Experimental and theoretical investigations of low-temperature specific-heat anomalies at electronic topological transitions in Cd-Mg alloys

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An experimental investigation was made of the low-temperature specific heat of $\mathrm{Cd}_{1-x}\mathrm{Mg}_x$ alloys in the range of compositions $x = 0$–0.18. The specific heat was divided into the electron and phonon components. The composition dependence of the electron specific heat $C_e = \gamma T$ had a strong anomaly at $x \approx 0.11$, which was attributed to an electronic topological transition. Calculations of the energy band structure predicted satisfactorily the position of this transition and the composition dependence $\gamma(x)$. The low-temperature phonon specific heat C_{ph} showed no anomalies associated with the electronic topological transition (this was true within the limits of the experimental error), although theoretical estimates of the relative scale of the anomalies of C_{ph} gave the same values as for C_e.

1. INTRODUCTION

Anomalies of the properties of metals and alloys near electronic topological transitions[1] are attracting much attention, especially because they provide an opportunity for deliberate changes of these properties. For example, it is pointed out in Ref. 2 that the diffusion thermoelectric power can change greatly as a result of small strains or changes in the composition of an alloy near an electronic topological transition (ETT). These predictions were confirmed in Ref. 3 and in several subsequent investigations.[4–7] The likelihood of strong anomalies of elastic and thermodynamic properties associated with ETT was discussed in Refs. 8 and 9. Recently strong composition anomalies of this type were observed in the case of the elastic moduli and the thermal expansion of $\mathrm{Nb}_{1-x}\mathrm{Mo}_x$ alloys.[10] The authors of Ref. 10 attributed these anomalies to a possible ETT in these alloys at $x \approx 0.4$, but this has not been confirmed.

It would therefore be of interest to investigate the anomalies of thermodynamic properties of systems in which the existence of an ETT has been established sufficiently reliably. A classical example of such a system is that formed by $\mathrm{Cd}_{1-x}\mathrm{Mg}_x$ alloys. In the composition range $0 < x \lesssim 0.18$ these alloys form a continuous series of hcp solid solutions in which the ratio c/a decreases monotonically on increase in x (Ref. 11). An investigation of the energy-band structure[12] showed that such a reduction in c/a may give rise to a number of ETT as x is varied. Svechkarev *et al.*[13] observed composition-dependent anomalies of the magnetic susceptibility of these alloys, and an analysis of these anomalies in Ref. 14 agreed with the hypothesis of the occurrence at $x \lesssim 0.1$ of one or two ETT associated with the structure in the vicinity of the point K in the Brillouin zone. Experiments on positron annihilation in $\mathrm{Cd}_{1-x}\mathrm{Mg}_x$ alloys[15] suggested the occurrence at $x \sim 0.1$ of an ETT due to the formation of a new electron sheet at the point L. Measurements of the electrical conductivity and thermoelectric power[4] confirmed that such an ETT occurs at $x = x_{c2} \approx 0.11$ and they revealed also a much smaller anomaly at $x_{c1} \approx 0.06$. Therefore, investigations of the low-temperature specific heat of $C(T)$ of $\mathrm{Cd}_{1-x}\mathrm{Mg}_x$ alloys provide reliable information on the nature and scale of the anomalies associated with ETT. A comparison of the results obtained with the band structure calculations should make it possible to identify the nature of the observed ETT, as well as to estimate the precision of the calculation methods, which is one of the urgent tasks in the theory of metals and alloys.

The low-temperature specific heat of $\mathrm{Cd}_{1-x}\mathrm{Mg}_x$ alloys had been determined earlier.[16] However, Bucher *et al.*[16] used large steps ($\Delta x \gtrsim 0.05$) on the composition scale and failed to detect ETT. Grechnev[12] analyzed theoretically ETT in $\mathrm{Cd}_{1-x}\mathrm{Mg}_x$ alloys but limited his treatment to estimates of the positions of ETT obtained using empirical pseudopotentials. We shall report below the results of complete self-consistent calculations both of the band structure and of the density of states in these alloys, and we shall compare them with the experimental results. In Sec. 2 we shall give the results of the measurements and in Sec. 3 we shall give the results of our energy band structure calculations. A comparison of the experimental and calculated results will be made in Sec. 4 and the final conclusions will be drawn in Sec. 5.

