

Approximations made in evaluating the residual electrical dc resistivity of disordered alloys

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The residual electrical dc resistivity of the transition-metal-alloy system Cu-Pt is evaluated by making use of the relativistic version of the Korringa-Kohn-Rostoker-coherent potential approximation and the one-electron Kubo-Greenwood formula for disordered systems. Starting from the results of a previous calculation the influence of truncation of the angular momentum expansion, the effects of self-consistency of the alloy potential, the importance of vertex corrections, and the difference between the nonrelativistic and the relativistic current operator are examined.

I. INTRODUCTION

The Korringa-Kohn-Rostoker coherent-potential approximation (KKR-CPA) has been used for calculating quite a number of physical properties of disordered alloys in the past. Beside equilibrium properties such as the total energy or magnetic properties the calculation of nonequilibrium transport properties is of great interest. Among these the residual electrical resistivity (or conductivity) is one of the most thoroughly investigated nonequilibrium quantity. For metallic systems the Kubo-Greenwood formula^{1,2} is agreed to give an adequate description of the conductivity. It has been adapted to the formalism of the CPA alloy theory by several authors^{3,4} and applied to real systems, e.g., Cu-Zn, Cu-Ga and Ag-Pd,⁵ Al-V (Ref. 6), and Cu-Pt.⁷ However, some of these calculations suffer from various kinds of approximations: They are limited to a restricted angular momentum expansion of $\ell \leq 2$,^{5,7} do not^{5,6} or only partially⁷ take into account relativistic effects, neglect the vertex corrections,⁷ or are based on non-self-consistent potentials.⁷ In this paper, the effects of the various approximations are studied by successively removing them. The results for the alloy system Cu-Pt of Ref. 7 are used as a starting point for this study.

II. THE KUBO-GREENWOOD FORMULA

The basis for the calculation of the residual electrical dc conductivity of a disordered alloy system is a formula given by Greenwood [see Eq. (31) of Ref. 2] which in turn may be derived from the Kubo formula [see Eq. (5.12) of Ref. 1]. For zero temperature this so-called

Kubo-Greenwood formula reads (in a slightly generalized form)

$$\sigma_{\mu\nu} = \frac{\pi\hbar}{N\Omega_{\text{at}}} \left\langle \sum_{mn} J_{mn}^{\mu} J_{nm}^{\nu} \delta(\epsilon_F - \epsilon_m) \delta(\epsilon_F - \epsilon_n) \right\rangle$$

with $\mu, \nu \in \{x, y, z\}$, (1)

where $J_{mn}^{\mu} = \langle m | J_{\mu} | n \rangle$ denotes the matrix element of the current operator in the μ th spatial direction and $|m\rangle$ and $|n\rangle$ are the eigenfunctions of a particular configuration of the random system. The average, indicated by $\langle \dots \rangle$, has to be taken over all possible configurations of the system considered. Ω_{at} is the atomic volume and N is the number of the atoms.

Because in the present work the electronic structure of the alloy is expressed in terms of the one-particle Green function rather than in terms of wave functions and energy eigenvalues, these are replaced by using the following representation for the imaginary part of the Green function:⁸

$$\text{Im } G^+(\epsilon) = -\pi \sum_n |n\rangle \langle n| \delta(\epsilon - \epsilon_n), \quad (2)$$

where $G^+(\epsilon)$ is the positive side limit of the Green function (see below). Inserting this into Eq. (1) yields

$$\sigma_{\mu\nu} = \frac{\hbar}{\pi N \Omega_{\text{at}}} \text{Tr} \langle J_{\mu} \text{Im } G^+(\epsilon_F) J_{\nu} \text{Im } G^+(\epsilon_F) \rangle. \quad (3)$$

