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Temperature dependence of electrical resistivity in δ -plutonium alloys

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Abstract

The anomalous behaviour of the temperature dependence of the electrical resistivity in Pu-based dilute alloys (δ -Pu) has been considered within the Mott two-band conductivity model. It has been shown that the physical origin of the negative sign of the temperature coefficient of resistivity (TCR), observed in δ -Pu based alloys, is the interference between electron–impurity and electron–phonon interactions. A simple criterion for negative TCR observability at high temperatures ($T > \theta_D$) was found and applied to explain qualitatively the experimental data on the TCR in some Pu-based dilute alloys. To make a numerical evaluation of the electrical resistivity, the coherent potential approach to the Mott two-band conductivity model was combined with the *ab initio* obtained fcc-Pu density of states (as the starting point in the iteration procedure) and applied to the calculation of resistivity temperature dependence in pure Pu and Pu–5 at.% Al alloy. The results are compared with experimental data.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

The anomalous electronic and magnetic properties of plutonium and plutonium-based alloys have been exciting the physical community for more than fifty years. Some of these anomalies relate to crystal phase transitions; others are associated with the heavy-fermion character of the electron system. Recent progress in experimental and theoretical studies has allowed us to understand the nature of the plutonium ground state [1–4]. With this ground state plutonium has to be an ordinary metal, distinguished only by strongly localized f electrons and an empty d band. However, it becomes quite unclear from that point of view how to treat well-known anomalies in the temperature dependences of the electrical resistivity (ER) in plutonium-based dilute alloys [5–9].

In this paper we analyse from the most general point of view how the ER will behave in a simple model by considering ordinary scattering mechanisms; however, this is done without making any assumptions on the weakness of interaction. In this approach we managed to account consistently for the renormalization effects in the electron ground state by the phonon subsystem at the final temperatures. If this renormalization turns out to be strong then the anomalies in the resistivity temperature dependence, similar to those observed in experiments, may emerge by themselves.

The most general features of experimental ER behaviour that we managed to describe within the single model are the following. First, we explain the negative temperature coefficient of resistivity (TCR) observed experimentally in δ -Pu dilute alloys [5–9] and, second, the quadratic temperature dependence of the ER at low temperatures in these alloys. Thus we have avoided the necessity of using two separate models [5, 10] for the explanation of ER behaviour at low and high temperatures, and making any assumption concerning the specificity of the density of states (DOS) near the Fermi level [10–15]. It might be thought also that the application of modifications of the Kondo model looks unjustified as based on the conception of δ -Pu alloys as *pure metals* [13] and the rather debatable treatment of experimental data in [14] (see [16]).

The dynamic spin-density fluctuation model [15] predicts $\rho(T)/\rho_{\text{sat}} \sim aT^{-1}$ dependence (where ρ_{sat} is a resistivity value of saturation) at high temperatures and negative TCR at some particular values of Stoner theory parameters. However, the Stoner parameter values, which may provide negative TCR, look unreasonably high [11]. Although this model predicts true-like $\rho \sim T^2$ dependence at low temperatures, which correlates with experimental data, nothing can be said immediately about whether this correlation is physically based or fortuitous. The latter seems more probable since the expected suppression of spin fluctuations, and therefore, essential ER variations in an external magnetic field, following from this model have not been found in experiments [11, 9].

Therefore, we have chosen as the starting point in our reasoning the Mooij empirical rule [17], according to which the negative TCR correlates with high ER values (~ 100 – $140 \mu\Omega \text{ cm}$). Note, at first, that high ER values in the alloys are due to very high *residual resistivity*, rating above $80 \mu\Omega \text{ cm}$ [6–8]. Thus the residual resistivity contribution is dominating over the temperature interval of negative TCR. However, this fact has never been taken into account, but in our opinion its proper accounting is rather important.

