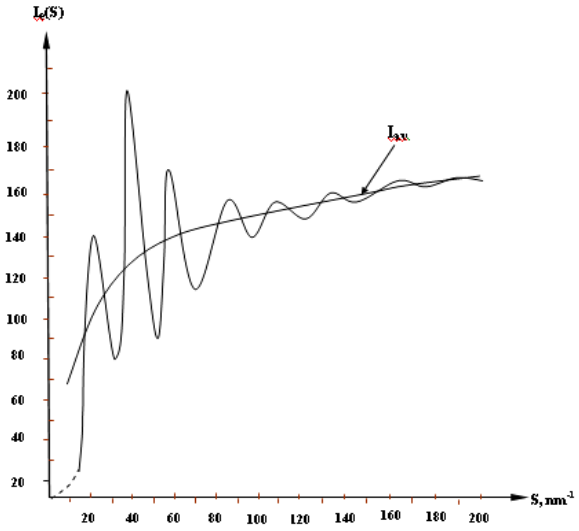

Fig.2. The curve of electron scattering intensity and curve of average intensity for amorphous films $Yb_{3(1-x)}Sm_xAs_4Se_9$.

The statistic method basing on the use of atomic density distribution function is the most effective method of structure description of amorphous and liquid states. The formula, given in [3] is in the base of above mentioned method, defining the curve of atom radial distribution (CARD) of amorphous substances, consisting of atoms of different sorts.

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

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

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

where $f_i(s)$ is atomic scattering factor of i-th element. The average atomic density ρ_o of investigated amorphous films is calculated by us by the formula:

$$\rho_o = \frac{\rho N_A}{\sum_I c_i A_i}, \qquad (3)$$

where ρ is density of crystalline substance in g/cm^3, A_i are atomic weights of elements, including in chemical formula, N_A is Avogadro's number, which is equal to $6\cdot10^{23}$ mol^{-1}. The normalization coefficient (α) is defined by extrapolation of near-angular region of structural factor, which is equal to 0,097. The average atomic density and effective scattering powers of ytterbium (Yb), arsenic and selenium are calculated on technique [4] and are equal to: ρ_o=0,0429 cm^{-3}; $K_{Yb}^{av.}$=1,530; $K_{As}^{av.}$=0,829; $K_{Se}^{av.}$=0,824 correspondingly. The curve of atom radial distribution for amorphous $Yb_{3(1-x)}Sm_xAs_4Se_9$ is calculated after α definition and construction of interference function on special program. The two strong and several few maximums are observed on CARD (fig.3).

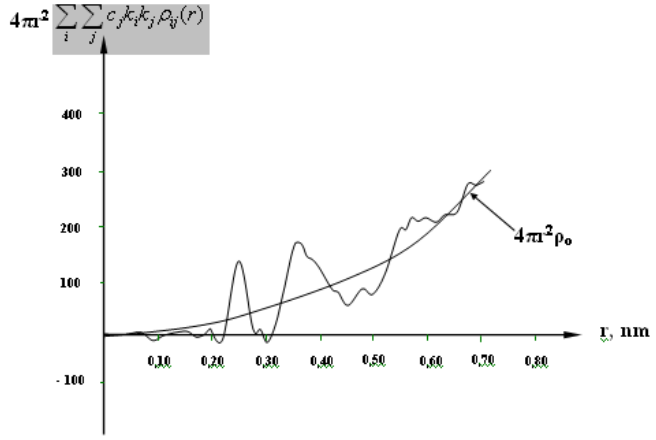

Fig. 3. The curve of atom radial distribution for $Yb_{3(1-x)}Sm_xAs_4Se_9$.

