

## *Ab initio* calculations of the deviations from Matthiessen's rule for dilute ternary alloys

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We report *ab initio* calculations of the residual resistivity and the deviations from Matthiessen's rule for dilute ternary alloys. We consider nonmagnetic (Cu) as well as ferromagnetic host materials (Ni) with an admixture of simple-metal (*4sp*, *5sp*) or transition-metal (*3d*, *4d*) impurities. The calculations are performed within the frame of density functional theory and the Korringa-Kohn-Rostoker Green's-function method. The transport is described quasiclassically by means of the Boltzmann equation. In the case of a ferromagnetic host a two-current model is applied. Both impurity atoms are considered as noninteracting and the scattering properties of each impurity atom are calculated self-consistently including in addition to the impurity potential one shell of perturbed host potentials around the impurity. Our results show satisfactory agreement with experiments and confirm the validity of Matthiessen's rule in nonmagnetic systems. In ferromagnetic systems the two-current model is confirmed.

### I. INTRODUCTION

We often wish to calculate transport properties of a solid where several different scattering processes are going on at the same time, for example, where electrons are being scattered by two different noninteracting impurities *A* and *B*. A crude argument suggests that the resulting resistivity is the sum of the resistivities due to each type of scattering separately. This is only true in certain special circumstances, and we then say that Matthiessen's rule is satisfied. How deviations from this rule occur is easily understood from the following considerations. The two types of elastic scattering, defined by two equilibrium transition probabilities, lead to two scattering operators  $\mathbf{P}_A$  and  $\mathbf{P}_B$ . Whereas the total scattering operator is the sum of both contributions

$$\mathbf{P}_{AB} = \mathbf{P}_A + \mathbf{P}_B, \quad (1)$$

this is not true, e.g., for the resistivity. Substituting the scattering operator in the variational expression of the Boltzmann transport theory<sup>1</sup> we find for the resistivity

$$\rho_{AB} = \frac{\langle \Phi, \mathbf{P}_A \Phi \rangle + \langle \Phi, \mathbf{P}_B \Phi \rangle}{\langle \Phi, \mathbf{X}(\mathbf{E} = 1) \rangle^2}, \quad (2)$$

where  $\Phi$  is the exact solution of the Boltzmann equation involving the operator  $\mathbf{P}_{AB}$  and  $\mathbf{X}$  is the generalized force in a unit electric field ( $\mathbf{E} = 1$ ). In general,  $\Phi$  is not the exact solution of the Boltzmann equation for the scattering operators  $\mathbf{P}_A$  or  $\mathbf{P}_B$ . Thus we obtain from the variational expression

$$\rho_{AB} \geq \rho_A + \rho_B, \quad (3)$$

and the equality sign only holds when the same function  $\Phi$  is a solution of the Boltzmann equation for all three scattering operators, i.e.,  $\mathbf{P}_A$ ,  $\mathbf{P}_B$ , and  $\mathbf{P}_{AB}$ , apart from

some constant multiplier. Only then is Matthiessen's rule satisfied.

Even when Matthiessen's rule is not exactly true, the deviations are not expected to be large. By the variational principle, a first-order error in  $\Phi$  leads to a second-order error in the value of the resistivity. This seems to be confirmed for (*A, B*) impurities in nonmagnetic hosts, but in ferromagnetic hosts, such as Ni or Fe, large deviations of Matthiessen's rule are obtained experimentally.<sup>2-4</sup>

The origin of these deviations can be explained within the two-current model.<sup>5,6</sup> In ferromagnetic metals the electrons can be classified as having spin up ( $\uparrow$ , parallel to the saturation magnetization  $M_s$ ) or spin down ( $\downarrow$ , antiparallel to  $M_s$ ). The conduction can be described as taking place by two currents in parallel. Even if Matthiessen's rule is satisfied for each current separately, this does not guarantee that it is satisfied for the total resistivity.

Owing to the developments of density-functional theory and sophisticated numerical techniques we are now able to perform realistic *ab initio* calculations, and we can check the reliability of such model studies mentioned above. Within the Korringa-Kohn-Rostoker (KKR) Green's-function method a detailed analysis of the range of charge and magnetization perturbations around impurities in either a nonmagnetic or a magnetic host was performed.<sup>7-10</sup> The same formalism was applied to calculate the transport properties of dilute Ni alloys.<sup>11</sup> For this purpose the microscopic transition probability for an impurity atom with perturbed neighboring potentials around the impurity is calculated and fed into the Boltzmann equation. The formalism is now extended to calculate the deviations from Matthiessen's rule for dilute ternary alloys *ab initio*, that is, without introducing any free parameter.

