ABOUT DIFFUSION OF PHASE TRANSITION OF $AgSbTe_2$

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It was investigated the influence of second phase on the electrical conductivity, thermo-e.m.f. and Hall coefficient of $AgSbTe_2$ in 200-450K temperature interval. It was shown, that the phase transition in $AgSbTe_2$ related by presence of p-Ag_2Te is diffuse and encompasses ~70% from all phase transition. It was established, that the $\alpha \rightarrow \beta$ phase transition has exponential character.

Introduction

In [1] was conducted the detailed research of thermoelectric properties of samples of Ag-Sb-Te system. Samples were obtained by a method of zone crystallization. The experiments have shown that from a beginning part to middle of an ingot samples are monophase and correspond to $Ag_{19}Sb_{29}Te_{52}$. Starting from middle of an ingot on temperature dependencies of electrical conductivity $\sigma(T)$, Hall coefficients $R(T)$ and thermo-e.m.f. $\alpha(T)$ the anomalies were observed. These results were analyzed within the framework of the theory of kinetic phenomena for two-phase systems [2]. Was proposed, that in investigated samples the matrix is $Ag_{19}Sb_{29}Te_{52}$, and second phase p-Ag_2Te. Was established, that really these structures are two-phase and the contents of the second phase changes within the limits of 11-13 vol. %. In [3] is established, that in crystals of Ag_2Te the structural phase transition (SFT) has diffusion nature. Was calculated the parameters of diffusion phase transition (DFT) T_0, a, $L_0(T)$, dL_0/dT, and is determined the area and degree of diffusion of phase transition (FT).

In this work was put the problem to consider the influencing of the second phase Ag_2Te on electrical properties of a system Ag-Sb-Te at more high temperature encompassing area of FT and to study the contents Ag_2Te on electrical properties in FT area.

Experimental results

In a fig. 1 the temperature dependencies of coefficients of electrical conductivity $\sigma(T)$, Hall $R(T)$ and thermo-e.m.f. $\alpha(T)$ of $AgSbTe_2$ are shown. As it is visible, since 390K the discontinuous change of all three factors takes place that unconditionally, is connected with FT Ag_2Te containing in $AgSbTe_2$.

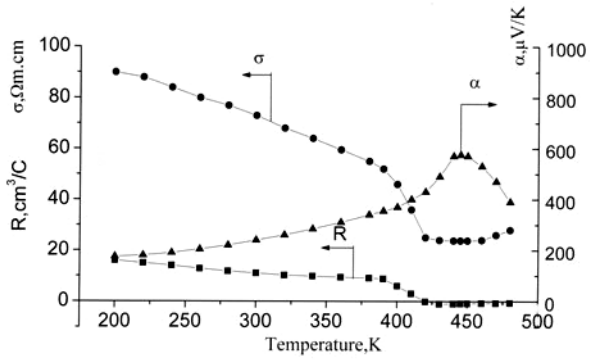

*Fig.1.*The temperature dependences of electrical conductivity (σ), thermo-e.m.f. (α) and Hall coefficient (R) of $AgSbTe_2$.

For a quantitative analyze of the obtained data it is necessary on basis of experimental data in FT region to find mass distribution of α and β- phases, according to the data m_α and m_β to calculate FT parameters: temperature of FT -T_0, at which one $m_\alpha = m_\beta$; a temperature-dependent constant a of FT, function of inclusion $L_0(T)$ of a β-phase in an α-phase and temperature speed dL_0/dT of FT.

The theory and analysis of experimental results

The theory of diffusion phase transition (DFT) is particularized in [4,5]. It as well as theory of other phase transitions, is base of thermodynamic reasons. The characteristic peculiarity of DFT is the absence of sharp jumps of physical quantities, which indicates coexisting of two phases in a certain interval ΔT. It means that thermodynamic potential and other additive values of a system in DFT area contain the conforming characteristics of both phases. Thus it is possible to use general results obtained at construction of thermodynamic potential for condensate systems, according to which one:

$$\Phi(T)=\Phi_\alpha(T)+\Delta\Phi(T)\cdot L(T) \qquad (1)$$

where $\Delta\Phi(T)=\Phi_\beta(T)-\Phi_\alpha(T)$, $\Phi_1(T)$- thermodynamic potential of the first phase, $\Phi_2(T)$ of the second phase, $L(T)$ - function of inclusion. For finding $L(T)$ it is necessary to take into account, that in DFT it is necessary conditionally to distinguish three temperature interval: $T<T_1$, $T_1<T<T_2$ and $T>T_2$. Therefore

$$\Phi(T)=\begin{cases}\Phi_1, & T<T_1\\ \Phi_{12}=\Phi_1+L_{12}(\Phi_2-\Phi_1), & T_1<T<T_2\\ \Phi_2 & T>T_2\end{cases} \qquad (2)$$