2. EXPERIMENTAL RESULTS

We determined the specific heat $C(T)$ of eleven samples of $\mathrm{Cd}_{1-x}\mathrm{Mg}_x$ alloys at temperatures $T = 1.5$–20 K with compositions in the range $0 \leqslant x \lesssim 0.18$, where these alloys were disordered right down to low temperatures T. The preparation and analysis of the samples and the method used to determine $C(T)$ were described briefly before.[17]

Figure 1 shows the results of our measurements of the specific heat of four samples of $\mathrm{Cd}_{1-x}\mathrm{Mg}_x$ alloys. At low temperatures the specific heat of metals can be described by

$$C = C_e + C_{ph} = \gamma T + \alpha T^3 \qquad (1)$$

representing a linear relationship. However, in the case of cadmium and its alloys this law is obeyed only at very low temperatures in the range $T \lesssim 2$ K. Above 2 K there are deviations of the dependence $C(T)$ from the law given by Eq. (1) and, as shown in Ref. 18, these deviations are due to a large density-of-states peak of cadmium at low energies $E \sim 4$ meV (Ref. 19). Therefore, in the separation of the specific heat into the electron and phonon components C_e

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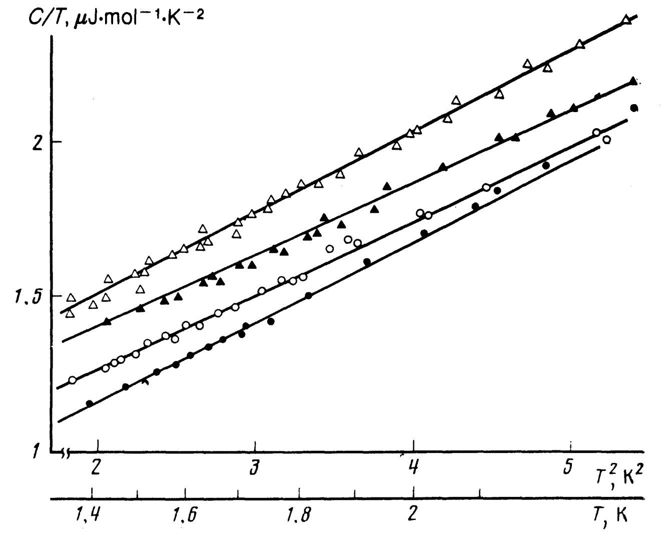

FIG. 1. Temperature dependences of the specific heat of $Cd_{1-x}Mg_x$ alloys with different values of x: (●) $x = 0$; (○) 0.119; (▲) 0.138; (△) 0.176.

and C_{ph} we can use only the experimental data obtained in the narrow temperature range $T \lesssim 2$ K. In this case the errors in the determination of the coefficients γ and α in Eq. (1) are considerably greater than indeterminacy of the specific heat $C(T)$ itself. For example, the errors in γ and α represent 5% and 10–15%, respectively, whereas the error in $C(T)$ in our experiments does not exceed 3%.

Figure 2 shows the composition dependences of the total specific heat $C(x)$ at several temperatures T, as well as the composition dependences of the coefficients $\gamma(x)$ and $\alpha(x)$. We can see that the nonmonotonic behavior (inflection) of the dependence $C(x)$ becomes significant only at temperatures $T \lesssim 3$ K. The narrowness of the temperature range where the specific heat anomaly associated with the ETT is manifested was the reason why this anomaly was not observed in our previous investigation.[18] However, using the low-T data for the composition dependences of the total specific heat $C(x)$ and of the coefficient γ (Fig. 2b), we found clear inflections at $x \approx 0.11$, in agreement with the positions of the anomalies reported earlier[4] for the transport coefficients. On the other hand, in the case of the phonon specific heat C_{ph} the composition dependence of the coefficient α was not observed (within the limits of our experimental error) although one should stress that the relative error in finding α was in our case almost three times as large as the error in γ.

