PHYSICAL REVIEW B VOLUME 53, NUMBER 11 15 MARCH 1996-I

Pressure dependence of the electrical residual resistivity of disordered alloys

John Banhart
Fraunhofer-Institute for Applied Materials Research, Lesumer Heerstrasse 36, D-28717 Bremen, Germany

(Received 25 April 1995; revised manuscript received 26 September 1995)

The pressure dependence of the electrical residual resistivity was calculated for a series of disordered Au-Pd alloys by using the Korringa-Kohn-Rostoker coherent-potential approximation and the Kubo-Greenwood equation. The changes of the density of states and of the Fermi surface caused by an external pressure applied to the alloy are discussed and related to the change in residual resistivity. The volume coefficient of the residual resistivity is calculated from the pressure-dependent resistivity and found to be in accordance with experimental findings.

I. INTRODUCTION

The theoretical understanding and the ability to calculate electronic properties of disordered alloys has greatly improved in the last ten years. The key for this success has been the Korringa-Kohn-Rostoker (KKR) coherent-potential approximation (CPA), which allows for a rigorous, parameter-free description of the electronic structure of disordered systems.[1,2] Historically the KKR-CPA was first used to determine equilibrium observables such as the linear coefficient of the low-temperature specific heat, magnetic properties, or total energies.[2] Then the calculations were extended to non-equilibrium transport properties, namely, the electrical conductivity,[3,4] the thermoelectric power,[3,5] the ordinary[6] and extraordinary[7] Hall coefficient or the spontaneous resistance anisotropy in ferromagnetic alloys.[7] In most cases theory was seen to yield numerical values that were in good agreement with experimental findings.

A future task will be the extension of the theory to other, more complicated transport coefficients in order to find out whether the theoretical concepts are still appropriate for the description of the corresponding phenomena. We want to contribute to this task in the present paper by calculating the pressure dependence of the residual resistivity for the exemplary alloy system gold-palladium.

It is well known that the interatomic distance is an important parameter in metal physics and that measurements of the pressure dependence of electronic observables provide a wealth of information.[8] The most common investigations carried out for pure metals at high pressures are electrical resistance measurements or, more precisely, measurements of the resistance caused by lattice vibrations at various temperatures and pressures. This quantity is a very sensitive probe of the lattice spacing due to the change of the Debye temperature under pressure. However, impurities or grain boundaries, e.g., can also affect the measurements and make the interpretation in terms of theoretical models difficult. In contrast to pure metals, experimental investigations on concentrated alloys at low temperatures, where disorder scattering is the prime source of resistance, are rather scarce (e.g., Ref. 9).

It is the objective of this paper to show how the residual resistivity of a series of Au-Pd alloys changes under the influence of pressure. It is the first computation of this quantity that is completely parameter free and treats the electronic structure problem of the alloy and the electrical conductivity problem on a high level of sophistication. There have been calculations of the change of the band structure of pure metals under the influence of pressure (e.g., Refs. 10–12) and simple calculations of the pressure effect on the resistivity of alloys. Povey,[13] e.g., determined the residual resistivity of an alkali-metal alloy for various lattice volumina using a muffin-tin model and simple transport theory.

Until the present there have been, to our knowledge, no experimental investigations of the pressure dependence of the residual resistivity for Au-Pd alloys at low temperatures. The pressure dependence in palladium diluted with nickel, however, has been measured for low temperatures and shall be compared to the calculated values for palladium-rich Au-Pd alloys. Moreover, there are room-temperature investigations for $\underline{\text{Au}}$Pd alloys ($x_{\text{Pd}}<4$ at.%) (Ref. 14) and for the isoelectronic system Ag-Pd (Ref. 15) that can be used for interpretation.

By presenting the calculations on Au-Pd, I wish to stimulate interest in experimental investigations of the pressure dependence of the electrical resistivity at low temperatures.

