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A calculation of the temperature dependence of thermopower in amorphous alloy Ca_xAl_{1-x}

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Abstract. The temperature dependence of the thermopower in amorphous alloy Ca_xAl_{1-x} is calculated in the framework of the dynamic concentration excitation (DCE) concept. The results are in good agreement with experimental data.

The thermopower of non-magnetic amorphous alloys is known to be positive over the whole temperature range, and the curve of the thermopower temperature dependence $S(T)$ itself changes slope not far off 50–100 K for various amorphous alloys [1]. As this takes place, the 'knee' in $S(T)$ is displaced when the alloy component concentration changes [1, 2].

In [3–5] we proposed the theory of the low-temperature anomalous electrical resistivity $\rho(T)$, thermopower and heat conductivity $k(T)$, which was based on the concept of the DCEs. These excitations describe the specific atomic dynamics in amorphous metallic systems connected with the dynamic short-range order and the peculiarities of electronic structure in these materials [6]. In [3–5] it was shown that the renormalization of the electron–electron interaction by the multiple elastic scattering on the DCEs results in the formation of the minimum in $\rho(T)$ [3], the 'knee' in $S(T)$ and the 'plateau' in $k(T)$ [5]. As follows from [3–5], the change of the alloy composition should lead to the displacement of the temperature range where the electron kinetic properties are anomalous.

The aim of the present work is to illustrate the possibilities of our theory [4] in the calculation of $S(T)$ in the concrete amorphous alloy Ca_xAl_{1-x} for different component concentrations.

The calculation of $S(T)$ was carried out using the Mott formula in the relaxation-time approximation [4]

$$S(T) = (k_B^2\pi^2 T/3|e|)\left[\tilde{\tau}(\epsilon)\frac{\partial}{\partial\epsilon}\tilde{\tau}^{-1}(\epsilon)\right]_{\epsilon=0} \tag{1}$$

where k_B is the Boltzmann constant, ϵ is the electron energy counting from the Fermi level and $\tilde{\tau}$ is the effective relaxation time of electrons, which is calculated taking into account the interference of electron–electron and electron–DCE scattering [4]

$$\tilde{\tau}^{-1}(\epsilon, T) = (m/2(2\pi)^3\nu_0\tau D^{3/2})[1 + (T/T_0)^2]^{-1/4}J(\epsilon, T). \tag{2}$$

Here

$$J(\epsilon, T) = \int -\frac{dx}{\sqrt{x}}\left\{\frac{N[(x + 1/2\tau - \mu_0)T]}{\sqrt{x + 1/2\tau - \mu_0 - \epsilon}} - \frac{N[(x + 1/2\tau + \mu_0)/T]}{\sqrt{x + 1/2\tau + \mu_0 - \epsilon}}\right\}$$

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and

$$N(x) = [\exp x - 1]^{-1}.$$

Then m and τ are the electron mass and relaxation time;

$$D = v_F^2 \tau / 3$$

is the coefficient of the electron diffusion (v_F is the Fermi velocity) and ν_0 is the original density of states at the Fermi level.

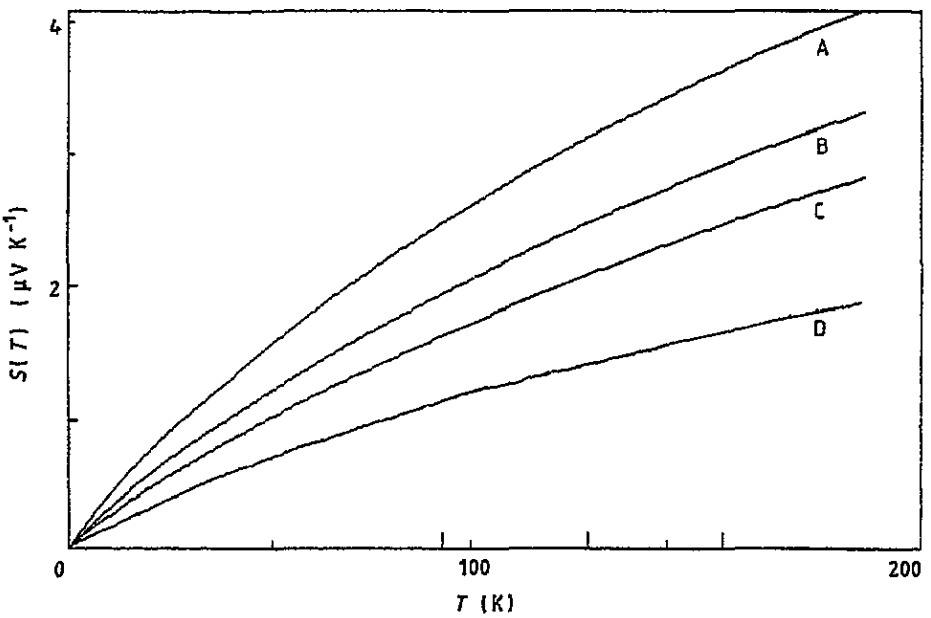

Figure 1. The calculated temperature dependences of thermopower in amorphous Ca_xAl_{1-x}: $x = 0.55$ (curve A), 0.65 (B), 0.70 (C) and 0.75 (D).