The outline of the paper is as follows. In Sec. II the microscopic scattering probability is derived within the Green's-function method and fed into the transport equation to calculate the resistivity. In Sec. III methodical aspects are presented, and in Sec. IV the results are discussed and compared with experimental data.

## II. THEORY

The scattering of host electrons at one impurity potential leads to a transition from a state  $k$  into a state  $k'$ , where  $k$  is a shorthand notation for the wave vector  $\underline{k}$  and the band index  $\nu$ . The corresponding microscopic scattering probability is given by

$$P_{kk'} = 2\pi c |T_{kk'}|^2 \delta(\varepsilon_k - \varepsilon_{k'}) \quad (4)$$

where  $c$  is the atomic concentration of impurities. Within the powerful KKR Green's-function formalism<sup>12-15</sup> the transition matrix elements  $T_{kk'}$  for the scattering of Bloch electrons by an impurity cluster embedded in an ideal host crystal are

$$T_{kk'} = \frac{\hbar^2}{2m} \frac{1}{\sqrt{E_F}} \sum_{Ln} C_L^n(k) Q_L^n(k'). \quad (5)$$

$L$  denotes a pair of angular-momentum indices, i.e.,  $L = (l, m)$  and  $n$  characterizes the sites of the perturbed potentials in the cluster.  $C_L^n(k)$  and  $Q_L^n(k)$  are generalized wave function coefficients for the host and the alloy, respectively. The latter are connected by the relation

$$Q_L^n(k) = \sum_{L'n'} T_{LL'}^{nn'} C_{L'}^{n'}(k). \quad (6)$$

Neglecting lattice distortion effects the  $T$ -matrix coefficients  $T_{LL'}^{nn'}$  contain the structural Green's-function matrix elements  $G_{LL'}^{nn'}$  (Refs. 13-15) of the perturbed system

$$T_{LL'}^{nn'} = e^{-i\eta_l^0} \Delta t_l^n (\delta_{LL'}^{nn'} + G_{LL'}^{nn'} \Delta t_l^{n'}) e^{-i\eta_{l'}^0}. \quad (7)$$

Here  $\eta_l^0$  are the scattering phase shifts of the unperturbed potentials, and  $\Delta t_l^n$  represents the differences between the single-site  $t$  matrices of the perturbed potentials and the unperturbed ones. The structural Green's-function matrix  $G_{LL'}^{nn'}$  contains all the information about multiple scattering between the perturbed muffin tins and can be related to its counterpart for the host crystal by an algebraic Dyson equation.<sup>9,10</sup> Substitution of Eqs. (5), (6), and (7) in Eq. (4) results in

$$P_{kk'} = c \left( \frac{\hbar^2}{2m} \right)^2 \frac{1}{E_F} \delta(\varepsilon_k - \varepsilon_{k'}) \times \sum_{LL'nn'} Q_L^n(k) Q_{L'}^{n'}(k) C_L^n(k') C_{L'}^{n'*}(k'). \quad (8)$$

The electron lifetime due to impurity scattering is given by

$$\tau_k^{-1} = \sum_{k'} P_{kk'} = -2c \text{Im} T_{kk}^{\sigma\sigma}. \quad (9)$$

The second equality in Eq. (9) expresses the optical the-

orem connecting diagonal elements of the transition matrix  $T_{kk'}$  to a sum over all transition probability rates for scattering out of state  $k$ .