Second, the negative TCR in Pu-based dilute alloys was observed only either for very *light* (Al, Si, Ga and others) or very *heavy* (Np) impurities. Such specific sensitivity to impurity mass gives evidence that the effect of the ion mass defect (i.e. electron–phonon interaction) may be a pointer not only to understanding the problem of plutonium crystal lattice stability under doping [18], but also to understanding the anomalous ER behaviour. The fact that the negative TCR emerges only near and above the Debye temperature ($\sim 100 \text{ K}$) gives an additional argument in favour of this point of view.

2. Model

Let us consider within the Mott model [19] the systems of s and (d)f electrons, performing intra- and inter-band transitions as a result of their scattering at the randomly distributed Coulomb fields of impurity ions at finite temperature. The Hamiltonian of the electron subsystem can be written in the following form [20]:

$$\hat{H} = \sum_l E_l a_l^\dagger a_l + \frac{1}{N} \sum_{n,l,l'} e^{-i(\vec{k}-\vec{k}', \vec{R}_n)} \hat{B}_{ll'}(n) a_l^\dagger a_{l'}, \quad (1)$$

where E_l is the periodical part of the electron energy. The quantum number l includes the band index j ($j = s, d, f$) and wavevector \vec{k} ; \vec{R}_n is a radius-vector of the n th site of a crystal lattice.

$$\hat{B}_{ll'}(n) = v(n)\Delta V_{ll'} + \sum_{\alpha} a_{\alpha}(n)\hat{Q}_{\alpha,l,l'}(n), \quad (2)$$

where $\Delta V_{ll'} = V_{ll'}^A - V_{ll'}^B$ describes the intensity of the electron–impurity part of the interaction and the periodical part of this interaction is included into E_l . The factor $v(n) = \alpha_B(n)c_A - \alpha_A(n)c_B$ randomly distributes the ions of alloy components along the sites of a crystal lattice; $\alpha_{A(B)}(n) = 1$ if the n th site is occupied by an ion of the $A(B)$ type, and equals zero in opposite case, where c_A and c_B are alloy component concentrations. The operator $\hat{Q}_{\alpha,l,l'}(n)$ describes the intensity of the electron–phonon interaction.

If the thermal displacements of the ions are small, then the operator $\hat{Q}_{\alpha,l,l'}(n)$ can be written as

$$\hat{Q}_{\alpha,l,l'}(n) = Z_{\alpha,ll'} \frac{-i}{\sqrt{N}} \sum_{\vec{q}} \sqrt{\frac{q_0}{q}} \left[e^{i(\vec{q}\vec{R}_n)} \hat{b}_{\vec{q}} - e^{-i(\vec{q}\vec{R}_n)} \hat{b}_{\vec{q}}^{\dagger} \right], \quad (3)$$

where

$$Z_{\alpha,ll'} = \left(\frac{\hbar K_F}{2M_{\alpha} S_{\alpha}} \right)^{1/2} \cdot \left(\frac{2K_F}{3q_0} \right)^{1/2} \cdot C_{\alpha,l,l'}, \quad (4)$$

are the constants of intensity of intra- and inter-band transitions due to electron–phonon scattering. M_{α} is the α -ion mass and S_{α} is the velocity of sound in α -type metal; q_0 is the maximum value of q and K_F is the Fermi wavenumber of the electron; $C_{\alpha,l,l'}$ is a (Bloch) constant of electron–phonon coupling. Note that the matrix elements of the electron–phonon interaction include two parts—dependent on and independent of the ions' stochastic distribution. Namely, the splitting of the electron–phonon coupling into two parts allows a clear understanding of the physical meaning of the impurity mass defect effect.

The s, p, d, and f bands overlap, and therefore hybridization effects have to be taken into account. However, these effects, as is well known, lead only to renormalization of the electron's ground state Hamiltonian and do not change its scattering part; therefore it will be assumed that these effects are accounted for in the electron's ground state. For the sake of simplicity we keep the same band names after renormalization.

As has been pointed out above, the electron–impurity interaction is not assumed to be weak. Therefore contributions from different types of scattering to the total ER may be not summed up in a simple additive way, since the *interference* between them is not negligible *a priori*. That is why one has to use calculation methods, whose validity is not limited by the interaction intensity and which are able to account for the complex structure of the d and f band DOS and the DOS deformation resulting from both electron–impurity interactions in δ -Pu systems, on the one hand, and blurring of singularities in the DOS curve due to electron–phonon scattering, on the other hand. Such a method is the multi-band coherent potential approach (CPA).