II. THEORY

The resistivity of an alloy can be split up into a temperature-dependent thermal contribution and the residual resistivity due to impurity or disorder scattering according to Matthiessen's rule:

$$\rho_{\text{tot}}(T)=\rho_{\text{ph}}(T)+\rho_0 . \tag{1}$$

A similar partition applies to the pressure coefficient of the resistivity:

$$\left(\frac{1}{\rho}\,\frac{\partial\rho}{\partial p}\right)_{\text{tot}}=\frac{\rho_{\text{ph}}}{\rho_{\text{tot}}}\left(\frac{1}{\rho}\,\frac{\partial\rho}{\partial p}\right)_{\text{ph}}+\frac{\rho_0}{\rho_{\text{tot}}}\left(\frac{1}{\rho}\,\frac{\partial\rho}{\partial p}\right)_0 . \tag{2}$$

In general, the pressure dependence of the thermal and of the residual resistivity can be quite different and must be determined separately by choosing such conditions that either ρ_{ph} or ρ_0 is negligible. In this paper I perform electronic structure calculations on static lattices with various lattice spacings; i.e., the resistivity does not contain any temperature-dependent contributions so that one is able to assess the pressure coefficient of the residual resistivity.

All one needs to be able to evaluate this coefficient is the electrical resistivity for varying lattice constants. The resistivity can be calculated by means of the Korringa-Kohn-Rostoker coherent-potential approximation (KKR-CPA) and the Kubo-Greenwood equation. The KKR-CPA describes the electronic structure of the disordered alloy in terms of an averaged Green function, which represents an effective medium approximating the true disordered system. From this Green function all important observables can be calculated. Whereas the determination of simple quantities such as the density of states is rather straightforward, the electrical resistivity leads to complicated equations. The starting point for the conductivity calculation is given by an expression of the form

$$\sigma = \frac{1}{\rho} \propto \langle\, \mathrm{Im}GJ\ \mathrm{Im}GJ \rangle_{\mathrm{conf}}, \tag{3}$$

where the G are one-particle Green functions and the J electrical current operators. The brackets denote an average over all possible configurations of the (infinite) disordered system, which has to be performed analytically. A scheme for this was developed by Butler.[16] It allows for the full calculation of the electrical conductivity tensor without having to make a semiclassical approximation and without neglecting important contributions to the conductivity such as the vertex corrections. The derivation of the Kubo-Greenwood equation in the framework of the KKR-CPA shall not be repeated here. The reader should refer to the literature for details.[2,16] The formalism has been shown to yield good and reliable results for a number of alloy systems (e.g., Refs. 4, 5, and 17) and has been adapted to deal with fully relativistic electronic structure calculations.[7,18]

III. CALCULATIONS

The KKR-CPA equations were solved for a number of gold-palladium alloys of various compositions. For each composition the lattice constant was varied with values around the known experimental lattice spacing. The calculation was carried out relativistically in order to take account of the relativistic effects known to be important for gold. The lattice potentials were determined in a self-consistent manner in the usual way. Examples of relativistic KKR-CPA calculations for Au-Pd alloys are found in the literature.[19,20]

Figure 1 shows the density of states for three $Au_{25}Pd_{75}$ alloys with various lattice constants. Because in the alloys with the smaller lattice constant the muffin-tin zeroes are shifted to lower energies, the energy scale in Fig. 1 was chosen in a way that the Fermi energies of all alloys coincide in order to allow for a better comparison of the various pressure levels.

Naturally, the density of states at the Fermi energy level is of major interest. Figure 2 shows this quantity for some of the alloys as a function of the lattice constant.

For each composition and lattice constant the residual resistivity was calculated by means of the Kubo-Greenwood equation. The relativistic version of this formalism was used as described in Ref. 18. The results of the calculations are shown in Fig. 3 for three selected alloys. From the values shown in this figure the quantity $d\rho/da|_{a_{\mathrm{exp}}}$ can be calculated, where a_{exp} is the experimental lattice constant at normal conditions (atmospherical pressure 10^5 Pa). The values for the residual resistivity and its derivative are shown in Table I.