Finally, the characteristic temperature T_0 is determined as follows:

$$T_0 \simeq \frac{(2\pi\hbar)^3 \mu_0^{1/2} \rho_0^2 w_0}{x^2(1-x)^2(\Delta E)^2(2m)^{3/2}\kappa^3} \tag{3}$$

where μ_0 is the electron chemical potential, ρ_0 and x are the alloy density and component concentration, respectively, and ΔE is the energy of alloy formation; $\kappa^2 = 4\pi e^2 \nu_0$ and ω_0 is the boundary frequency of the DCEs [5].

To estimate ω_0 one could assume that in the range of low energies the dispersion relation for the DCEs $\omega_k \sim v_s k$ takes place, Here v_s is the sound velocity in the amorphous metal ($\sim 2 \times 10^5$ cm s^{-1} [1]) and $k \sim 10^8$ cm^{-1} characterizes the structure of short-range-ordered regions in the amorphous system structure. Thus a reasonable value of the DCE boundary frequency is $\omega_0 \sim 100$ K.

Reasonable values of the electronic characteristics are the following: $\mu_0 \sim 10^4$ K; $\tau \sim 10^{-14}$ s and $m \sim 9.1 \times 10^{-28}$ g [7].

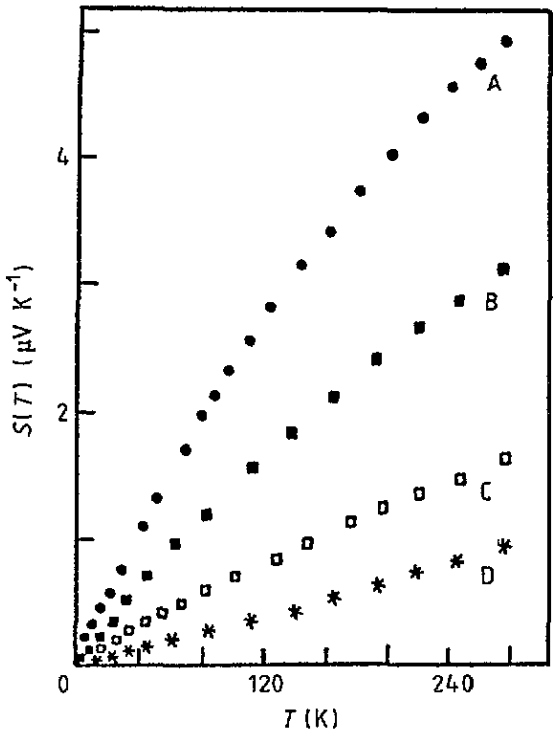

Figure 2. The experimental data on thermopower in amorphous alloy Ca_xAl_{1-x} for $x = 0.55$ (curve A), 0.67, (B) 0.70 (C) and 0.75 (D) [2].

As is seen from (3), the temperature T_0 dividing the ranges of more and less intensive electron scattering on the DCEs is determined by the material characteristics (x, ρ_0 and ΔE) as well as by the electronic ones (μ_0, τ and m) and by the DCE characteristics (ω_0). Apparently, the variation of the alloy component concentration x should lead to change in ρ_0, ΔE and ω_0, and, hence, in T_0. This is why the temperature range where $S(T)$ is non-linear should be displaced when the component concentration of the alloy changes.

In fact, as is seen from figure 1, where the results of the calculation of $S(T)$ in Ca_xAl_{1-x} for $x = 0.55$, 0.65, 0.70 and 0.75 based on (1)–(3), are represented, the temperature of the 'knee' in $S(T)$ depends significantly on the alloy component concentration.

The experimental data on $S(T)$ in Ca_xAl_{1-x} for $x = 0.55$, 0.67, 0.70 and 0.75 [2] are represented in figure 2. The comparison of figures 1 and 2 shows not only good qualitative but also good quantitative agreement of our results with experiment.

Thus we can conclude that the nature of low-temperature anomalous thermopower can be connected with the electron scattering on the other electrons and on the DCEs.

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