If to designate temperature of FT beginning through T_1, and the temperature of FT end through T_2, then for $L(T)$ we have:

$$L(T)=\begin{cases}0 & T<T_1\\ 0<L<1 & T_1<T<T_2\\ 1 & T>T_2\end{cases} \qquad (3)$$

In case of diffused FT

$$L(T)=\frac{1}{1+exp[-a(T-T_0)]} \quad (4)$$

and

$$\partial L/\partial T = \frac{a}{2}\frac{1}{1+ch[-a(T-T_0)]} \quad (5)$$

From (4) and (5) it is seen, for their determination the parameters a_0 and T_0 are necessary found. A technique of determination a_0 and T_0 in detail are described in [3]. If to take into account, that $L(T)$ characterizes a part of phases in the region of their coexisting, it can be determined and as:

$$L(T)=\left[1+\frac{m_\alpha(T)}{m_\beta(T)}\right]^{-1} \quad (6)$$

Values m_α and m_β it is necessary to determine directly from temperature dependences of investigated physical phenomena in FT region. From the joint solution (4) and (6) in the supposition $a=a_0$ we obtain:

$$ln\frac{m_\alpha}{m_\beta}=a(T_0-T) \quad (7)$$

From (7) follows, that at constant value a $ln(m_\alpha/m_\beta=y)$ is a linear function T.

In work [3], enabling, that in FT region the abruptly change of electrical and thermal properties of Ag_2Te is related by a quantitative change α and β phases, m_α and m_β were calculated. On temperature dependences of electrical and thermal properties, the dependence lny on T are constructed and T_0 and a are determined. For this purpose it was proposed to achieve linear change T in transition zone. Then from a beginning up to the end of FT the interval $\Delta T=T_e-T_b$ can be divided into equal intervals and corresponding values of measured coefficients to attribute to suspected phases, for example:

$$\Delta T_y=T_{y,\alpha}(1-m_\beta/m_\alpha)+\Delta T_{y,\beta}(m_\beta/m_\alpha) \quad (8)$$

By such method distribution m_α and m_β were determined in FT region, T_0, a, then $L(T)$, dL/dT are calculated and it is shown, that for determination of FT parameters the most sensible to FT electronic processes can be used.

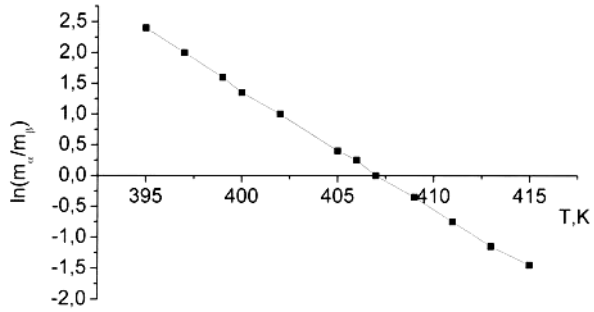

Fig.2. The temperature dependence of $ln(m_\alpha/m_\beta)$, obtained from electrical conductivity data.

In a fig. 2 the dependence lny on T, obtained on the data $\sigma(T)$ and $R(T)$ for $AgSbTe_2$ are shown. The interception of these straight lines with an axis T gives value T_0, at which one $m_\alpha=m_\beta$, and relation $\Delta lny/\Delta T=a$. Under the data T_0 and a according to the formulas (4) and (5) the temperature dependence of a function of inclusion $L(T)$ and speed dL/dT of FT are calculated. The temperature dependence $L(T)$ and dL/dT are shown in a fig. 3 and 4.

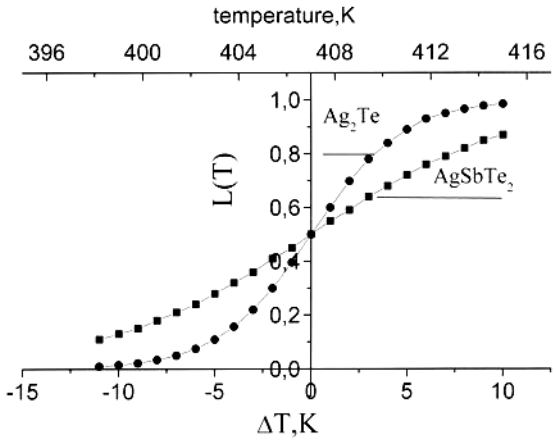

*Fig.3.*The temperature dependence of inclusion function L.