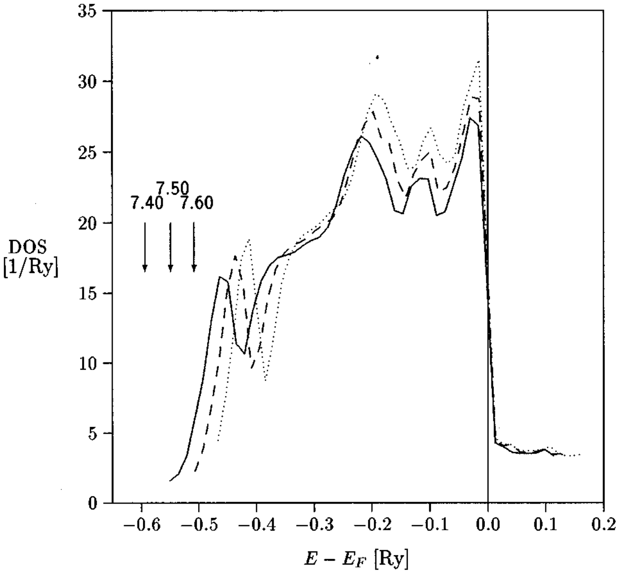

FIG. 1. Density of states for $Au_{25}Pd_{75}$ alloys with three different lattice constants (full line: 7.40 a.u.; dashed: 7.50 a.u.; dotted: 7.60 a.u. The muffin-tin zeroes for the three lattice constants are indicated by vertical arrows.

IV. DISCUSSION

The effect of pressure on the electronic structure of the disordered alloy $Au_{25}Pd_{75}$ can be seen from Fig. 1: pressure,

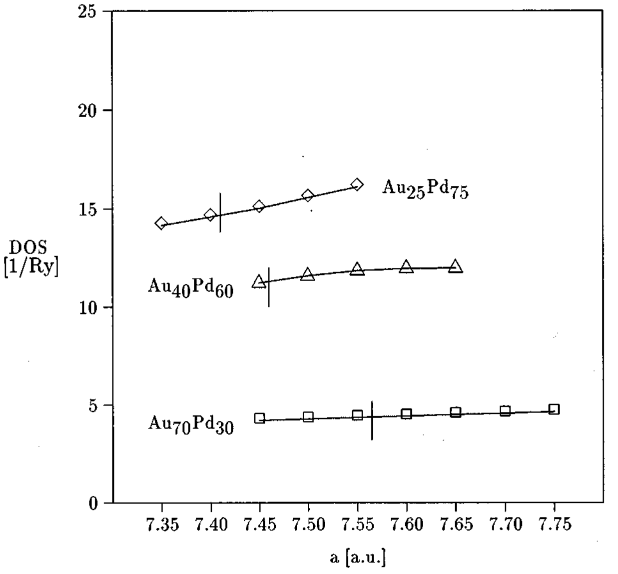

FIG. 2. Density of states of various Au-Pd alloys as a function of the lattice constant. The full lines serve as a guide for the eye. The short vertical bars denote the experimental lattice constants at atmospherical pressure $p_0 = 10^5$ Pa.

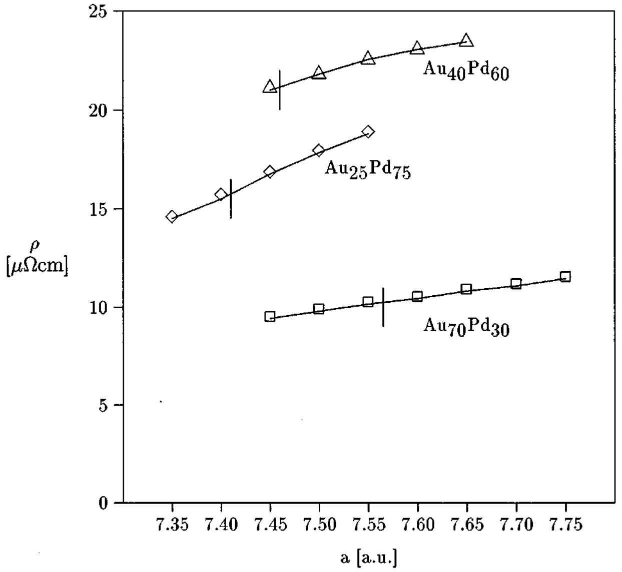

FIG. 3. Residual resistivity of various Au-Pd alloys as a function of the lattice constant. The full lines serve as a guide for the eye. The short vertical bars denote the experimental lattice constants at atmospherical pressure $p_0 = 10^5$ Pa.