To simulate a dilute ternary alloy we use the following ansatz for the microscopic transition probability

$$P_{kk'} = (1-x) P_{kk'}^A + x P_{kk'}^B, \quad (10)$$

with two types of noninteracting impurities,  $A$  and  $B$ , being statistically independently distributed. Correspondingly, the electron lifetime becomes

$$\frac{1}{\tau_k} = (1-x) \frac{1}{\tau_k^A} + x \frac{1}{\tau_k^B}. \quad (11)$$

In the dilute limit  $c \ll 1$  the residual resistivity of impurities can be obtained from the solution of the linearized Boltzmann equation

$$\underline{\Lambda}_k = \frac{\tau_k^A \tau_k^B}{(1-x)\tau_k^B + x\tau_k^A} \times \left( \underline{v}_k + \sum_{k'} [(1-x)P_{kk'}^A + xP_{kk'}^B] \underline{\Lambda}_{k'} \right) \quad (12)$$

for the vector mean free path  $\underline{\Lambda}_k$ . Here  $\underline{v}_k$  is the Fermi velocity.

Obviously, Eq. (12) is an integral equation, which we solve by iteration.<sup>11</sup> For a ferromagnetic host, where  $k$  includes also the spin quantum number  $\sigma$  Eq. (10) represents a system of coupled integral equations for the vector mean free path  $\underline{\Lambda}_k$ . Assuming, that for the considered Ni alloys the spin-flip scattering can be neglected the Boltzmann equation decouples for both spin directions and can be solved separately.

The resistivity can be obtained from

$$(\rho_{AB})_{ij}^{-1} = e^2 \sum_k \delta(\varepsilon_k - \varepsilon_F) v_{ki} \Lambda_{kj}.$$

For cubic systems we have  $\hat{\rho}_{AB}^\sigma = \rho_{AB} \delta_{ij}$ . This equation can be used for each spin separately in ferromagnetic hosts leading to  $\rho_{AB}^\uparrow$  for the majority electrons and  $\rho_{AB}^\downarrow$  for the minority ones.

Due to the parallel addition of the two currents the total resistivity becomes for ferromagnetic cubic systems

$$\rho_{AB}^{-1} = \frac{\rho_{AB}^\uparrow + \rho_{AB}^\downarrow}{\rho_{AB}^\uparrow \rho_{AB}^\downarrow}. \quad (13)$$

In the limit  $x = 0$  the residual resistivity of the impurity  $A$ ,  $\rho_A$ , and in a ferromagnetic host the corresponding anisotropy ratio of the subband resistivities  $\alpha_A = \rho_A^\downarrow / \rho_A^\uparrow$  are reached. Analogously, for  $x = 1$  the residual resistivity  $\rho_B$  of impurity  $B$  with the anisotropy ratio  $\alpha_B = \rho_B^\downarrow / \rho_B^\uparrow$  will be obtained.

Finally, the deviations from Matthiessen's rule are defined as

$$\Delta\rho_{AB} = \rho_{AB} - \rho_A - \rho_B, \quad (14)$$

and the relative deviations are defined as  $\Delta\rho_{AB}/(\rho_A + \rho_B)$ .

### III. METHOD

This section specifies the numerical details in the calculation. A basic ingredient are the self-consistent potentials for pure Cu and Ni, which are taken from Moruzzi *et al.*<sup>16</sup> The KKR method with an angular-momentum truncation at  $l_{\max} = 4$  was used.

The imaginary part of the structural Green's-function was generated within the same KKR method by means of a Brillouin-zone integration using the tetrahedron method.<sup>22,10</sup> The real part of the Green's-function was calculated by a Hilbert transformation<sup>10</sup> with a truncation energy of 2.0 Ry.

The self-consistent impurity calculations are performed within the frame of density functional theory<sup>17,18</sup> using the local spin-density approximation as proposed by von Barth and Hedin<sup>19</sup> with parameters as chosen by Moruzzi *et al.*<sup>16</sup> To obtain the Green's-function of the perturbed system the algebraic Dyson equation is solved. The dimension of this equation is made finite by truncating the angular-momentum expansion at  $l = 3$  and by assuming potential perturbations only at the impurity site and at the first shell atoms around the impurity.