3. CALCULATIONS OF THE BAND STRUCTURE AND OF THE DENSITY OF ELECTRON STATES IN Cd-Mg ALLOYS

The nature of the composition-dependent anomalies of the specific heat of Cd-Mg alloys was identified by self-consistent calculations of the band structure of these alloys. In these calculations we used the linearized muffin-tin orbital (LMTO) method in the atomic sphere approximation (ASA),[20,21] i.e., we considered spherically symmetric self-consistent potentials in the geometry of overlapping Wigner-Seitz spheres. The exchange-correlation potential was used in the Barth-Hedin form,[22] whereas the valence-electron wave functions were calculated by a semirelativistic method,[20] i.e., allowing for all the relativistic terms apart from the spin-orbit contributions. We used the two-center approximation in the LMTO-ASA method.[21] The procedure was made self-consistent using a potential $V(r)$ with a convergence criterion $|\delta V/V| \leqslant 10^{-6}$, where δV is the difference between the last and last but one iterations; this precision required ~ 100 iterations. In numerical integration with respect to the quasimomentum $\mathbf{k}$ we used $n_{\mathbf{k}} = 396$ points in the Brillouin zone; an increase in the number of these points from $n_{\mathbf{k}} = 225$ to 396 altered the band energies $\varepsilon_\nu = \varepsilon(\mathbf{k})$ and the density of states $N(\varepsilon)$ by less than 0.1%. In the case of the d states we made use of a "two-panel" calculation,[21] i.e., the basis of the valence states included not only the $5s$, $5p$, $4d$, and $4f$ orbitals, but also the almost-free $5d$ states. This made it possible to refine the description of the lower states: in agreement with a nonlinearized calculation,[23] but in contrast to one-panel calculations (such as those reported in Ref. 24), the filled $4d$ band of Cd was separated from the conduction band by a gap of width Δ (in our case this gap was $\Delta \approx 10^{-2}$ Ry). We also achieved an improvement with the experimental results in the case of the states near the Fermi level ε_F. For example, the rate of rise of $N_F = N(\varepsilon_F)$

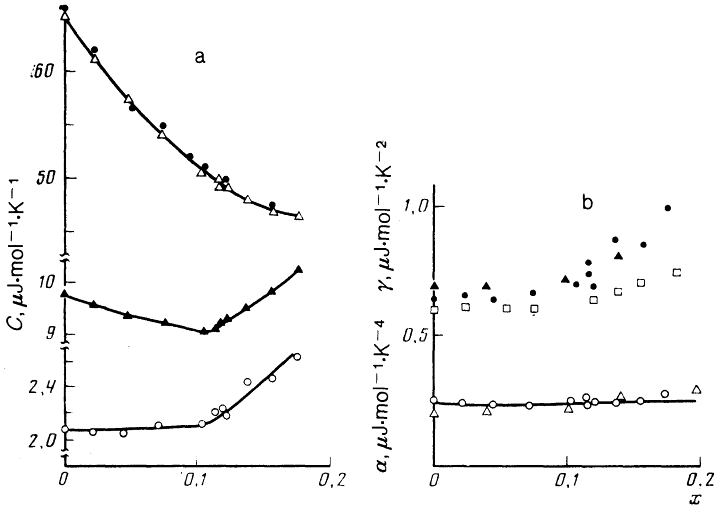

FIG. 2. a) Composition dependences of the specific heat of $Cd_{1-x}Mg_x$ alloys at different temperatures T (K): (●) 1.6, (▲) 3, (△) 5, all obtained in the present study; (●) 5, taken from Ref. 18. b) Composition dependences of the coefficients γ and α in Eq. (1): (●) γ, our experimental results; (▲) γ taken from Ref. 16; (□) γ, calculated using Eq. (2a) and using our calculated values of N_F and the experimental values of λ from Ref. 16; (○) α, our experimental results; (△) α, taken from Ref. 16.

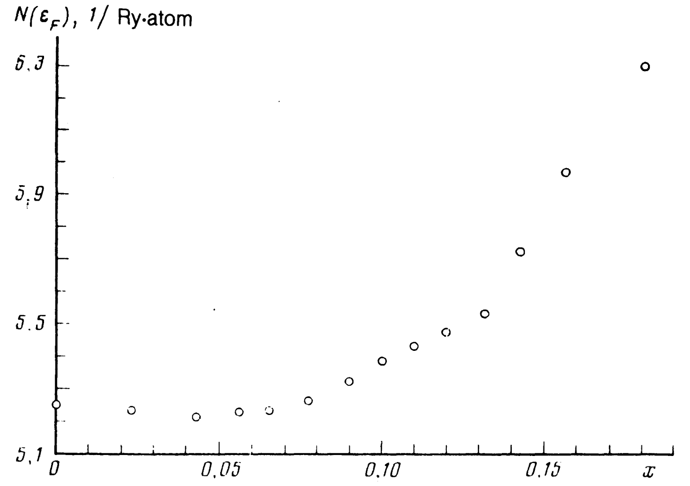

FIG. 3. Density of states at the Fermi level $N_F(x) = N(\varepsilon_F, x)$ calculated for $Cd_{1-x}Mg_x$ alloys.