accompanied by a reduction of the lattice spacing, leads to a broadening of the alloy d band and a corresponding reduction of the density of states of the d band. The reduction of the density of states is more pronounced for low-lying states and rather small for the states near the Fermi energy. In Fig. 2 the density of states at the Fermi energy level is shown as a function of the lattice constant for various different alloy compositions. Pressure leads to a slight reduction of the Fermi energy density of states for all the alloys. The reduction is strongest for the palladium-rich alloys where the Fermi level runs through the upper edge of the d band and small for the gold-rich alloys where the Fermi energy is in a region of relatively constant density of states. For the alloy $\mathrm{Au}_{25}\mathrm{Pd}_{75}$, e.g., a lattice constant change from 7.6 to 7.4. a.u. decreases the s density of states (DOS) n_s by about 14%, the d DOS n_d by about 11% and the product $n_s n_d$ by about 26% (see below).

The behavior of the residual resistivity as a function of the lattice constant shown in Fig. 3 is similar to that of the density of states because the electrical conductivity is also a property related to the electronic structure at the Fermi energy level. The most obvious feature is that the resistivities increase with increasing lattice constant for all alloy compositions or, in an equivalent formulation, pressure reduces the electrical resistivity. For the said alloy $\mathrm{Au}_{25}\mathrm{Pd}_{75}$ a lattice reduction from 7.6 to 7.4 a.u. reduces the electrical resistivity by 25%, a value that is almost identical to the reduction of $n_s n_d$. This allows a link to the traditional sd picture of electrical conduction in transition-metal alloys, where the resistivity is mainly caused by scattering from s to d states for Pd-rich alloys and the resistivity is therefore proportional to $n_s n_d$. Of course this picture is only true in limited cases and does, e.g., not apply to gold-rich Au-Pd alloys.

TABLE I. Experimental lattice constants and calculated resistivities and their derivatives for disordered Au-Pd alloys.

at.% Au	a_{exp}	$\rho(a_{\mathrm{exp}})$	$d\rho/da\|_{a_{\mathrm{exp}}}$
20	7.395	12.8	20
25	7.410	15.8	22
30	7.425	18.0	13
40	7.460	21.2	13
50	7.495	17.2	2
60	7.525	12.5	3.3
70	7.565	10.2	5.3
75	7.580	9.1	5
80	7.600	7.4	5

A discussion of the electrical resistivity in terms of the DOS can be misleading. The reason for this is that the DOS merely gives the number of states that may contribute to dissipative scattering events but does not contain any information about how inelastic such events are and how much they contribute to the resistivity. This is most obvious for pure palladium, which has the highest DOS in the system Au-Pd, but has no residual resistivity at all.

From a more formal viewpoint this can be seen as follows: the DOS, defined by

$$n(E) = -\frac{1}{\pi}\,\mathrm{Im}\,\mathrm{Tr}\langle G(E)\rangle_{\mathrm{conf}} \tag{4}$$

contains an average over a single Green function, whereas the Kubo-Greenwood equation [Eq. (3)] contains a product of two Green functions and current operators. There is no reason to believe that the two expressions should behave in a similar fashion except for very limited cases.

The effect of a change of the lattice constant on the resistivity is difficult to trace directly from the Kubo-Greenwood equation, because there are many matrix elements involved in this equation and most of the elements vary with the lattice constant. However, there is a quantity that is closely related to the electrical resistivity: the Bloch spectral function (BSF). The BSF, $A_B(\vec{k},E)$, is a k-resolved density of states.[2] For a translationally invariant system it is a collection of δ functions that maps the dispersion relation $E(\vec{k})$. For random alloys, however, the δ-function peaks are broadened due to impurity scattering, thus expressing the fact that the wave vector $\vec{k}$ is no longer a good quantum number. Therefore, in contrast to the ordinary DOS, the BSF carries information not only about the number of states but also about the level of disorder in the system. In particular, the BSF at the Fermi energy $A_B(\vec{k},E_F)$ defines an alloy Fermi surface by the positions of its (broadened) peaks. The half width of these peaks is a measure of disorder. Provided that the BSF along a particular ray $\vec{e}$ in the Brillouin zone can be approximated by a Lorentzian function,

$$A_B(k\cdot\vec{e},E) = \frac{a}{[(k_F-k)^2+\gamma^2]}, \tag{5}$$

a mean free path for the particular $\vec{e}$ can be defined as $l(\vec{k}_F) \propto 1/2\gamma$, where $\overrightarrow{k_F} = k_F \cdot \vec{e}$ defines the positions of the Fermi surface. If $l(\vec{k}_F)$ is sufficiently large in comparison