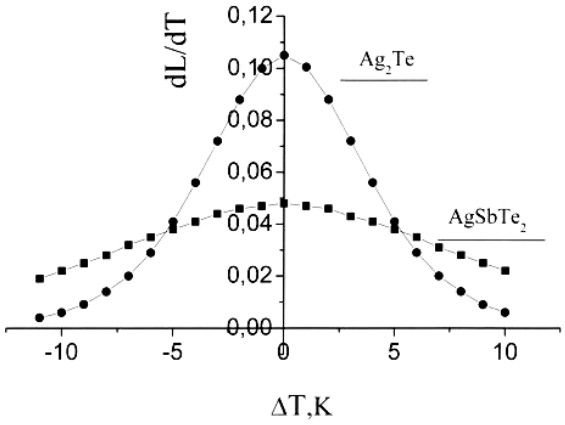

Fig.4. The temperature dependence of speed of change of inclusion function dL/dT.

In these figures for comparison, the data for Ag_2Te are presented also. These data visually demonstrate a diffuse FT in Ag_2Te and $AgSbTe_2$. According to the DFT theory the region of FT diffusion ΔT is determined by interception of a straight line conducted from half of maximum value dL/dT parallel to axis ΔT, from a curve dL/dT. In a fig. 4 these straight lines are indicated by broken lines. For Ag_2Te the region of diffusion encompasses $2\Delta T$=8,5K, and in $AgSbTe_2$ the diffusion encompasses $2\Delta T$=18K. From the formula (5) follows, that maximum value dL/dT corresponds to $a/4$, i.e. degree of diffusion is the temperature-dependent constant of FT. From the obtained data also it is follows, that in the region of diffusion the transition of an α-phase in a β-phase goes on exponential law $m_\alpha/m_\beta=e^{a(T_0-T)}$.

The calculations demonstrate, that the region of FT diffusion encompasses ~70% of all phase change ($\Delta T=T_e-T_b$)

The mechanism leading to diffusion of FT is fluctuations of physical states in matter. The main causes of the fluctuation

at structural FT are as follows: irregularity of distribution of temperature, owing to an allocated significant amount of heat at SFT, in particular in Ag_2Te, polycrystalline of a low temperature phase of argentums chalcogenides, distorting of crystal lattice, high impurity concentration, deviation from a stoichiometry etc. irregularity of physical states.

It is necessary to pay the special attention that diffusion of FT in $AgSbTe_2$ more, than twice surpass diffusion in Ag_2Te. It means that at FT Ag_2Te, arranged inside $Ag_{19}Sb_{29}Te_{52}$ as the second phase, additional source of fluctuations takes place. Certainly, it could be expected, as distribution 11-13 weights. % Ag_2Te inside a matrix should result to additional heterogeneities: temperature at FT, heterogeneities of distribution Ag_2Te on volume basis, on borders of two phases etc. We shall note that more detailed research of two-phase systems can expand knowledge about mechanisms of FT diffusion in solids. Some results about it are obtained at research of a problem of diffusion FT in HTSC [6-9]. In these works the FT region of a lot known HTSC is considered and influence of magnetic field on a degree of FT diffusion is determined. Is shown, that the dual states (normal and superconducting), created by a magnetic field in a transition zone, hardly enhances a fluctuation, a source by which one is vortex current. However, number of vortexes in SC of the second kind, though grow with increasing of a magnetic field, but they as against of phase - Ag_2Te in a matrix $Ag_{19}Sb_{29}Te_{52}$ are distributed uniformly.

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$AgSbTe_2$–DƏ FAZA KEÇİDİNİN YAYILMASI

200-450K temperatur intervalında $AgSbTe_2$–nin elektrikkeçiriciliyinə, termo e.h.q. və Xoll əmsalına ikinci fazanın təsiri tədqiq edilmişdir. p-Ag_2Te -un olması ilə əlaqədar olan $AgSbTe_2$- nin faza keçidinin yayınıq olması və bütün faza keçidinin 70% əhatə etməsi göstərilmişdir. α–fazanın β-fazaya keçidinin eksponensial qanun ilə baş verməsi göstərilmişdir.

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О РАЗМЫТИИ ФАЗОВОГО ПЕРЕХОДА В $AgSbTe_2$

Исследовано влияния второй фазы на электропроводность, термоэдс и коэффициент Холла $AgSbTe_2$ в температурной области 200-450K. Показано, что фазовый переход в $AgSbTe_2$, обусловленный присутствием p-Ag_2Te, является размытым и охватывает ~70% от всего фазового перехода. Установлено, что переход α–фазы в β-фазу происходит по экспоненциальному закону.

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