The strong isolation of first maximum evidences about bond covalence between atoms, the distances between which it reflects. As it is seen on CARD, the distance 0,24nm corresponds to first maximum. The radius of first coordination sphere reflects the distance between atoms of arsenic and selenium, connected between each other by covalent bond:

$$r_{As}^{cov.} + r_{Se}^{cov.} = 0{,}121 + 0{,}117 = 0{,}238\ nm$$

The second maximum on CARD, which corresponds to distance r_2=0,365 nм is radius of second coordination sphere and is caused by distance As-Yb^{2+}, caused by the fact that sum of first coordination sphere radius and ion bond radius is equal to:

$$r_1 + r_{Yb}^{2+} = 0{,}24 + 0{,}107 = 0{,}347\ nm$$

The radii of coordination spheres in $Yb_{3(1-x)}Sm_xAs_4Se_9$ are less in comparison with ones in $Yb_3As_4Se_9$. The differences in atomic spacings in $Yb_3As_4Se_9$ compounds and ones, doped by Sm atoms are probably explained by influence of Sm impurity atoms. The decrease of atomic spacings is observed for others compounds of Yb – As – Se system, doped by Sm atoms [5]. As the atomic spacings are the one of the main parameters of structure of amorphous substances, then it is possible to suggest that coordination numbers of amorphous compounds $Yb_{3(1-x)}Sm_xAs_4Se_9$ also change. The partial coordination numbers for $Yb_{3(1-x)}Sm_xAs_4Se_9$ are defined in terms of formula (4), applied as for amorphous films of $Yb_3As_4Se_9$ compounds [1].

$$\sum_{i=1}^{3}\sum_{j=1}^{3} c_i k_i k_j n_{ij} = Q_1, \qquad (4)$$

where

Q_1 – square under first maximum, calculated on Simpson method

n_{ij} – atom number of j sort round one atom i

c_i – relative content of element, including in chemical formula of investigated compound

k_i – relative average scattering power of i sort atom.

The averaging "k_i" is carried out on the formula:

$$< k_i >= \frac{1}{s_m}\int_o^{s_m} k_i(s)ds, \qquad (5)$$

s_m is maximum from considered values $s=4\pi\sin\theta/\lambda$ (θ is scattering angle).

On the assumption of relative element concentrations and averaged scattering powers of elements, including in chemical formula, the coordination numbers in amorphous $Yb_{3(1-x)}Sm_xAs_4Se_9$ are defined.

It is established that 3 selenium atoms are in amorphous $Yb_{3(1-x)}Sm_xAs_4Se_9$ near ytterbium ions, also as in amorphous $Yb_3As_4Se_9$.

Thus, the difference in atomic spacings, i.e. the decrease of radiuses of coordination spheres in the comparison with atomic spacings in $Yb_3As_4Se_9$ [1] is observed at investigation of structure of short-range order in amorphous films $Yb_{3(1-x)}Sm_xAs_4Se_9$, that is explained by influence of Sm impurities on atomic spacings.

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Sm AŞQARLARININ $Yb_3As_4Se_9$ BİRLƏŞMƏLƏRİNİN AMORF NANOQALINLIQLI TƏBƏQƏLƏRDƏ ATOMLARARASI MƏSAFƏYƏ TƏSİRİ

Elektronoqrafiya üsulu ilə $Yb_{3(1-x)}Sm_x$ As_4Se_9 (x=0,2 at.%) amorf təbəqələrindən elektronların səpilmələrinin intensivlik əyriləri alınmışdır (S_{max}=210 nm^{-1}). Nanoqalınlıqlı amorf təbəqələrində atomların radial paylanma əyrisi qurulmuş və onların yaxın nizam quruluşu parametrləri təyin edilmişdir. Göstərilmişdir ki, Sm atomunun aşqarları $Yb_3As_4Se_9$ birləşməsinin amorf nazik təbəqələrindəki atomlararası məsafənin dəyişməsinə səbəb olur.

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ВЛИЯНИЕ ПРИМЕСЕЙ Sm НА МЕЖАТОМНЫЕ РАССТОЯНИЯ В АМОРФНЫХ НАНОТОЛЩИННЫХ ПЛЕНКАХ СОЕДИНЕНИЙ $Yb_3As_4Se_9$

Получена кривая интенсивности рассеяния электронов в зависимости от угла рассеяния до S_{max}=210$нм^{-1}$ для тонких аморфных пленок $Yb_{3(1-x)}Sm_xAs_4Se_9$ (x=0,2 ат.%). Построена кривая радиального распределения атомов. Определены радиусы координационных сфер и парциальные координационные числа атомов в $Yb_{3(1-x)}Sm_xAs_4Se_9$. Показано, что примеси атомов Sm влияют на межатомные расстояния в $Yb_3As_4Se_9$.

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