The Boltzmann equation is solved by iteration.<sup>20,21,11</sup> The necessary Fermi surface integrations were performed with a modified tetrahedron method.<sup>15</sup>

### IV. RESULTS AND DISCUSSION

#### A. Nonmagnetic host

As examples we considered Cu diluted with  $4sp$  impurities (Zn,As), with  $3d$  transition metal impurities (Co,Ti) and with a combination of  $4sp$  and  $3d$  impurities (Cr,As). The results for Cu(Zn,As) are shown in Table I. The calculated relative deviations from Matthiessen's rule are smaller than 1% for all compositions of dilute Cu(Zn) with Cu(As). Although Zn and As have different  $4p$  occupation numbers, their scattering properties can be essentially described by pseudopotentials differing only by the different excess charges  $\Delta Z$ , so that the microscopic scattering probabilities  $P_{kk'}^{Zn} \simeq C_0 P_{kk'}^{As}$  and also

TABLE I. Calculated residual resistivities  $\rho_{ZnAs}$ , prediction of Matthiessen's rule  $\rho_{Zn} + \rho_{As}$  and relative deviations from Matthiessen's rule for Cu(Zn<sub>1-x</sub>,As<sub>x</sub>) in dependence on the composition  $x$ . All resistivities are given in  $\mu\Omega$  cm/at. %.

$x$	$\rho_{ZnAs}$	$\rho_{Zn} + \rho_{As}$	$\Delta\rho/(\rho_{Zn} + \rho_{As})$
0.0	0.250	0.250	0.0
0.1	0.864	0.862	$2.0 \times 10^{-3}$
0.2	1.483	1.474	$6.2 \times 10^{-3}$
0.3	2.094	2.086	$3.8 \times 10^{-3}$
0.4	2.704	2.698	$2.2 \times 10^{-3}$
0.5	3.312	3.310	$0.6 \times 10^{-3}$
0.6	3.924	3.922	$0.5 \times 10^{-3}$
0.7	4.536	4.534	$0.4 \times 10^{-3}$
0.8	5.147	5.146	$0.2 \times 10^{-3}$
0.9	5.758	5.758	$0.0 \times 10^{-3}$
1.0	6.370	6.370	0.0

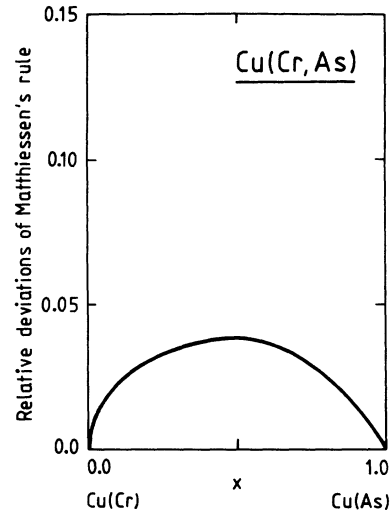


FIG. 1. Relative deviations from Matthiessen's rule against composition  $x$  for Cu(Cr<sub>1-x</sub>,As<sub>x</sub>). The calculated residual resistivities of the binary systems are  $10.00 \mu\Omega$  cm/at. % for Cu(Cr) and  $6.37 \mu\Omega$  cm/at. % for Cu(As).

the relaxation time  $\tau_k^{Zn} \simeq C_0 \tau_k^{As}$  of both scatterers, Zn and As, are comparable apart from a constant multiplier  $C_0 \simeq (\Delta Z_{Zn}/\Delta Z_{As})^2$ . Nearly the same situation was obtained for all compositions of dilute Cu(Co) with Cu(Ti) as representatives for  $3d$  transition-metal scatterers. Although Co and Ti have different  $3d$  occupation numbers, the scattering behavior in a Cu matrix is obviously so similar that the calculated relative deviations from Matthiessen's rule are smaller than  $1\%$ . Only the combination of dilute Cu(Cr) with dilute Cu(As), with Cr as a representative of  $3d$  transition-metal impurities and As as a simple-metal impurity, differ in their scattering behavior in a more pronounced way, so that the relative deviations from Matthiessen's rule increase to about 4% for a fifty-fifty admixture (see Fig. 1). Finally, we can conclude that Matthiessen's rule is a good approximation for combined scattering of two noninteracting impurities embedded in a nonmagnetic host, like Cu.