for $Cd_{1-x}Mg_x$ alloys with $x \gtrsim 0.12$ was in our one-panel calculation approximately half that obtained in a two-panel calculation, the results of which are plotted in Fig. 3, and approximately half the experimental values of $\gamma(x)$ (Fig. 2). On the other hand, we ignored the "combined" correction for the overlap of the atomic spheres,[20] which was clearly small. Thus, the structure of the valence band of Cd calculated in Ref. 24 allowing for this correction was very close to that obtained by our calculations as shown in Fig. 4; the values of N_F for Cd obtained in our one- and two-panel calculations and reported in Ref. 24 were, respectively, 2.45, 2.62, and 2.55 1/(Ry.atom).

The energy band structure of Cd-Mg alloys was calculated in the rigid band approximation, i.e., we calculated the band structure of pure Cd with the lattice parameters of $Cd_{1-x}Mg_x$ alloys taken from Ref. 11. This approximation was justified by, firstly, the previous experience in the calculations of the band structure of these alloys,[12,14] which demonstrated that the structure was governed primarily by variation of the geometric parameter c/a. Secondly, the validity of this approximation (at least at low values of x) was confirmed by our values of $N(\varepsilon)$ calculated for an isolated Mg impurity in Cd. The density of states found in this way was almost identical with $N(\varepsilon)$ for pure Cd and no additional singularities appeared in the region of interest to us near the Fermi level.

The results of calculations of $N(\varepsilon)$ and ε_v for $Cd_{1-x}Mg_x$ alloys are presented in Figs. 3–5 and in Table I. We shall now consider these results. It is clear from Fig. 4 that if $x = 0$, i.e., in the case of pure Cd, the Fermi level passes near a series of extrema of the band energy ε_c: a minimum at the point L and two saddle points near the point K and along the direction GM for $|\mathbf{k}| \approx 0.8|\mathbf{k}_M|$ (we shall denote the last point by Σ). The smallness of the differences $\varepsilon_c - \varepsilon_F$ suggest the possibility of several ETT in Cd under the influence of deformation or doping.[12] For example, according to our calculations, an increase in x in $Cd_{1-x}Mg_x$ alloys induces the first ETT at $x = x_{c1} \approx 0.065$ and this transition is associated with filling of the saddle point at the point K, whereas at $x = x_{c2} \approx 0.123$ there is a second ETT associated with the appearance of a new sheet at the point L. On the other hand, our calculations indicate that the level ε_Σ is filled at all values of x; if $x \lesssim 0.06$, an increase in x causes this level to approach ε_F, but at higher values it moves again away from the Fermi level.

A comparison of our results with other calculations of the band structure of Cd (Refs. 23–25) and of Cd-M alloys[12] shows that all the calculations predict the same main features of the band structure. However, the signs and magnitudes of small differences $\Delta_{cF} = \varepsilon_c - \varepsilon_F$, governing the existence and position of an ETT, vary from one calculation to another. For example, a one-panel LMTO calculation reported for Cd in Ref. 24 gives values of Δ_{LF} and $\Delta_{\Sigma F}$ similar to those obtained by us, but it predicts $\Delta_{KF} < 0$, which (as pointed out already), corresponds to the absence of an ETT associated with the point K in the case of $Cd_{1-x}Mg_x$. A

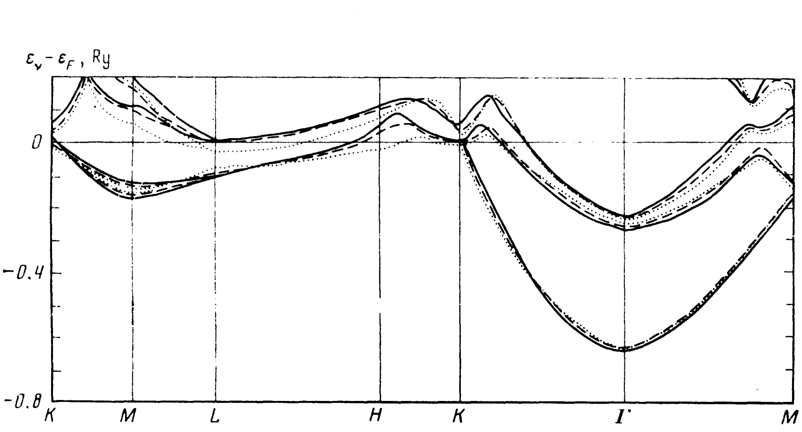

FIG. 4. Structure of the conduction band of $Cd_{1-x}Mg_x$ alloys with different values of x: the continuous curves correspond to $x = 0$, the dashed curves to $x = 0.077$, and the dotted curves to $x = 0.183$.