Having to take the imaginary part of the Green function in Eq. (3) makes the final expressions (see below) somewhat awkward to evaluate. Using positive and negative side limits of the Green function one can avoid this and may express the electrical conductivity as

$$\sigma_{\mu\nu} = \frac{1}{4} [\tilde{\sigma}_{\mu\nu}(\epsilon^+, \epsilon^+) + \tilde{\sigma}_{\mu\nu}(\epsilon^-, \epsilon^-) - \tilde{\sigma}_{\mu\nu}(\epsilon^+, \epsilon^-) - \tilde{\sigma}_{\mu\nu}(\epsilon^-, \epsilon^+)], \quad (4)$$

where the complex energies ϵ^+ and ϵ^- are defined in terms of the Fermi energy ϵ_F :

$$\epsilon^+ = \epsilon_F + i\eta, \quad \epsilon^- = \epsilon_F - i\eta, \quad \eta \rightarrow 0 \quad (5)$$

and

$$\tilde{\sigma}_{\mu\nu}(\epsilon_1, \epsilon_2) = \frac{\hbar}{\pi N \Omega_{\text{at}}} \text{Tr} \langle J_\mu G(\epsilon_1) J_\nu G(\epsilon_2) \rangle \quad (6)$$

with $\epsilon_1, \epsilon_2 \in \{\epsilon^+, \epsilon^-\}$.

Dealing with cubic systems we may drop the indices μ and ν because for that case the conductivity tensor is diagonal with three identical elements, as long as we deal with nonmagnetic systems.

The CPA approximation primarily aims to supply the configuration average for the Green function $\langle G \rangle$ of a random alloy system.⁹ Butler⁴ derived a scheme to evaluate the configuration average of the product of two Green functions occurring in Eq. (6), that is consistent with the CPA (see also Ref. 10). In his formulation the Green function does not occur explicitly. Instead of dealing with $\langle G \rangle$ the information is carried by the scattering-path operator τ^{CPA} of the CPA medium which is closely related to the Green function $\langle G \rangle$.⁹ The quantity $\tilde{\sigma}$ of Eq. (6) can then be expressed by

$$\begin{aligned} \tilde{\sigma}(\epsilon_1, \epsilon_2) = & -\frac{4m^2}{3\pi\hbar^3\Omega_{\text{at}}} \sum_{\mu} \left(\sum_{\alpha, \beta} c^\alpha c^\beta \tilde{j}_\mu^\alpha(\epsilon_2, \epsilon_1) \right. \\ & \times \underbrace{\{1 - \chi w\}^{-1}}_A \chi(\epsilon_1, \epsilon_2) \tilde{j}_\mu^\beta(\epsilon_1, \epsilon_2) \\ & + \sum_{\alpha} c^\alpha \tilde{j}_\mu^\alpha(\epsilon_2, \epsilon_1) \tau^{\text{CPA}}(\epsilon_1) J_\mu^\alpha(\epsilon_1, \epsilon_2) \\ & \left. \times \tau^{\text{CPA}}(\epsilon_2) \right). \quad (7) \end{aligned}$$

The matrix of the scattering-path operator τ^{CPA} is related to the CPA t matrix and the structure constants $G(\mathbf{k})$ by an integral of the inverted KKR matrix, $\tau(\mathbf{k}, \epsilon)$, over the Brillouin zone (BZ)

$$\begin{aligned} \tau^{\text{CPA}}(\epsilon) &= \frac{1}{\Omega_{\text{BZ}}} \int_{\text{BZ}} \tau(\mathbf{k}, \epsilon) d^3k \\ &= \frac{1}{\Omega_{\text{BZ}}} \int_{\text{BZ}} \{[t^{\text{CPA}}(\epsilon)]^{-1} - G(\mathbf{k}, \epsilon)\}^{-1} d^3k \quad (8) \end{aligned}$$

and χ is essentially the BZ average of a pair of the matrices $\tau(\mathbf{k}, \epsilon)$

$$\chi(\epsilon_1, \epsilon_2) = \frac{1}{\Omega_{\text{BZ}}} \int_{\text{BZ}} \tau(\mathbf{k}, \epsilon_1) \tau(\mathbf{k}, \epsilon_2) d^3k - \tau^{\text{CPA}}(\epsilon_1) \tau^{\text{CPA}}(\epsilon_2). \quad (9)$$

The operator w in Eq. (7) contains the single-site t matrices for the CPA medium and the components α , t^{CPA} , and t^α , respectively, as well as the CPA scattering-path operator τ^{CPA} .⁴ J in Eq. (7) is the current operator and $\tilde{J} = D^t J D$, where D is the CPA impurity operator and D^t its transposed operator.⁴ The integration in Eq. (9) can be restricted to 3/48 parts of the Brillouin zone in the case of cubic symmetry of the crystal lattice. If the vertex corrections are neglected by setting the matrix A to unity, one 1/48 part is sufficient. The summation in Eq. (7) extends over the components $\alpha, \beta \in \{A, B\}$ of a binary alloy and the spatial coordinates $\mu \in \{x, y, z\}$.