As shown in [21], systems of CPA equations may be obtained using the identity

$$\hat{\Delta} = \left[\hat{V}\hat{G}\hat{V} + \hat{V}\hat{G}\hat{V}\hat{G}\hat{V} + \dots \right]_D, \quad (5)$$

where $\hat{G} = (z - \hat{H}_0 - \hat{\Delta})^{-1}$ and the index D means that in $[\dots]_D$ only strictly diagonal terms in the \hat{H}_0 representation are kept and items containing the blocks are omitted.

Assuming $B_{n,jj'}(u) = v(n)\Delta V_{jj'} + Q_{jj'}(u)$ values independent of the wavevectors (\vec{k} , \vec{k}') and functions of fluctuating variable u [22], using matrix representation of the band indices

for B_{jj} and the Green function, the series (5) may be summed up within single-electron and single-site approaches [23]. Finally, for the coherent potentials of s-band electrons one obtains

$$\langle \Delta_s \rangle_{\text{ph}} = \frac{1}{N} \sum_n \int_{-\infty}^{+\infty} du P_n(u) \frac{B_{n,s}^2(u) F_s (1 - F_f B_{n,f}(u)) + (1 + F_s B_{n,s}(u)) B_n^2(u) F_f}{(1 - F_s B_{n,s}(u))(1 - F_f B_{n,f}(u)) - B_n^2(u) F_s F_f}, \quad (6)$$

where

$$P_n(u) = \frac{1}{\sqrt{2\pi\beta_n}} e^{-u^2/2\beta_n}$$

is the Gauss distribution function with $\beta_n = Z_{\alpha,jj'} 6T/\Theta_n$ [22, 20] and Θ is the Debye temperature. $B_{jj}(u) = B_j(u)$ and $B_{jj'}(u) = B_{j'}(u) = B(u)$. Full equations for Δ_s may be found from (6) after summation over sites $n \in A$ and $n \in B$. The equation for the coherent potential of f-band electrons is the same as (6) with only the replacement of band indices $s \rightleftharpoons f$.

Neglecting with inter-band transitions, i.e. assuming $B = 0$, then as follows from (6), two independent equations corresponding to the single-band model of CPA can be obtained:

$$\begin{aligned} \langle \Delta_f \rangle = & \int_{-\infty}^{+\infty} du c_A P_A(u) \frac{(c_B \Delta V + Q_{A,f}(u))^2 F_f}{1 - F_f (c_B \Delta V + Q_{A,f}(u))} \\ & + c_B P_B(u) \frac{(c_A \Delta V - Q_{B,f}(u))^2 F_f}{1 + F_f (c_A \Delta V - Q_{B,f}(u))}. \end{aligned} \quad (7)$$

The second equation may be derived from the above by replacement of band indices $f \rightarrow s$.

Note that the equations (7) for the coherent potentials essentially differ from the main equation in [22], since the latter was obtained assuming that the average over configuration single-site scattering T matrix is zero ($\langle \langle T_n \rangle_{\text{ph}} \rangle_c = 0$).

As is well known from the band structure *ab initio* calculations, the DOS for d and f electrons in actinides is significantly higher than that for s (p) electrons. Therefore it is reasonable to assume that $|B_s F_s| \ll 1$, $|B F_s| \ll 1$ and $|B_s F_s|/|B_f F_f| \ll 1$, $|B F_s|/|B F_f| \ll 1$. Then the system of equation (6) can be simplified, since the f-electron's coherent potential equation coincides with (7) and an expression for the s-electron's coherent potential can be written from (7) by the substitution $Q_{\alpha,f}(u) \rightarrow Q_{\alpha}(u)$.