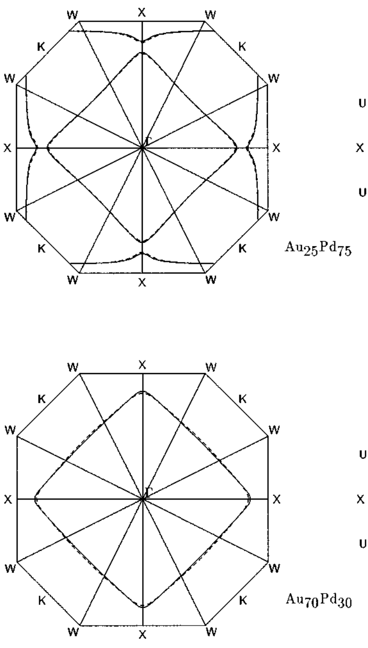

FIG. 4. Fermi surface cuts for $Au_{25}Pd_{75}$ (top) and $Au_{70}Pd_{30}$ (bottom) alloys. Left panels: (100) plane; right panels: (111) plane. Full lines: lower lattice constant; dashed line: higher lattice constant.

with the lattice spacing, a simple version of the Boltzmann equation can be applied to calculate the electrical conductivity:[21,22]

$$\sigma \propto \int\int_{\mathrm{FS}} l(\vec{k})\, dS. \tag{6}$$

However, the Kubo-Greenwood equation is superior to this approach so that the BSF are merely used to locate the Fermi surface and to determine the degree of disorder in this work. Figure 4 shows the Fermi surface of two Au-Pd alloys calculated from BSF. The Fermi surfaces are represented by cuts through the (100) and the (111) plane in this figure and for each alloy the Fermi surface for two different lattice constants is given.

The (111) plane (right-hand side) contains the necks, which are typical for noble metals and which intersect the Brillouin zone boundary only for the gold-rich alloys. Moreover, the gold-rich alloys have a connected Fermi surface, whereas alloys with more than 30% palladium show a second sheet in the first Brillouin zone. The Fermi surfaces in the (100) plane (left-hand side) are simpler: the inner sheet is closed and has flat portions in the K directions. There is an outer sheet intersecting the Brillouin zone between the K and W points for Pd-rich alloys.

In the context of the present paper it is interesting to see how a variation of the lattice constant changes the Fermi surface: for $Au_{25}Pd_{75}$ the Fermi surface corresponding to the higher lattice constant (dashed lines) lies closer to the Γ point for all k directions shown in Fig. 4 and both sheets, i.e., all k vectors $\vec{k}_F$ are smaller for the higher lattice constant. The changes are rather small and are therefore not easy to see. As the strongest reductions occur in the X and L directions, the Fermi surface becomes "rounder" and smaller for increasing lattice constant. For the alloy $Au_{70}Pd_{30}$ the higher lattice constant is also associated with smaller k vectors in the X and L directions, whereas the Fermi surface expands around the K direction. As for the Pd-rich alloy the Fermi surface is rounder and therefore closer to the free electron surface for the higher lattice constant.

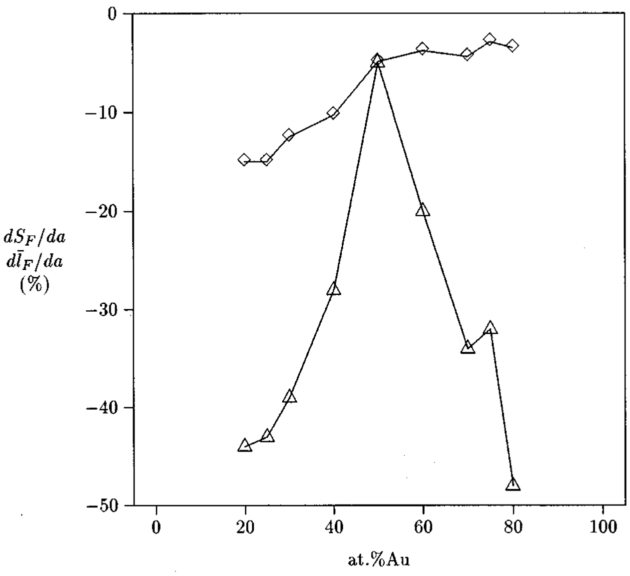

FIG. 5. Change of Fermi surface area S_F (◇) and averaged mean free path $\bar{l}_F$ (△) with lattice constant for Au-Pd alloys.