We deal with the above equations within the fully relativistic Dirac formalism. By adopting the corresponding relativistic angular momentum representation all matrix elements occurring are labeled with the spin-orbit and magnetic quantum numbers κ and m_j , respectively, which are combined to $\Lambda = (\kappa, m_j)$. In Ref. 7, the non-relativistic expression for the current operator $\mathbf{J} = \frac{e\hbar}{m} \nabla$ was adapted to the relativistic calculation by merely using the relativistic representation. In this representation the matrix elements of the current operator are of the form

$$J_{\Lambda, \Lambda'}^{\alpha, \mu}(\epsilon_1, \epsilon_2) = \frac{e\hbar}{m} \int_{\text{WS}} d^3r Z_{\Lambda}^{\alpha \dagger}(\mathbf{r}, \epsilon_1) \frac{\partial}{\partial r_\mu} Z_{\Lambda'}^{\alpha}(\mathbf{r}, \epsilon_2), \quad (10)$$

where $Z_{\Lambda}^{\alpha}(\mathbf{r}, \epsilon)$ is the regular solution of the Dirac equation for the component α for the energy ϵ and the set of quantum numbers Λ and μ is the spatial coordinate. The integration is performed over the Wigner-Seitz cell (integration over the muffin-tin sphere is not sufficient). Although the use of the nonrelativistic current operator was expected to be sufficient, in the present work the correct fully relativistic expression was evaluated as well in order to study a possible effect on the electrical conductivity. With the relativistic current operator $\mathbf{J} = ec\boldsymbol{\alpha}$ the corresponding expression for the matrix elements is

$$J_{\Lambda, \Lambda'}^{\alpha, \mu}(\epsilon_1, \epsilon_2) = ec \int_{\text{WS}} d^3r Z_{\Lambda}^{\alpha \dagger}(\mathbf{r}, \epsilon_1) \alpha_\mu Z_{\Lambda'}^{\alpha}(\mathbf{r}, \epsilon_2), \quad (11)$$

where α_μ are the standard 4×4 Dirac matrices.¹¹

Once the KKR-CPA equations have been solved yielding the CPA t matrix and the scattering-path operator τ^{CPA} the Kubo-Greenwood conductivity (and resistivity) can be calculated by means of Eqs. (4), (7), (9), and either (10) or (11).

III. CALCULATIONS

In Ref. 7, the KKR-CPA equations were solved for various compositions of the alloy system Cu-Pt restricting the angular momentum expansion of all quantities to $\ell \leq 2$. The potentials used had been constructed in a non-self-consistent manner (see Refs. 12 and 13 for

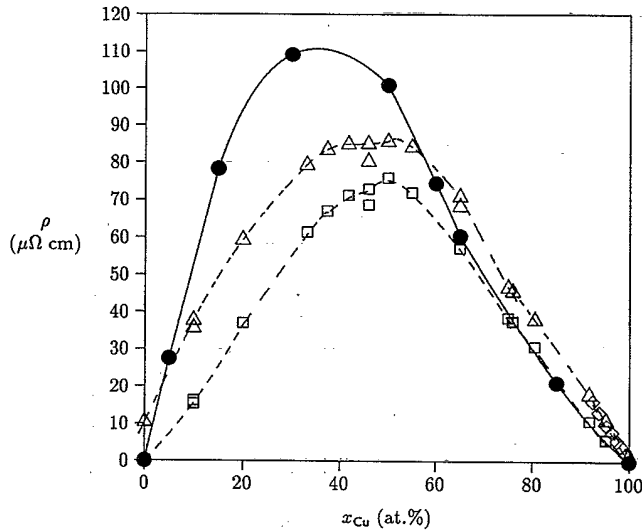


FIG. 1. Residual dc resistivity of disordered Cu-Pt alloys. Full circles: calculated values taken from Ref. 7; triangles: experimental values for $T=273$ K; squares: estimated values for $T=0$ K, using Eq. (12) and data from Ref. 15; diamonds: experimental values for $T=4.2$ K (Ref. 16).