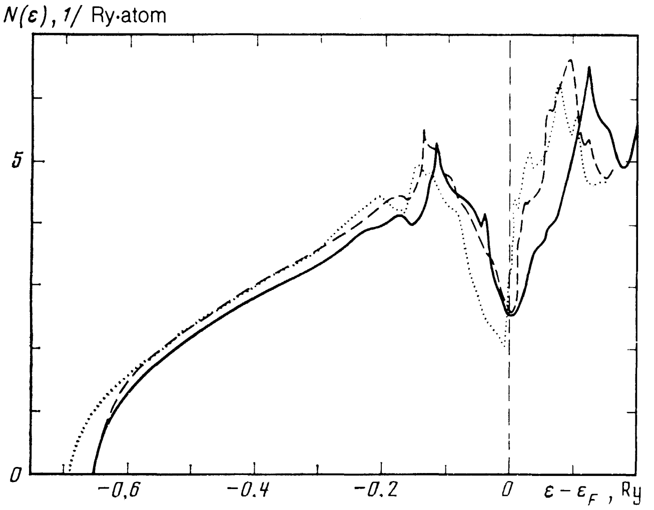

FIG. 5. Density of states $N(\varepsilon)$ calculated for $Cd_{1-x}Mg_x$ alloys with different values of x. The curves are labeled in the same way as in Fig. 4.

calculation carried out by the augmented plane wave (APW) method reported for Cd in Ref. 23 predicts signs of all the differences Δ_{cF} in Table I which are opposite to those obtained by us, corresponding to the absence of both ETT in $Cd_{1-x}Mg_x$ mentioned earlier. Calculations carried out using pseudopotentials fitted to the data on the Fermi surface[12,25] give values of Δ_{LF} and Δ_{KF} similar to those found by us and a similar variation with x (Table I), but at low values of x these calculations predict an additional ETT associated with the point Σ. It should also be mentioned that in calculations of Refs. 12 and 25 an allowance is made for the spin-orbit splitting, in contrast to our calculations and those reported in Refs. 23 and 24, which complicate somewhat the level structure near the point K (see Ref. 14 and the literature cited there). However, this splitting is small and an extremum ε_K discussed by us corresponds to a level $\varepsilon_L \approx \varepsilon_{K2}$ in the notation adopted in Ref. 14.

We shall consider manifestations of ETT in the density of states $N(\varepsilon)$. A comparison of Fig. 5 with the values of Δ_{cF} in Table I shows that, firstly, the Van Hove singularities associated with the points K and Σ are very weak and are hardly manifested in $N(\varepsilon)$. True, the dependence $N_F(x)$ in Fig. 3 has a barely detectable singularity at $x = 0.065$, although in numerical calculations the square-root singularity of the $\delta N_F(K) \propto (x_{c1}-x)^{1/2}\theta(x_{c1}-x)$ type [where $\theta(x) = 1$ if $x > 0$ and $\theta(x) = 0$ if $x < 0$] smears out into a weak inflection. On the other hand, a singularity associated with the point L is manifested clearly by $N(\varepsilon)$ in Fig. 5 and by an anomaly of $N_F(x)$ nearer $x_{c2} = 0.123$ in Fig. 3, although again a singularity of the $\delta N_F(L) \propto (x-x_{c2})^{1/2}\theta(x-x_{c2})$ type is smeared out in numerical calculations (in the case of a real disordered alloy a corresponding smearing appears because of nonconservation of the electron quasimomentum and a corresponding smearing of the Fermi surface[2,3,12]). As pointed out in Ref. 9, the smallness of $\delta N_F(K)$, compared with $\delta N_F(L)$, is due to the presence in the expression for $\delta N_F(K)$ of an additional small factor $(V/\varepsilon_F)^{1/2}$ [where $V = V(2\mathbf{k}_M)$ is the Fourier component of the pseudopotential] and it is also due to a lower statistical weight of the singularity (there are 6 points of the K type in the Brillouin zone compared with 12 points of the L type) and also due to numerical factors. We shall note additionally that the "climb" of the Fermi level on top of the $N(\varepsilon)$ peak, demonstrated in Fig. 5 for $x \approx 0.18$, should increase strongly the "band" energy of the investigated disordered phase as x is increased. This is correlated with the experimentally observed loss of the stability of this phase in the range $x \gtrsim 0.2$, giving rise to an intermetallic compound Cd_3Mg.