The described changes in the Fermi surface shape do certainly affect the electrical resistivity. In the picture based on the mean free path $l(\vec{k}_F)$ [Eq. (6)] there are two possibilities for the resistivity to change: by increasing the mean free path or by increasing the Fermi surface area. The area may either vary continuously when the Fermi surface moves in or out with respect to the origin Γ, or discontinuously when the topology of the Fermi surface changes. This may happen when new sheets of the Fermi surface appear. Such so-called electronical topological transitions[23] were not observed for Au-Pd when the lattice constant was changed in the narrow range that plays a role for the present paper. The change of the area of the inner sheet of the Fermi surface, which contributes predominantly to the electrical conductivity, is shown in Fig. 5. The area was determined by calculating BSF along 1176 rays originating from the Γ point of the Brillouin zone, locating the Fermi surface on these lines, and finally calculating the area of the Fermi surface numerically. This calculation was performed for each alloy composition and for the lowest and highest lattice constant for each alloy. As already said, the Fermi surface shrinks with increasing lattice constant for all the alloys, the change being largest for the palladium-rich alloys.

The mean free path averaged over the Fermi surface, $\bar{l}_F$, also decreases for increasing lattice constants for all the alloys. However, here the effect is largest for the palladium- and gold-rich alloys and small for the alloy $Au_{50}Pd_{50}$. This finding is perfectly compatible with the results for $d\rho/da$ obtained in the rigorous calculation listed in Table I: the resistivity of the alloy $Au_{50}Pd_{50}$ is less sensitive to lattice constant changes than that of the other alloys. The change of

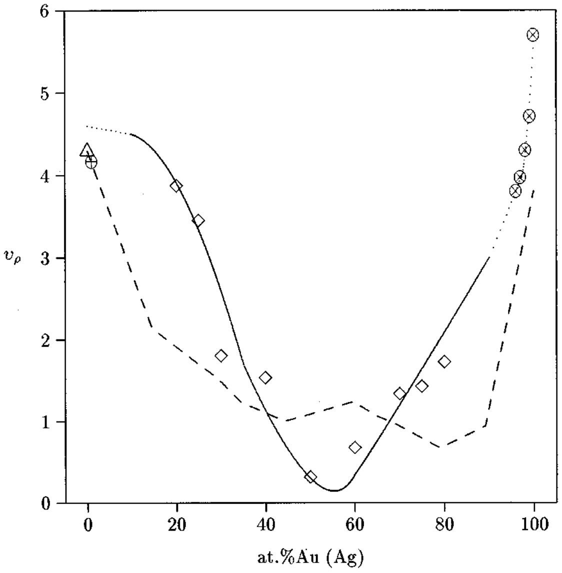

FIG. 6. Volume coefficient of the residual resistivity of Au-Pd. ◇: calculated values; ⊕: experimental value for PdNi1 ($T=4.2$ K); ⊗: experimental values for Au-Pd (300 K); △: experimental value for Pd (300 K). Dashed line: volume coefficient for Ag-Pd (300 K).

the mean free path obviously is the main reason for the resistivity change and is enhanced by the reduction of the Fermi surface area.

Turning back to Fig. 3 one can see that within the range of lattice constants considered the resistivity varies approximately linearly with the applied pressure. The pressure range associated with the range of lattice constants used is about -50 to 100 kbar for the alloy $Au_{25}Pd_{75}$ and similar for the other alloys. This range is comparable to the pressures usually applied in measurements (only $p>0$).