details). The electrical conductivity was calculated using Eq. (7) neglecting the vertex corrections by setting $A = 1$. This facilitates the calculation very much because the Brillouin-zone integration has to be performed for a scalar quantity only in this case [see Eq. (3) of Ref. 7]. Moreover, the nonrelativistic version of the current operator defined in Eq. (10) was applied. The results of this calculation are shown in Fig. 1. The resistivity $\rho = \sigma^{-1}$ is displayed instead of the conductivity for matters of convenience. Comparison to experimentally determined resistivities is somewhat difficult because for Cu-Pt only room-temperature measurements are available.¹⁴ Only for some Cu-rich alloys measurements at $T=4.2$ K have been done.¹⁶ To get a rough idea of the zero-temperature resistivity, the values measured at $T=273$ K were extrapolated to $T=0$ K by using the measured ratio $\rho(T=4.2 \text{ K})/\rho(T=273 \text{ K})$ of the alloy system Au-Pd:¹⁵

$$\rho_{\text{est}}^{\text{CuPt}}(0 \text{ K}) \approx \frac{\rho^{\text{AuPd}}(4.2 \text{ K})}{\rho^{\text{AuPd}}(273 \text{ K})} \rho^{\text{CuPt}}(273 \text{ K}). \quad (12)$$

Here it is implicitly assumed that the low-temperature behavior of the electrical resistivity is similar for the iso-electronic alloy systems Au-Pd and Cu-Pt. Of course this is not a reliable way to estimate the residual resistivity from room-temperature data. But, as no temperature dependent data are available, we choose this way to get an indication about the approximate magnitude of this quantity. The resulting values are displayed in Fig. 1. Comparison with the experimental data for $T=4.2$ K demonstrates that the extrapolation yields quite reasonable results. Of course, the estimated zero-temperature resistivity is lower than the room-temperature resistivity for all compositions. Obviously the agreement between the extrapolated and theoretical values is only satisfactory for alloys that contain more than 60% copper,

whereas the calculated resistivities for the platinum-rich alloys are much too large. This failure can be attributed to various sources: First of all the non-self-consistency of the alloy potentials could affect the accuracy of the calculation. Furthermore, the use of the nonrelativistic current operator may lead to incorrect results. This may be important especially for the Pt-rich side of the alloy composition range. Also the vertex corrections may have an influence on the results for the conductivity, although their contribution to the Pt-rich alloys is expected to be small. Finally, the restriction of the angular momentum expansion to $\ell \leq 2$, which leads to satisfactory results for properties related to the density of states, e.g., the linear coefficient of the low-temperature specific heat or the spin-lattice relaxation time,¹³ may lead to an underestimate for the electrical conductivity.

Equation (12), of course, is a very crude estimate. But it certainly gives the correct sign and order of magnitude of the resistivity change between room temperature and $T=0$ K. For this reason the calculated results of Ref. 7 definitively do not match the experimental findings. In the following, the importance of each of the possible sources of the deviation is examined.

A. Self-consistency of the alloy potentials

In order to check the effect of charge and potential self-consistency the potentials of all alloy compositions were recalculated using the non-self-consistent potentials as starting values. The full KKR-CPA equations were iterated in order to achieve self-consistency in both the potential iteration and the CPA iteration cycle. The electrical conductivity was then calculated in the same manner as in Ref. 7, i.e., the angular momentum expansion was restricted to $\ell \leq 2$, the vertex corrections were neglected, and the nonrelativistic current operator of Eq. (10) was used. Figure 2 shows the results of this improved calculation and the relative deviation of the results based on the non-self-consistent and self-consistent potentials. Obviously the changes are quite pronounced except for the Cu-rich alloys with $x_{\text{Cu}} \geq 85$ at.%. This finding is in accordance with the observations of Ref. 17 who find a difference up to 30% between resistivities of Ag-Pd calculated via the Boltzmann equation using a self-consistent and a non-self-consistent potential, respectively. This shows that it is important to use self-consistent potentials in resistivity calculations even if one gets satisfactory results for other quantities using non-self-consistent potentials.

