THE BLUR OF THE ORDER PARAMETER IN ARGENTUM CHALCOGENIDE IN THE REGION OF THE PHASE TRANSITION

S.A. ALIYEV
Institute of Physics of NASA, Baku-1143, G. Javid av., 33

The temperature dependence of the order parameter η in argentums chalcogenides is defined using the temperature differential coefficient of the inclusion function in the zero approximation. It is revealed, that η in the region of the phase transition (PT) is strongly blurred. It is established, that Ag_2Te, Ag_2Se and Ag_2S achieve only 69%, 52% and 49% in the phase disorder region PT correspondingly.

The order parameter η, characterizing the physical state of the phases in PT region takes the important place among the parameters, describing the PT. That's why the investigation of the temperature dependence $\eta(T)$ in PT region can add the current information about PT nature in argentums chalcogenides and give the comprehensive data about phase disorder in PT process.

According to the classic theory of PT, the η parameter is considered for the ordered system $\eta \neq 0$, and for the unordered system $\eta=0$. In such interpretation PT can be considered as the system transfers from the ordered state into unordered one. The η parameter depends on T at the constant pressure, and achieves the zero meaning in PT-T_0 point, when the ordering disappears.

However, in the common case the change of η near PT can be as in spurts, so constantly. These questions had been considered in the refs [1-3], in which Landau developed his theory for PT of II type, considering them more interesting as physical ones. But the main conditions are applied for another PT also. Taking under the consideration the small meaning of η near PT-T_0, analyzing the thermodynamic potential $P(\eta)$, depending on η, we obtain:

$$\Phi=\Phi_0+\alpha\eta^2+\beta/2\,\eta^4\,, \qquad (1)$$

Where Φ_0 is thermodynamic potential of the disordered phase, α and β are decomposition coefficients. Using the equilibrium conditions for the thermodynamic potential of the ordered phase at the given pressure, we obtain:

$$\alpha(T)=\alpha_0(T-T_0)\,, \qquad (2)$$

where $\alpha_0>0$. As β changes weakly near PT-T_0 point, so changed it on $\beta_0>0$ and limited by the quadratic member, we obtain

$$\eta^2=\alpha_0(T_0-T)/\beta_0\,, \qquad (3)$$

being the main result of Landau theory for PT II.

But it is need to note, that the fluctuation of the compound and other physical values, order parameter η, also as PT parameters and the thermodynamic parameters, can be blurred because of the existing the microgeterogeneities in the solid bodies. The given question is discussed in the ref [4] and the model of the elementary subsystems (ES) is supposed to use for its decision. Toward this end the system can be divided on the big number of ES with the similar volumes v_0 near PT point. Such system is characterized by the macroscopic temperature T and macroscopic point PT-T_0. The separate ES have local temperature τ, differed from all T sample. If change of T carries out slowly enough, then the definite distribution of ES on the local temperatures carries out at the each meaning of the temperature. For comfort of the calculations, the local temperature of ES τ is accounted from average T as $\theta=T-\tau$. Designating the being probability of ES through $W(\theta)$ with the local temperature in the limits from θ till $\theta+d\theta$, we obtain

$$dW(\theta)=\varphi(\theta)d\theta\,, \qquad (4)$$

where $\varphi(\theta)$ presents the probability density, the norm of which is equal to one. Knowing the distribution probability of $dW(\theta)$, it is possible to calculate the temperature dependence $\eta(T)$. Designated the order parameter through $\eta^2(\tau, \theta)$ at the macroscopic temperature $t=T-T_0$ of that part of the system, the local temperature of which is in the limits from θ till $\theta+d\theta$, then at t we obtain:

$$\eta^2(t)=\int \eta^2(t\bullet\theta)d\theta=\int \eta^2(t\cdot\theta)\varphi(\theta)d(\theta) \qquad (5)$$

As it is seen it is need to know the distribution function of ES on the local temperatures $\varphi(\theta)$ and the order parameter of the separate ES for the calculation of square of order parameter $\eta^2(t)$. It is supposed, that the first from them can be defined on the base of the common introduction of the fluctuation theories, and second one is defined by PT character in the separate ES (PT of I and PT of II type). In the case, when ES consist on the PT of II type, without taking under consideration of effects of anisotropy and elastic stresses on the base of formulae (3), we obtain:

$$\eta^2(T,\theta) = \alpha_0/\beta_0\,(\theta- t), \quad (\text{at } t\le\theta) \qquad (6)$$

And consequently

$$\eta^2(t)= \alpha_0/\beta_0\int_t^\infty \varphi(\theta)\cdot(\theta-t)d\theta. \qquad (7)$$

As it was mentioned, it is need to apply the fluctuation theory for the calculation of $\varphi(\theta)$. In [4] the case of small fluctuations, realizing on practices very often is considered, at which

$$dW(\theta)=\frac{1}{\nu\sqrt{n}}\exp(-\frac{\theta^2}{\nu^2})d\theta\,, \qquad (8)$$

where ν parameter characterizes the given distribution. Considering ν as the constant value, we obtain:

$$\eta^2(t)= \frac{\alpha_0 \nu}{2\beta_0\sqrt{\pi}}\exp\left(-\frac{t^2}{y^2}\right)-\frac{t\alpha_0}{2\beta_0}\left[1+\Phi\left(\frac{\sqrt{2}}{y}|t|\right)\right], \quad (t<0)$$

$$\eta^2(t)= \frac{\alpha_0 \nu}{2\beta_0\sqrt{\pi}}\exp\left(-\frac{t^2}{y^2}\right)-\frac{t\alpha_0}{2\beta_0}\left[1-\Phi\left(\frac{\sqrt{2}}{y}|t|\right)\right], \quad (t>0) \qquad (9)$$

where

$$\Phi(x)=\sqrt{\frac{2}{\pi}}\cdot\int_0^x exp\left(-\frac{x^2}{2}\right)dx$$

In ref. [4] the calculations $\eta(t)$ for PT of II type had been carried out. For this the definite simplifications and admissions, defensible for the common theoretical evaluation $\eta(t)$ had been carried out. The obtained data are compared with the calculated curves, carried out on Landau classic theory (on formulae 3). It is shown, that the blur of order parameter η has place in the case of the heterogeneity in the solid bodies in region of PT of II type. At the same time, it is observed, that the blur of η can take place at the other PT.