The quantity that can be determined experimentally is the pressure coefficient of the resistivity

$$\frac{1}{\rho}\left(\frac{d\rho}{dp}\right)_T.$$

In order to be able to compare experimental values with calculated ones, it is useful to define a dimensionless volume coefficient v_ρ:

$$v_\rho=\frac{V}{\rho}\left(\frac{d\rho}{dV}\right)_T=-\frac{1}{\rho}\left(\frac{d\rho}{dp}\right)_T\frac{1}{\kappa_T}, \tag{7}$$

where κ_T is the isothermal compressibility of the alloy. Because the volume V is proportional to a^3 one can also write

$$v_\rho=\frac{a}{3\rho}\left(\frac{d\rho}{da}\right)_T. \tag{8}$$

By inserting the values of Table I into Eq. (8), the volume coefficient can be calculated. Its composition dependence is shown in Fig. 6. The values are all positive, reflecting the fact that the resistivity decreases with increasing pressure for all compositions. Alloying gold to palladium leads to a rapid decrease of the volume coefficient and a minimum around 50% Au. Further addition of gold slightly increases v_ρ again.

TABLE II. Experimental low-temperature values for the volume coefficient of the residual resistivity v_ρ of pure Pd and PdNi alloys (calculated from Ref. 24). For comparison: room-temperature value for pure Pd (Ref. 15).

Ni concentration	v_ρ
0 (pure Pd)	0.77
0.32	3.76
0.55	4.00
1.0	4.17
0 (pure Pd), $T=300$ K	4.30

As was already mentioned, there are experimental sources for the pressure coefficient of pure palladium and Pd-Ni alloys at low temperatures.[24] Using experimental values for the isothermal compressibility[25] of Pd, the volume coefficient can be calculated by means of Eq. (7) from these data ($\kappa_T=5.4\times10^{-12}$ Pa^{-1} was used for Pd). The resulting experimental quantities v_ρ are summarized in Table II.

Obviously, addition of Ni to Pd leads to a rapid increase of v_ρ as the source of resistivity shifts from thermal to disorder scattering upon addition of Ni. v_ρ seems to saturate out for small contents of the nickel impurities already. The value for 1% Ni (4.17) is compared to the calculated volume coefficients of Au-Pd in Fig. 6. Apparently, this experimental low-temperature value for "dirty" palladium fits nicely to the calculated ones on the palladium-rich side if one extrapolates the calculated values (see the dotted line). Also, the room-temperature value for pure palladium (4.3) is very close to this figure, showing that thermal and disorder induced v are comparable in this particular case.

For the gold-rich side of the alloy system there is a series of experimental room-temperature values of v for AuPd ranging between 3.5 and 5.6. This fits to a (rather speculative) curve obtained by extrapolating the calculated values to pure gold (dotted line in Fig. 6). However, this comparison is doubtful because for pure gold v is strongly temperature dependent: for temperatures higher that room temperature it is seen to vary slowly[26] and for low temperatures ($1-5$ K) the sign of $d\rho/dp$ can even change: application of pressure then increases the residual resistivity and v_ρ is negative.[27] In the latter case the effect is caused by lattice defects, which are influenced by pressure changes and cause a pressure dependence this way. This demonstrates that the pressure dependence induced by other mechanisms than disorder scattering cannot be compared with the pressure coefficient of the disorder-induced resistivity in a straightforward way.

Figure 6 also shows room-temperature measurements of v for the alloy system Ag-Pd. As this system is isoelectronic to Au-Pd, one can expect that the composition dependence of v at least resembles that for Au-Pd. This is indeed the case: for Ag-Pd the maximum values for v are found for the pure components and a minimum is observed that is slightly shifted to Ag-rich alloys. This is exactly what was calculated for Au-Pd. Of course the agreement cannot be perfect because two different alloy systems are compared. Moreover, the measurements were made at room temperature.