B. Relativistic current operator

The use of the nonrelativistic current operator of Eq. (10) (in the relativistic Λ representation) instead of the correct relativistic one of Eq. (11) was suspected to be a further source of errors. The matrix elements of the correct relativistic operator were, therefore, evaluated and the electrical conductivity again calculated by means of Eqs. (4), (7), and (9). The self-consistent potentials were used but the vertex corrections were again

neglected. The results are to be seen in Fig. 3. The difference between the results corresponding to the non-relativistic and the relativistic operator, respectively, are not very large. The resulting resistivity is smaller for the relativistic operator in all cases. The difference is more pronounced on the Pt-rich side of the composition range than on the copper side. This result is perfectly understandable in terms of the increasing importance of relativistic effects for the heavy elements. The correct relativistic operator of Eq. (11) can be expanded in a series with increasing order of $1/c$ yielding the operator of Eq. (10) as the leading term while the first correction term of the order of $1/c^2$ contains the spin-orbit coupling operator¹⁸

$$\mathbf{J} = \frac{e}{m} \left[\frac{\hbar}{i} \nabla + \frac{\hbar}{4mc^2} \boldsymbol{\sigma} \times \nabla V + \dots \right]. \quad (13)$$

The comparison shows that both operators lead to comparable results for the electrical resistivity, thus demonstrating that the spin-orbit coupling has only a small influence on the electrical conductivity in this case. This is consistent with calculations of the optical conductivity where the operator in Eq. (13) has been used with the second term contributing about 10% to the matrix elements.^{18,19}

C. Vertex corrections

Calculating the vertex correction makes the evaluation of Eq. (7) a lot more difficult because first, large matrices

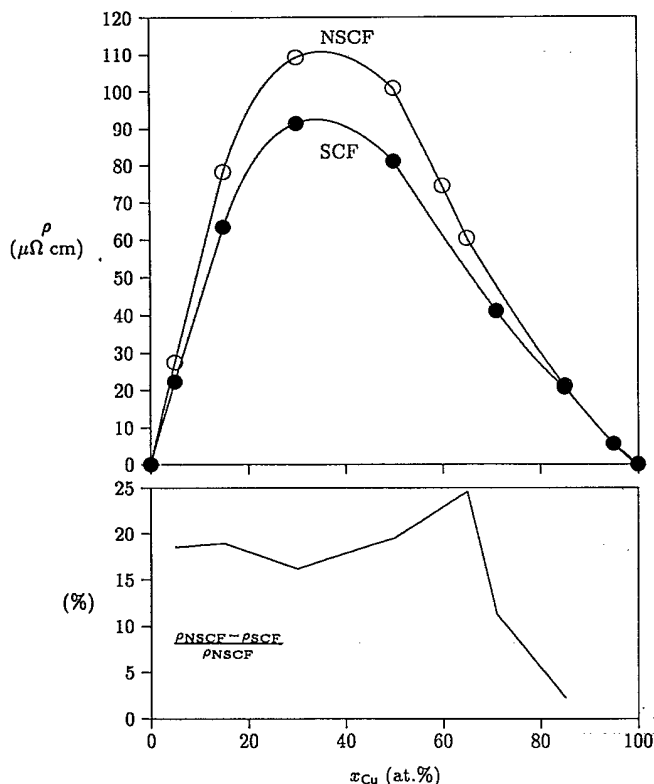


FIG. 2. Upper part: comparison between the resistivity of Cu-Pt calculated using non-self-consistent (NSCF) and self-consistent (SCF) potentials. Lower part: relative difference between the two calculated values.

of the order $n^2 \times n^2$, where n is determined by the angular momentum expansion [$n = 2 \times (\ell_{\max} + 1)$, thus $n=18$ for $\ell \leq 2$ and $n=32$ for $\ell \leq 3$], have to be multiplied and inverted and second, the Brillouin-zone integral has to be carried out over 3/48 parts of the zone instead of the 1/48 part. This was the reason why in the early study of Ref. 7 the vertex corrections were neglected. However, the calculation is feasible and the results for the calculations based on the self-consistent potentials and the relativistic current operator are presented in Fig. 4. As could be expected the effect is largest for the copper-rich alloys and rather minute for the Pt-rich side of the composition range. The vertex corrections are small when the effective range of the alloy potentials is small and when the electronic states are more localized to one particular lattice site.³ This is definitely more the case for the Pt-rich alloys which have more localized d -like states at the Fermi surface than for the Cu-rich alloys with more free electron like s and p states. However, as the major differences between the calculated and the experimental resistivities are found on the Pt-rich side, the inclusion of the vertex corrections does not eliminate the remaining discrepancy, because it merely changes the resistivity on the copper-rich side where the deviations are small.