The task in the given ref. leads to the selection method for the definition of the order parameter η and the degree of its blur in PT region of argentums chalcogenides, having the structural PT. In principle, ES model can be applied to the argentums chalcogenides, considering α-phase till phase transition through the ordered system, and the inclusion of germs of β-phase in each PT point through elementary subsystems, having local temperatures $\theta=T-\tau$ and creating the disordering of phase system. However, as it is seen from (9) the ν parameter, characterizing the distribution of small fluctuations, thermodynamic potential $\Phi(x)$, the local temperatures of germs, and other parameters, the values of which in the difference from the theoretical evaluations η is hard to define for the concrete crystal, enter in their expressions. At the same time, it is known, that the differences in the character of the phase transitions is more clear revealed with the help of the physical values, connected with the differential coefficients of parameters, characterizing PT. The $L_0(T)$ and dL_0/dT have been investigated for the argentums chalcogenides in refs [5-8] and it is shown, that PT are strongly blurred in them. That's why the blur of order parameter η in PT region can be considered by the introduction of dL_0/dT in the formulas (3) or (9) in the form:

$$\eta^2(t)=\frac{\alpha_0}{\beta_0}\cdot\left(\frac{dL_0}{dT}\right)^{-1}=\frac{\alpha_0}{\beta_0}\frac{2}{a_0}\left\{1+ch\left[a_0(T-T_0\right]\right\} \quad (10)$$

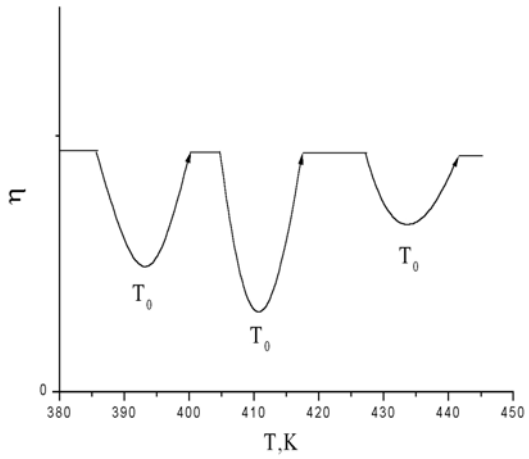

Fig.1. Temperature dependence of order parameter in argentums chalcogenides: a-Ag_2Te, в-Ag_2Se и с-Ag_2S.

where a_0 is temperature constant of PT, characterizing the blur degree of PT. Then the temperature motion $\eta(t)$ in the ordered region is defined by the formula (3), and in PT region is defined by formulae (10). The calculation results, carried out for the Ag_2Te, Ag_2Se and Ag_2S samples (with excess Te≈0,75at.%) in SPT (α'-β') with the use of a_0 and dL_0/dT parameters [5-8], are presented on the fig.1. At the calculations β_0 was considered constant ($\beta_0>0$), and α_0 was selected analogically to the theoretical calculations, carried out in ref [4]. The ration α_0/β_0in PT region didn't influence significantly on $\eta(T)$. As it is seen from the figure, the change of $\eta(T)$ at PT hasn't clearly spasmodic type, has the wide interval ΔT, the curve $\eta(T)$ is strongly blurred near PT-T_0 point and η_0 meaning is more bigger than zero. All this shows on the strongly blur of order parameter. Physically it means that disordering of the phases at PT in the argentums chalcogenides doesn't carry out totally, as it is followed from the classical theory. In Ag_2Te, Ag_2Se and Ag_2S the disordering of phases in PT region achieves only 69%, 62% and 49% correspondingly.

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S.A. Əliyev

FAZA KEÇİDİ OBLASTINDA GÜMÜŞ XALKOQENİDLƏRDƏ NİZAMLILIQ PARAMETRİNİN YAYINIQLIĞI

Sıfırıncı yaxınlaşmada daxilolma funksiyasının törəməsinin temperatur asılılığından istifadə edilərək gümüş xalkoqenidlərdə η nizamlılıq parametrinin temperatur asılılığı təyin edilmişdir. Faza keçidi (FK) oblastında η-nin kəskin yayınıq olması müşahidə edilmişdir. FK oblastında Ag_2Te, Ag_2Se, Ag_2S –də fazaların yayınıqlığının uyğun olaraq 69%, 52% və 49% olduğu göstərilmişdir.

С.А.Алиев

РАЗМЫТИЕ ПАРАМЕТРА УПОРЯДОЧЕНИЯ В ХАЛЬКОГЕНИДАХ СЕРЕБРА В ОБЛАСТИ ФАЗОВОГО ПЕРЕХОДА

Используя температурную производную функции включения в нулевом приближении определена температурная зависимость параметра неупорядоченности η в халькогенидах серебра. Обнаружено, что в области фазового перехода (ФП) η сильно размыт. Установлено, что разупорядочение фаз, в области ФП Ag_2Te, Ag_2Se и Ag_2S достигает только 69%, 52% и 49% соответственно.

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