Using the above assumptions and assuming also the $\Delta V_{jj'} = 0$ in (7) one can obtain coherent potentials in the pure metal:

$$\langle \Delta_f \rangle = \int du P(u) \frac{Q_f^2(u) F_f}{1 - Q_f(u) F_f}, \quad \langle \Delta_s \rangle = \int du P(u) \frac{Q^2(u) F_f}{1 - Q(u) F_f}. \quad (8)$$

In this cause $\beta = Z_{jj'} 2T/\Theta$.

The CPA equations include several parameters of the theory. Parameters $\Delta V_{jj'}$ equal the difference in positions of the gravity centres on the total energy scale of the alloy component bands. Usually within CPA they are approximated as $\Delta V_{jj'} \approx \Delta V$, and the latter can be estimated from the data of *ab initio* calculations. Other parameters ($Z_{\alpha,jj'}$ in (6)–(8)) can be estimated based on available experimental data.

To account in a reliable way for the effect of the individual electronic DOS of the alloy components on the alloy kinetic properties, the CPA equations have to be solved numerically using a realistic, *ab initio* calculated DOS of the alloy components. The initial alloy DOS may be chosen according to the approach described in [23].

Model simplifications used in the derivation of equation (7) are equivalent to the main Mott's conductivity model assumptions, where only the inter-band electron transitions have been considered, since the probabilities of the others turn out to be very low as compared to that of $s \rightarrow (d)f$ transitions. As a result of such simplifications, all numerical calculations

within the Mott conductivity model for metals and alloys at high temperature can be carried out in well-known manner, using the Kubo formula for electrical conductivity.

The full system of the CPA equation (6) is very difficult for direct analysis and solution. However, several simple estimations can help to analyse the ER temperature dependence qualitatively. For our reasoning it is sufficient to consider only the main terms that are linear with temperature in the perturbation theory row, taking into account terms only of the second and third order per interaction. Since the ER is proportional to the imaginary part of the shift operator, then from (6) one obtains an expression consisting of three terms:

$$\begin{aligned} \rho / \text{Im } F_j(E_F) \sim & c_A c_B \Delta V^2 + \{c_A Z_A^2(T/\theta_A) + c_B Z_B^2(T/\theta_B)\} \\ & + 2c_A c_B [2\Delta V (Z_{jA} Z_A(T/\theta_A) - Z_{jB} Z_B(T/\theta_B)) \\ & + \Delta V_{sj} (Z_A^2(T/\theta_A) - Z_B^2(T/\theta_B))] \text{Re } G_j(E_F) \end{aligned} \quad (9)$$

where $F_j(E_F)$ is the Green function at the Fermi level. The first term in (9) describes only electron–impurity scattering and it determines the value of residual resistivity. The second term corresponds to electrons scattered at the ‘pure’ phonons. The term in the quadratic brackets describes the *interference* between electron–impurity and electron–phonon couplings. Assuming additionally that $Z_{j,\alpha} \approx Z_\alpha$, $\Delta V_j \approx \Delta V$ the following simple criterion for negative TCR observability at high temperatures, i.e. ($T > \theta$), can be found:

$$1 + 6c_A c_B \Delta V \frac{Z_A^2/\theta_A - Z_B^2/\theta_B}{c_A Z_A^2/\theta_A + c_B Z_B^2/\theta_B} \text{Re } F_f(E_F) \leq 0. \quad (10)$$

Thus the values of ΔV , the difference between electron–phonon coupling constants of solvent and impurity, and the real part of the Green function at the Fermi level, which are available from experimental data and *ab initio* calculations, determine the sign of the TCR.

3. Results and discussion

It is reasonable to imply that in *dilute* alloys ($c_B \leq 5$ at.%) the solvent band structure and elastic properties are almost the same as in the pure metal, and for the qualitative estimates one can assume that $\theta_B \approx \theta_A$ and $S_B \approx S_A$. In this case only the distinction between solvent and impurity ion masses determines the difference between the elastic constants of solvent and impurity.

The first parameter ΔV can be evaluated according to Harrison [24] as $\sim (-10)$ eV. The numerical value of $\text{Re } F(E_F)$ has been determined from *ab initio* DOS calculations in pure fcc-Pu by the LSDA+ U method [25, 26], and it equals (-1) eV $^{-1}$. Using simple Bloch estimation, as $C_{sf,\alpha} \sim 2/3 E_{F,\alpha}$, the difference between electron–phonon constants of solvent and impurity can be evaluated.