D. Inclusion of f states

As the calculated resistivity still seems too much too high on the Pt-rich side of the composition range, finally

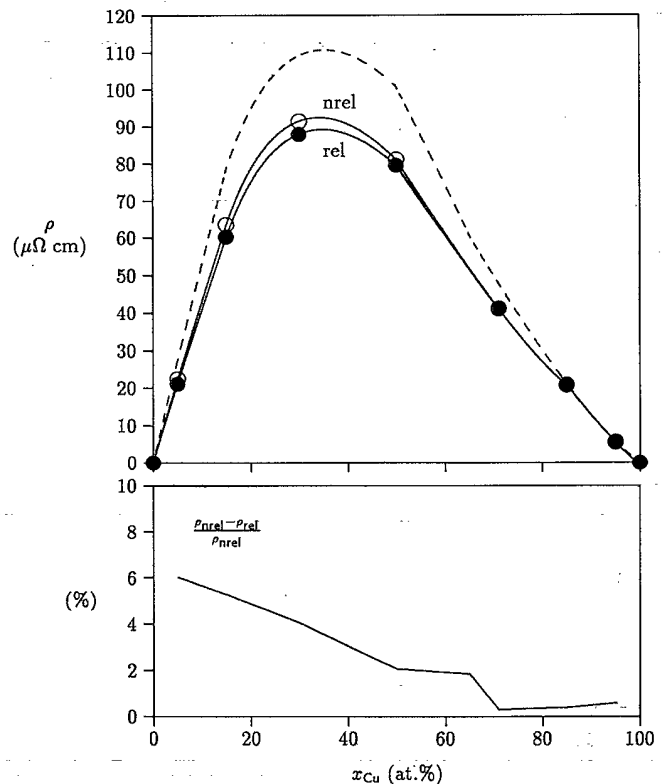


FIG. 3. Upper part: Comparison between the resistivity of Cu-Pt calculated using the nonrelativistic (nrel) and the relativistic (rel) current operator; dashed line: results from Ref. 7. Lower part: relative difference between the two calculated values.

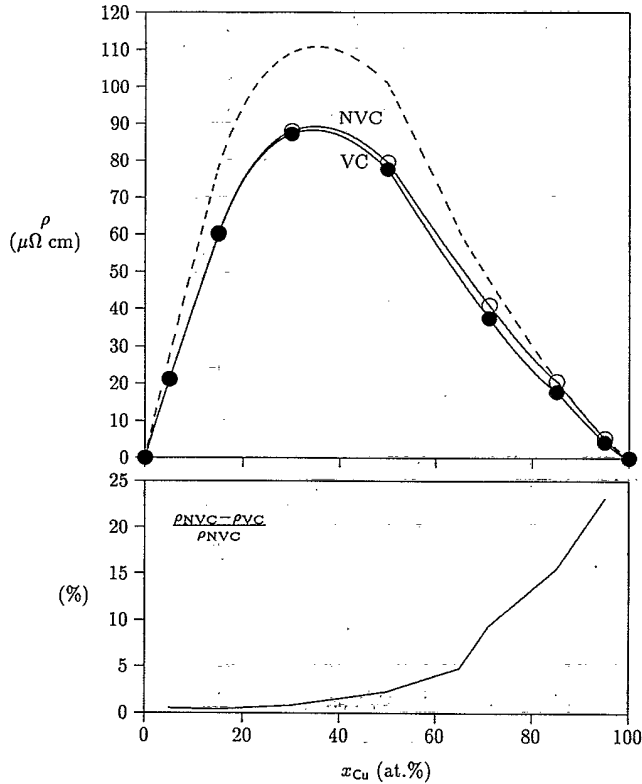


FIG. 4. Upper part: comparison between the resistivity of Cu-Pt without (NVC) and including (VC) vertex corrections; dashed line: results from Ref. 7. Lower part: relative difference between the two calculated values.