#### B. Ferromagnetic host

In this section we present calculated deviations from Matthiessen's rule for a variety of dilute ternary Ni alloys in comparison with experimental results (see Fig. 2). The columns in each figure illustrate the relative subband contributions to the conductivity in the binary alloys hatched parts belong to minority spin contributions and the black part to majority spin contributions. The general trend is that larger differences

$$\left| \frac{\sigma_A^\sigma}{\sigma_A} - \frac{\sigma_B^\sigma}{\sigma_B} \right|$$

between the relative subband conductivities of the dilute binary systems lead to larger deviations from Matthiessen's rule. In order to understand the origin of

these deviations we can compare our results with results predicted by the two-current model<sup>2,3</sup>

$$\rho_{AB} = \frac{[(1-x)\rho_A^\uparrow + x\rho_B^\uparrow][(1-x)\rho_A^\downarrow + x\rho_B^\downarrow]}{(1-x)\rho_A^\uparrow + x\rho_B^\uparrow + (1-x)\rho_A^\downarrow + x\rho_B^\downarrow}, \quad (15)$$

where it is supposed that the impurities *A* and *B* add their resistivity in each current, so that Matthiessen's rule is valid for the subband resistivities. Using the anisotropy ratios  $\alpha$  and the two-current model Eq. (13)

we can transform Eq. (15) into the following expression for the deviations from Matthiessen's rule

$$\Delta\rho = \frac{(\alpha_A - \alpha_B)^2 \rho_A \rho_B}{(1 + \alpha_A)^2 \alpha_B \rho_A + (1 + \alpha_B)^2 \alpha_A \rho_B}, \quad (16)$$

which is more comfortable for the comparison with experiments. The predictions of Eq. (16) are illustrated in Table II for Ni(Cr,Ti), in comparison with our calculation. The differences for the relative changes are about