V. SUMMARY

The pressure dependence of the residual resistivity of disordered alloys can be calculated first principles by applying the Kubo-Greenwood equation in the framework of the Korringa-Kohn-Rostoker coherent-potential approximation. For the alloy sytem Au-Pd the calculations show a strong pressure dependence of the residual resitivity for Pd-rich alloys, a nearly pressure-independent resistivity for 50% Au and, as one approaches pure gold, a rise of the pressure dependence. The resistivities vary approximately linearly with the applied pressure. Experimental low-temperature values for PdNi alloys and room-temperature values for pure Pd agree well with the calculations, if one extrapolates the calculated coefficients to $\underline{\mathrm{Pd}}$Au. For gold-rich alloys, measured room-temperature values re compatible with the calculations, but the temperature dependence makes the comparison doubtful for very dilute alloys. The experimental data for Ag-Pd shows a composition behavior similar to that calculated for Au-Pd.

In conclusion the method presented in this paper yields excellent results for a transport quantity without any use of adjustable parameters. The very encouraging results demand futher applications of the method and will hopefully stimulate experimental low-temperature work.

ACKNOWLEDGMENTS

I would like to thank Peter Weinberger for generating the alloy potentials used for the calculations presented in this paper.

---

[1] G.M. Stocks and H. Winter, in *The Electronic Structure of Complex Systems*, Vol. 113 of *NATO Advanced Study Institute, Series B: Physics,* edited by P. Phariseau and W.M. Temmerman (Plenum, New York, 1984), p. 463.

[2] P. Weinberger, *Electron Scattering Theory for Ordered and Disordered Matter* (Oxford University Press, Oxford, 1990).

[3] W.H. Butler and G.M. Stocks, Phys. Rev. B **29**, 4217 (1984).

[4] J.C. Swihart, W.H. Butler, G.M. Stocks, D.M. Nicholson, and R.C. Ward, Phys. Rev. Lett. **57**, 1181 (1986).

[5] J. Banhart and H. Ebert, Solid State Commun. **94**, 445 (1995).

[6] W.H. Butler, Phys. Rev. B **29**, 4224 (1984).

[7] J. Banhart and H. Ebert, Europhys. Lett. **32**, 517 (1995).

[8] H.G. Drickamer, in *Solid State Physics*, edited by F. Seitz and D. Turnbull (Academic, New York, 1965), Vol. 17, p. 1.

[9] A. Myers and N.D. Young, J. Phys. F **12**, 2641 (1982).

[10] Y. Kubo, J. Phys. F **17**, 383 (1987).

[11] R. Ahuja, A.K. Solani, and S. Auluck, Phys. Rev. B **39**, 9806 (1989).

[12] R. Ahuja, A.K. Solani, and S. Auluck, Phys. Rev. B **43**, 2401 (1991).

[13] M.J.W. Povey, J. Phys. F **8**, 231 (1978).

[14] P.W. Bridgman, Proc. Am. Acad. Arts Sci. **84**, 179 (1955).

[15] P.W. Bridgman, Proc. Am. Acad. Arts Sci. **84**, 131 (1955).

[16] W.H. Butler, Phys. Rev. B **31**, 3260 (1985).

[17] R.H. Brown, P.B. Allen, D.M. Nicholson, and W.H. Butler, Phys. Rev. Lett. **62**, 661 (1989).

[18] J. Banhart, H. Ebert, J. Voitländer, and P. Weinberger, Phys. Rev. B **50**, 2104 (1994).

[19] P. Weinberger, C. Blaas, B.I. Bennett, and A.M. Boring, Phys. Rev. B **47**, 10 158 (1993).

[20] P. Weinberger, J. Kudrnovski, J. Redinger, B.I. Bennett, and A.M. Boring, Phys. Rev. B **48**, 7866 (1993).

[21] W.H. Butler and G.M. Stocks, Phys. Rev. B **29**, 4217 (1984).

[22] J. Banhart, P. Weinberger, and J. Voitländer, J. Phys. Condens. Matter **1**, 7013 (1989).

[23] E. Bruno, B. Ginatempo, E.S. Giulano, A.V. Ruban, and Y. Vekilov, Phys. Rep. **249**, 353 (1994).

[24] R.A. Beyerlein and D. Lazarus, Phys. Rev. B **7**, 511 (1973).

[25] P.W. Bridgman, *Physics of High Pressures* (G. Bell, London, 1949), p. 160.

[26] R.R. Bourassa, D. Lazarus, and D.A. Blackburn, Phys. Rev. **165**, 853 (1968).

[27] J. Crone and E. Lüscher, Z. Phys. **30**, 287 (1978).