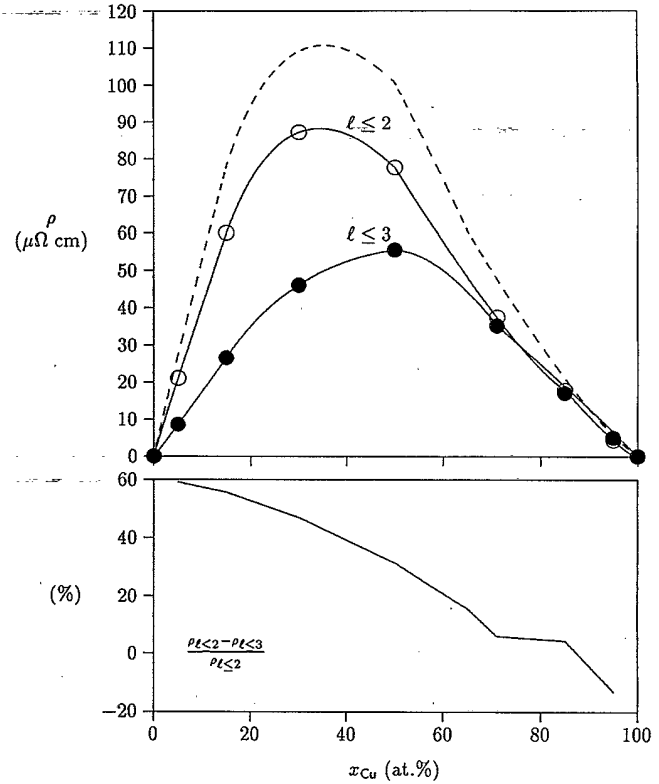


FIG. 5. Upper part: comparison between the resistivity of Cu-Pt calculated without ($\ell \leq 2$) and including ($\ell \leq 3$) f states; dashed line: results of Ref. 7. Lower part: relative difference between the two calculated values.

the extension of the calculation to an angular momentum expansion up to $\ell=3$ (f states) was attempted. Computationally, this extension is quite demanding because the size of the matrices in Eq. (7) increases to 1024×1024 compared to 324×324 for $\ell \leq 2$. For this reason, in order to limit the expenditure in computation time, the same alloy potentials and Fermi energies were used as for the calculations limited to $\ell \leq 2$. The results of the calculations are shown in Fig. 5. The resistivity is now much smaller for the Pt-rich alloys with a relative difference to the result for $\ell \leq 2$ of nearly 60% for $\text{Cu}_5\text{Pt}_{95}$. The reason for this dramatic effect is that the current operators of Eqs. (10) and (11) obey the selection rule $\Delta\ell = \pm 1 \dots$. Although the contribution of the f states to the density of states is quite small they may be important for the electrical conductivity by their coupling to the d states via the matrix elements of the current operator. This holds especially for the Pt-rich alloys because here the d elements of the scattering-path operator—corresponding to a high DOS at the Fermi energy level—are quite large. Naturally, for the Cu-rich alloy where both the d and the f elements are rather small, because the Fermi energy lies well above the d -band complex, this contribution is small and there is almost no difference between calculations restricted to $\ell \leq 2$ and those restricted to $\ell \leq 3$.

E. Comparison with measured values

Without doubt the results of the calculations discussed in the preceding sections lie closer to the extrapolated values of the measured zero-temperature resistivity (shown in Fig. 1) than the results of the calculations of Ref. 7 (also shown in this figure) which were calculated in a less sophisticated way. The agreement, however, is not all that good, a fact which might be due to the extrapolation in Eq. (12). The extrapolated results are not compared to the final theoretical resistivities in Fig. 5 in order not to suggest that a coincidence would be any measure of quality for the calculations. It is possible that the true experimental $T = 0$ K resistivity of Cu-Pt lies lower than the extrapolated zero-temperature curve in Fig. 1 and, therefore, matches the calculated curve of Fig. 5. Presently, measurements of the resistivity of Cu-Pt alloys at very low temperatures are in progress and will help to clarify the discussion when available.

IV. SUMMARY

The calculation of the residual electrical dc resistivity of disordered Cu-Pt alloys by means of the Kubo-

Greenwood formula and the relativistic KKR-CPA yields numerical values that are substantially smaller than the results of an earlier calculation based on a simplified version of the Kubo-Greenwood formula and on non-self-consistent alloy potentials. By removing successively the restrictions of our previous calculation it turned out that it is indispensable to use alloy potentials determined in a self-consistent manner in any case. The vertex corrections should be calculated in cases where the electronic states are not well localized at a specific lattice site, i.e.,

for alloys which have predominantly s and p states at the Fermi energy level. The use of the nonrelativistic and the relativistic form of the current operator yields differences just when heavy elements are involved. Finally, f states should be included in the calculation whenever the d -like component in the scattering operators is not negligible, i.e., whenever the d -like density of states is high at the Fermi energy level. As it turned out this demand may be even more important than the request for using self-consistent potentials.

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