We shall now consider the relationship between the calculated values of $N_F(x)$ and the specific heat $C(T,x)$. The coefficients γ and α in Eq. (1) for C are related to N_F and to the Debye temperature T_D, expressed in terms of the elastic moduli c_{ij}:

$$\gamma = {}^{1}\!/_{3}\pi^2(1+\lambda)N_F, \tag{2a}$$

$$\alpha = {}^{12}\!/_{5}\pi^4 T_D^{-3}, \tag{2b}$$

where $\lambda \geqslant 0$ is the electron-phonon interaction constant. Calculations of N_F allow us to estimate γ but in the case of similar estimates of α we need to carry out band calculations of the elastic moduli c_{ij}, which are fairly complex.[26,27] However, it should be noted that the singular contributions c_{ij}^s to the moduli c_{ij} associated with an ETT are proportional to the singular contributions to N_F and opposite in sign to the latter. These terms are due to the presence of a band contribution to the energy of a metal, which when differentiated twice with respect to the strains u_i allowing for self-consistency in the local density functional method yields the following expression[27]:

$$c_{ij} - c_{ij}{}^0 = c_{ij}{}^s$$

$$= -\sum_\nu \left[\frac{\partial \xi_\nu}{\partial u_i}\frac{\partial \xi_\nu}{\partial u_j} - \frac{1}{2}\left(\frac{\partial \xi_\nu}{\partial u_i}\frac{\partial V_\nu{}^{ee}}{\partial u_j} + \frac{\partial \xi_\nu}{\partial u_j}\frac{\partial V_\nu{}^{ee}}{\partial u_i} \right)\right] \delta(\xi_\nu). \tag{3}$$

Here, $\xi_\nu = \varepsilon_\nu - \varepsilon_F$; V_ν^{ee} is the average potential of the elec-

TABLE I. Calculated values of $\varepsilon_c - \varepsilon_F$ (mRy) at critical points of the electron spectrum of $Cd_{1-x}Mg_x$ alloys.

Calculation	x	$\varepsilon_L-\varepsilon_F$	$\varepsilon_K-\varepsilon_F$	$\varepsilon_\Sigma-\varepsilon_F$
Refs. 25 and 12	0 0,10	6 0	1 −9	−1,5 3
Present study	0 0.056 0.132	3.6 2.1 −0.3	1.6 0.2 −1.8	21.3 5 13

tron-electron interaction in a state ν; c_{ij}^0 are nonsingular contributions to c_{ij} which near an ETT become less singular than c_{ij}^s. A singularity of c_{ij}^s is due to states ν close to the state ν_c with an energy ε_c and it clearly is of the same form as a singularity in the density of states N_F, because the expression in the square brackets of Eq. (3) is regular at $\nu = \nu_c$ or (as in the case of terms with $\partial V_\nu^{ee}/\partial u_i$) contains singularities of the same type as those in N_F. Calculations carried out using the scheme of Ref. 27 demonstrate that the terms with $\partial V_\nu^{ee}/\partial u_i$ in Eq. (3) are usually much smaller than $\partial\xi_\nu/\partial u_i$, and in estimates they can be ignored. It is then clear from Eq. (3) that near an ETT the singular contribution δc_{ij}^s is opposite in sign to the singular term δN_F (at least in terms of the main diagonal components of c_{ij}). Bearing in mind that T_D is proportional to $(c_{ij})^{1/2}$, i.e., that $\delta T_D \propto \frac{1}{2}\delta c_{ij}^s$, we find that the signs and the nature of the singular terms in C_e and C_{ph} described by Eq. (1) are the same. Therefore, the nature of the composition anomalies near an ETT is the same for the electron and phonon contributions to the specific heat. This is illustrated in Figs. 2 and 5 of Ref. 9 using the model of almost-free electrons.