Using experimental data for the Debye temperature, velocity of sound [27], and lattice parameter in fcc-Pu, and applying criterion (10), one obtains the theoretical predictions for the TCR in δ -Pu alloys, doped with 5 at.% of various impurities; these are presented in figure 1. The TCR sign is negative in the case of doping with light impurities (Al, Ga, Ge, Si, Sc) and positive in the case of intermediate impurity masses (Ir, Rh, Pd, Pt, In). Almost all predictions agree with the available experimental data. Therefore it is very likely that the observed regularities of TCR sign variation with impurity mass come from the interference between electron–impurity and electron–phonon interactions. It is rather interesting to stress that a negative TCR is also predicted for plutonium doped with very heavy impurities, such as Np, Am, Cm, since the difference between their reciprocal masses is very small. However, the lack of reliable experimental data prevents us from making any accurate predictions on this account.

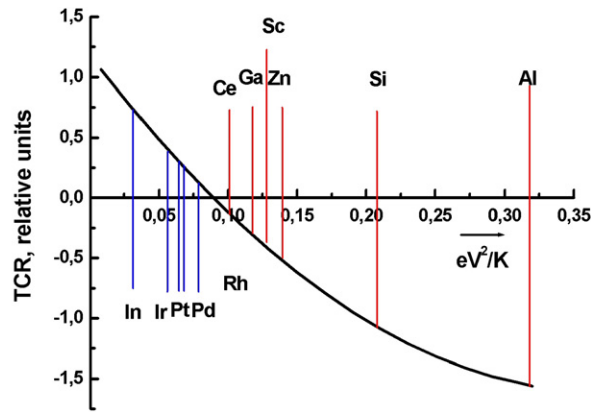


Figure 1. The relationship between the electron–phonon coupling constant and the sign of the TCR in dilute Pu-based alloys. The value of the electron–phonon coupling constant for different types of impurity in Pu is at the intersection of the vertical lines and the x-axis.

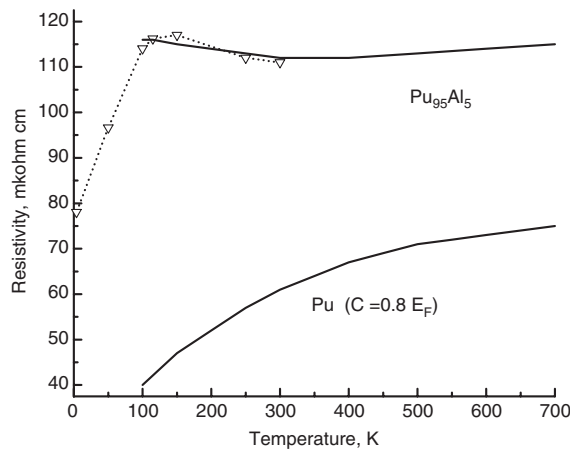


Figure 2. Temperature dependence of ER in pure fcc-Pu and $\text{Pu}_{0.95}\text{Al}_{0.05}$ alloy. Solid lines—results of calculations.

The results of CPA calculations for the ER in *pure* fcc-Pu using equations (8) and a Bloch constant value about $0.8E_F$ [27] are shown in figure 2. Experimental data for pure Pu ER are unknown. Compared to ER data in the other 4d (5d) transition and 4f (5f) rare-earth metals [8], the obtained ER demonstrates ordinary behaviour with temperature without any anomalies. The high value of ER is a result of $s \rightarrow d$ and $s \rightarrow f$ scattering and weak nonlinearity in the ER temperature dependence above θ_D and is caused by DOS erosion at the Fermi level due to electron–phonon interaction.