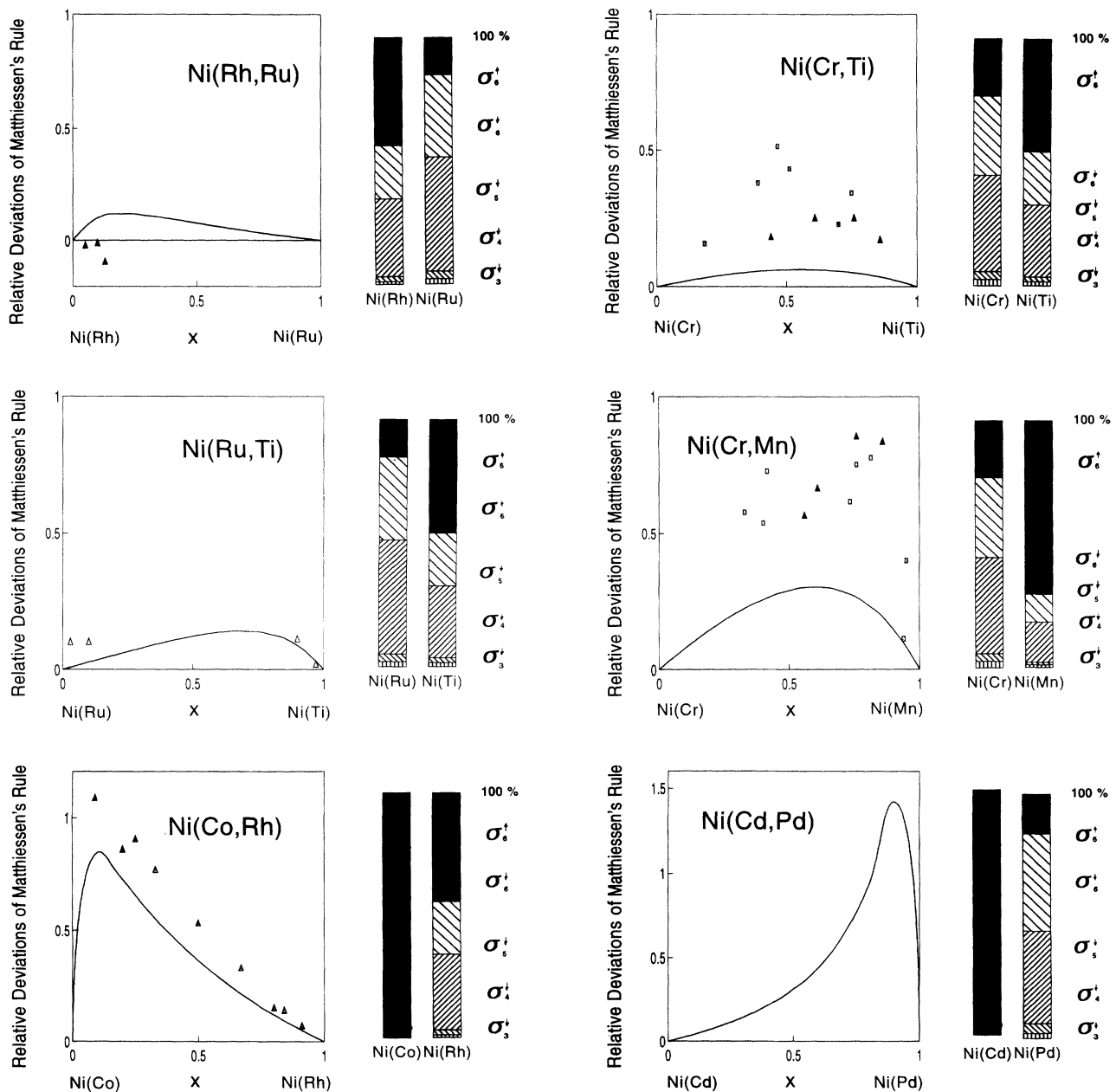


FIG. 2. Relative deviations from Matthiessen's rule against composition  $x$  for (a) Ni(Rh<sub>1-x</sub>Ru<sub>x</sub>), (b) Ni(Cr<sub>1-x</sub>Ti<sub>x</sub>), (c) Ni(Ru<sub>1-x</sub>Ti<sub>x</sub>), (d) Ni(Cr<sub>1-x</sub>Mn<sub>x</sub>), (e) Ni(Co<sub>1-x</sub>Rh<sub>x</sub>), (f) Ni(Pd<sub>1-x</sub>Cd<sub>x</sub>). The calculated residual resistivities and the  $\alpha$  ratios belonging to the dilute binary systems are given in Table III. The full line is our calculation. The triangles are experimental values as given in Ref. 2, for the rectangles see Ref. 3. The columns illustrate the relative subband contributions to the conductivity of the binary dilute systems, where the numbers indicate the number of the band and the arrows the spin direction.

TABLE II. Calculated residual resistivities  $\rho_{\text{CrTi}}$ , prediction of Matthiessen's rule  $\rho_{\text{Cr}} + \rho_{\text{Ti}}$  and relative deviations from Matthiessen's rule calculated by solving the Boltzmann equation for several compositions and due to the band model using Eq. (15) for  $\text{Ni}(\text{Cr}_{1-x}, \text{Ti}_x)$ . All resistivities are given in  $\mu\Omega \text{ cm/at. \%}$ .

$x$	$\rho_{\text{CrTi}}$	$\rho_{\text{Cr}} + \rho_{\text{Ti}}$	$[\Delta\rho/(\rho_{\text{Cr}} + \rho_{\text{Ti}})]_{\text{fit}}$	$[\Delta\rho/(\rho_{\text{Cr}} + \rho_{\text{Ti}})]_{\text{exact}}$
0.0	4.35	4.35	0.000	0.000
0.1	4.42	4.32	0.018	0.022
0.3	4.49	4.27	0.047	0.052
0.5	4.50	4.21	0.061	0.069
0.7	4.42	4.16	0.056	0.062
0.9	4.22	4.11	0.027	0.029
1.0	4.08	4.08	0.000	0.000

18% for  $\text{Ni}(\text{Cr}_{0.9}, \text{Ti}_{0.1})$  and smaller otherwise. Consequently, we can conclude that Matthiessen's rule is well satisfied (comparable to the nonmagnetic systems) for the subband resistivities,  $\rho_{AB}^{\alpha} = \rho_A^{\alpha} + \rho_B^{\alpha}$ .

In  $\text{Ni}(\text{Rh}, \text{Ru})$  [Fig. 2(a)] the calculated deviations from Matthiessen's rule for the total resistivity  $\rho_{AB}$  are generally small (up to 10%). The scattering behavior in the subbands is comparable, which can be seen from the similar relative conductivity contributions. A maximum is reached near  $\text{Ni}(\text{Rh})$  mixed with 15%  $\text{Ni}(\text{Ru})$ . The residual resistivities and also the  $\alpha$  ratios of both constituents agree with experiment (see Table III). The experimentally obtained negative deviations of Matthiessen's rule are impossible and can only be accepted with large error bars reaching the positive side. From the variational solution of the resistivity discussed in the Introduction it becomes clear that  $\rho_{AB} \geq \rho_A + \rho_B$ . That means, that  $\Delta\rho$  is always positive.