4. COMPARISON OF THE EXPERIMENTAL AND THEORETICAL RESULTS

In comparing the theory with experiments we shall begin from the electron specific heat C_e and point out that, firstly, the value of N_F can be calculated accurately for Cd by the LMTO method, whereas the precision of the APW calculations[23] is somewhat less. For example, if for λ of Eq. (2a) we use an experimental estimate from Ref. 16, which is $\lambda_{\rm Cd} = 0.39$, we find that the values of γ calculated in Refs. 23 and 24 and in the present study are, respectively (in units mJ·K^{-2}) 1.04, 0.62, and 0.63, whereas our experimental data for Cd give $\gamma = 0.65$ and the results reported in Ref. 16 give $\gamma = 0.69$. The composition dependences of N_F and $N(\varepsilon)$ calculated by us are also quite accurate. For example, the calculated positions of ETT $x_{c1} = 0.065$ and $x_{c2} = 0.123$ are in good agreement with $x_{c1} \approx 0.06$ and $x_{c2} \approx 0.11$ reported in Ref. 4.

As pointed out in Sec. 3, the results of the calculations for Cd reported in Refs. 23 and 24 correspond to the absence of one or both of these ETT. Therefore, the observed agreement with the experiments at x_{c1} allows us to assume that in our two-panel calculation the energy band structure near ε_F is described more accurately than in Refs. 23 and 24. The composition dependence $\gamma(x)$ can be calculated from Eq. (2a) using the computed values of $N_F(x)$ and the experimental values of $\lambda(x)$ from Ref. 16. The results of these calculations, presented in Fig. 2, are clearly also in agreement with the experimental results within the limits of the experimental error in the values of $\gamma(x)$ and $\lambda(x)$.

As pointed out above, the theoretical calculations predict that the ETT-associated anomalies in the coefficient $\alpha(x)$ in Eq. (1) or in the Debye temperature $T_D(x)$ in Eq. (2) should generally be not smaller than the anomalies in C_e or in N_F. However, our experiments showed that these anomalies are undetectable within the limits of the experimental error. Nevertheless, it would be premature to conclude that the theory and experiments disagree, because the relative error in the determination of α was in our experiments considerably greater than that in γ. On the other hand, if we use the results of Ref. 16 (where the errors could be less because of the use of larger samples), we find that the distribution of the corresponding experimental points in Fig. 2 is not in conflict with the existence of anomalies of α on the same scale as those of γ. It should also be noted that, as pointed out in Ref. 16, the reduction in $T_D(x)$ observed for $\rm Cd_{1-x}Mg_x$ on increase in x is in agreement with the considerable reduction in the elastic moduli $c_{ij}(x)$ reported in Ref. 28 when the composition is changed by going over from $x \approx 0$ to $x = 0.14$. Therefore, the final conclusion on the presence or absence of ETT-related anomalies in the phonon specific heat would clearly require further experiments.

5. CONCLUSIONS

The results of this and previous investigations[3,4,10] demonstrate that the ETT-related anomalies of the properties of alloys may be observed clearly in spite of the formal absence of the conserved electron quasimomentum and a corresponding smearing of the Fermi surface. In the present study we used the example of $\rm Cd_{1-x}Mg$ alloys which were the first for which an ETT-related anomaly of the electron specific heat $C_e = \gamma T$ was found to be considerable. In the range of x from $x_{c2} \approx 0.12$ to $x = 0.18$ the coefficient γ increased by 30–40%, whereas between $x = 0$ and x_{c2} it was hardly affected. Self-consistent calculations of the energy band structure were carried out in the present study and they demonstrated that the ETT at the point x_{c2} is due to the formation of a new sheet near the point L in the Brillouin zone. These calculations described satisfactorily the observed composition dependence $\gamma(x)$ and showed in particular that the anomaly of C_e at the ETT for a sample with the composition $x = x_{c1} \approx 0.06$ is weak and clearly does not exceed the experimental error. This agreement with the experimental results may indicate a high precision of a two-panel variant of the LMTO-ASA method and the validity of the rigid band approximation in the description of the density of states in the $\rm Cd_{1-x}Mg_x$ alloys. On the other hand, in the case of the low-temperature phonon specific heat C_{ph} we found no dependence on the composition (within the limits of the experimental error), although theoretical estimates predicted comparable anomalies of C_{ph} and C_e. More accurate measurements would be needed to identify these anomalies in C_{ph}.

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