Full solution of the CPA equations (7) in the case of δ -Pu alloy doped with 5 at.% Al, obtained with use of the *ab initio* plutonium DOS and the Green function [26] as the starting point in the numerical calculations, demonstrates that the electron–impurity and electron–phonon interactions significantly smoothen all initial fine singularities in the DOS curve and make the resultant DOS value at the Fermi level decrease with temperature. A similar result was observed experimentally by Lashley [28] in δ -Pu doped with 5 at.% Al in heat capacity

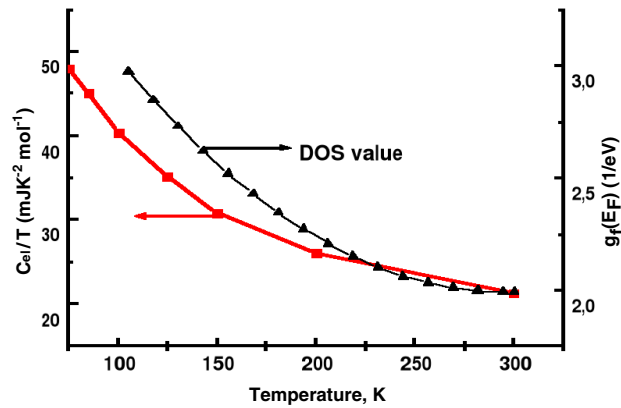


Figure 3. Comparison of calculated $g_F(E_F)$ in δ -Pu_{0.95}Al_{0.05} as a function of temperature (right axis) and experimental dependence of C_{el}/T [28] (left axis).

measurements. The comparison between the calculated DOS value at Fermi level and the ratio of the electronic part of heat capacity C_{el} to temperature T (C_{el}/T), extracted from experimental data [28] is presented in figure 3. The magnetic susceptibility data [14, 29] in the same alloy also demonstrate the drop of DOS values at the Fermi level with temperature.

The temperature dependence of ER in δ -Pu stabilized with 5 at.% Al, calculated with the Kubo formula in the same manner as mentioned above, is shown in figure 2. It is seen that the theoretical curve fits the experimental data well at $100 \text{ K} < T < 300 \text{ K}$ and predicts the TCR sign inversion at $T > 450 \text{ K}$. Thus the direct numerical calculation confirms the validity of criterion (10), obtained from a general qualitative consideration. The agreement between theoretical and experimental data in respect to the DOS as well as the ER behaviour with temperature gives evidence in favour of our approach taking into account the interference between electron–impurity and electron–phonon interactions.

Our approach allows avoiding various assumptions of unknown reliability, which have often been used previously to describe the negative TCR as $\sim T^2$ dependence. It is likely that the presented model also permits understanding the ER behaviour at low temperatures. It has been found earlier [30, 31] that in dilute alloys characterized by interference between electron–impurity and electron–phonon interactions, the Mott model predicts a $\rho(T) \sim T^2$ regularity at low temperatures in contrast to a $\rho(T) \sim T^3$ one, which is typical in alloys without interference. Thus all the observed features of ER behaviour, both at low and high temperatures, can be explained in a natural way within the single model without making any assumption about the DOS structure at the Fermi level.

Note, that our calculation of the ER in pure fcc-Pu at high temperatures, carried out in the same model using equations (8), predicts typical metallic behaviour of the ER over the whole temperature region (see figure 2). The comparison with experimental data in other actinides—Th, Pa, U, Am, Np (see for example [8]) demonstrating similar ER behaviour—shows that the ER in pure fcc-Pu has no specific peculiarities and that fcc-Pu is an ordinary metal in a row among other actinides.

A new unusual effect, which must correlate with the negative TCR and interference between different types of scattering, is the renormalization of a ground-state energy in Pu-based alloys. As a result of interference, a new energy local minimum is formed in these alloys. This effect may be very important for understanding the nature of Pu-based alloy stability.

As follows from our numerical calculations, s-electron scattering into d and f bands is nearly equiprobable, since the DOS values at the Fermi level in d and f accepting bands are

almost the same. Therefore mobile s-type electrons are able to scatter into and fill up the empty d states, thus leading to the probable emergence of weak magnetic moments observed in some Pu-based alloys. It looks rather interesting to seek for correlation between the above specific electron scattering and magnetic properties.

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