

ORDERING IN SE-TE ALLOYS

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Atomic short-range order was previously investigated in solid solutions of metals and semiconductors with closed-packed structure or with diamond-type structure, and the existence of a nonrandom relative placement of atoms of different sorts was observed in all the investigated systems. The presence of short-range order was registered also in liquid alloys. At the same time, experiment has not revealed to this day a similar type of order in structures, say, of chainlike character. Only recently [1] did an investigation of the distribution of diffuse scattering of X-rays in the Se-Te alloy show that atomic short-range order is produced in this alloy, with preferred neighborhood of unlike atoms. This follows from Fig. 1, which shows the distribution of the intensity of the diffuse scattering (as a function of the slip angle θ) for an Se-Te alloy of equiatomic composition.

It is seen that a maximum of diffuse scattering is observed near the possible superstructure line. It is interesting that this maximum has produced a rise on the plot of the intensity of the scattering by an amorphous alloy of Se with 4 at.% Te (Fig. 1). This rise is connected with the preservation of the predominant neighborhoods of the Se and Te atoms and on going into the amorphous phase.

This work was undertaken to explain the observed phenomena on the basis of pseudopotential theory. As shown in [2-4], the ordering energy is connected with the formfactors of the pseudopotentials of the alloy components by the relation

$$V(R) = \frac{\Omega_0}{\pi^2} \int F(q) q^2 \frac{\sin(qR)}{qR} dq, \quad (1)$$

where Ω_0 is the atomic volume, q is the modulus of the wave vector that connects the initial and final states of the electron, R is the interatomic distance, and $F(q)$ is a characteristic function given by

$$F(q) = \frac{\Omega_0}{8\pi} |\Delta w(q)|^2 q^2 \frac{\epsilon(q) - 1}{\epsilon^*(q)} + \frac{2\pi}{\Omega_0 q^2} |\Delta z|^2 e^{-q^2/4\eta}. \quad (2)$$

Here $\Delta w(q) = w_A(q) - w_B(q)$; $w_A(q)$ and $w_B(q)$ are the unscreened formfactors of the components; $\epsilon(q)$ is the permittivity, $\epsilon^*(q)$ is the permittivity corrected for exchange and correlation, Δz is the difference between the valences of the components, and η is the Ewald parameter. To calculate $F(q)$ we used the formfactors $w_A(q)$ and $w_B(q)$ calculated with the aid of the analytic expressions for $w(q)$ [5] and the parameters proposed by Animalu [6]. The validity of such a calculation was demonstrated in [7].

The results of the calculation of $V(R)$ are shown in Fig. 2. It is seen that $V(R)$ is positive near R_1 and large enough compared with the values of $V(R)$ on all the other coordination spheres. The parameter α_1 must therefore be negative, since the signs of $\alpha(R_1)$ and $V(R_1)$ are opposite.

To explain the constancy of the sign of $\alpha(R_1)$ on going from the crystalline to the amorphous phase, it is necessary to consider the pseudopotential approximation of atomic short-range order of crystalline alloys for amorphous alloys. It can be shown that the band energy, which depends on the atomic short-range order, of an amorphous or liquid alloy is given by

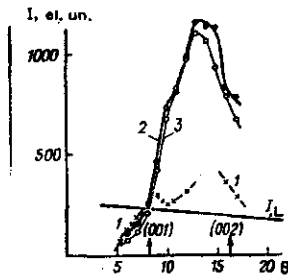


Fig. 1

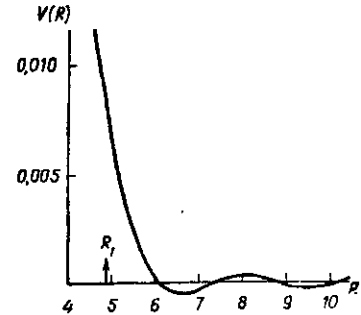


Fig. 2

Fig. 1. Intensity of diffuse scattering by a crystalline Se-Te alloy (1) and by amorphous Se + 4 at.% Te (2) and pure Se (3), (001) and (002) are the possible superstructure lines.

Fig. 2. Ordering energy of Se-Te alloy, calculated by the pseudopotential method.

$$E_{b.am.} = \frac{\Omega_0}{(2\pi)^3} \int dq 4\pi q^2 \left\{ 4\pi \int \alpha(R) \rho(R) \times \right. \\ \left. \times R^2 \frac{\sin(qR)}{qR} |\omega_A - \omega_B|^2 C_A C_B \frac{\epsilon(q) - 1}{\epsilon^*(q)} dR \right\} - 4\pi \alpha(R) \rho(R) R^2 V(R) dR. \quad (3)$$

Here $\rho(R)$ is the distribution function of the atoms in the interatomic distances; this function, as shown by numerous investigations of liquid and amorphous materials, is a modulated function and its maxima (at least at relatively small R) are located near the radii of the coordination spheres. For this function we have

$$C_i = \int_{R_i - \Delta R}^{R_i + \Delta R} 4\pi R^2 \rho(R) dR. \quad (4)$$

C_i is the coordination number, and R_i is the radius of the i -th coordination sphere. If (4) is taken into account, it is easily seen that (3) goes over into the expression for the band energy of a solid solution (we assume, of course, that in this case $\epsilon(q)$ does not change significantly).

Therefore, if on going from the crystalline to the amorphous phase $\rho(R)$ becomes smeared out relative to R_i in such a way that the sign of $V(R_i)$ remains unchanged in the smearing region, the sign of the short-range order should also be conserved in this transition. Judging from the form of $V(R)$ (Fig. 2), this condition is satisfied for the alloy in question. The sign of $\alpha(R_i)$ should therefore be conserved on going from the crystalline Se-Te alloy to the amorphous one, as was in fact observed.

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