For  $\text{Ni}(\text{Cr}, \text{Ti})$  [Fig. 2(b)] the calculated deviations from Matthiessen's rule are smaller than 10% for a nearly fifty-fifty composition in agreement with experiments.<sup>3</sup> The residual resistivities for the dilute binary systems agree well with experiments (see Table III), but the  $\alpha$  ratios, particularly for  $\text{Ni}(\text{Ti})$ , differ more from experiment. As a consequence of Eq. (16) our calculated devi-

TABLE III. Calculated residual resistivities  $\rho_{\text{calc}}$  and subband ratios  $\alpha_{\text{calc}}$  in comparison to experimental results ordered with increasing  $\alpha$ . The resistivities are given in  $\mu\Omega \text{ cm/at. \%}$ .

Impurity	$\rho_{\text{calc}}$	$\rho_{\text{expt}}$	$\alpha_{\text{calc}}$	$\alpha_{\text{expt}}$
Pd	0.03		0.19	
Ru	6.27	4.9 <sup>a</sup>	0.17	0.29 <sup>a</sup>
Cr	4.35	4.8 <sup>a</sup>	0.3	0.5 <sup>a</sup>
		5.0 <sup>b</sup>		0.45 <sup>b</sup>
Rh	2.23	1.79 <sup>a</sup>	0.77	0.65 <sup>a</sup>
Ti	4.08	3.4 <sup>a</sup>	0.85	1.1 <sup>a</sup>
		2.9 <sup>b</sup>		4.0 <sup>b</sup>
Mn	3.13	0.72 <sup>a</sup>	2.42	8.9 <sup>a</sup>
		0.61 <sup>b</sup>		15.0 <sup>b</sup>
Cd	0.39		15.2	
Co	0.04	0.145 <sup>b</sup>	92.4	30.5 <sup>b</sup>

<sup>a</sup>Reference 2.

<sup>b</sup>Reference 3.

ations from Matthiessen's rule can be expected to differ from the experimental results. But the experiments also differ by about 100%. The system  $\text{Ni}(\text{Ru}, \text{Ti})$  [Fig. 2(c)] shows deviations from Matthiessen's rule up to 20% for a composition of 70%  $\text{Ni}(\text{Ti})$  and 30%  $\text{Ni}(\text{Ru})$  in very good agreement with experiment.

The system  $\text{Ni}(\text{Cr}, \text{Mn})$  [Fig. 2(d)] shows stronger deviations from Matthiessen's rule, up to 30% in our calculation and up to 75% experimentally. The position of the maximum near to 70%  $\text{Ni}(\text{Mn})$  is well reflected in our calculation. The differences between the absolute theoretical and experimental values should be connected with the  $\alpha$  ratio of  $\text{Ni}(\text{Mn})$  which also differs strongly.

The system  $\text{Ni}(\text{Co}, \text{Rh})$  [Fig. 2(e)] is an example for large differences in the subband contributions to the conductivity.  $\text{Ni}(\text{Co})$  with exclusively majority band contributions and  $\text{Ni}(\text{Rh})$  with comparable majority and minority band contributions to the conductivity. The deviations from Matthiessen's rule reach up to 100% for a ternary alloy consisting of 90%  $\text{Ni}(\text{Co})$  and 10%  $\text{Ni}(\text{Rh})$ .

Finally, starting from our detailed analysis of the residual resistivity of dilute Ni alloys<sup>11</sup> we would like to predict some systems that should show about 300–400% deviations of Matthiessen's rule. In Ni all combinations of Pd impurities, which cause mostly minority conduction, with impurities like Cd, Ag, Fe, Co, or Cu, which show mainly conduction in the majority band, should deviate strongly from Matthiessen's rule. The calculated deviations for  $\text{Ni}(\text{Pd}, \text{Cd})$  [Fig. 2(f)] illustrate this fact.

## V. SUMMARY

We have shown that Matthiessen's rule is a very good approximation for the resistivity of two noninteracting impurities in a nonmagnetic host. For a ferromagnetic host Matthiessen's rule is valid for the subband resistivities, but due to the parallel conduction of the majority and minority currents large deviations of Matthiessen's rule occur which are determined by the differences between the relative subband conductivities of the considered scatterers.

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