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Residual electrical resistivity in dilute nonmagnetic alloys of transition metals

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The residual electrical resistivity in dilute alloys of nonmagnetic transition metals is calculated within Mott's two-band model without using the electron-impurity interaction as a small parameter. The linear dependence between reduced residual electrical resistivity and square of modulus of the nondiagonal element of the scattering T matrix is found for row transition metals dilute alloys. Experimental and calculation results are compared.

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I. INTRODUCTION

It is well known that in the majority of dilute alloys (up to 5 at.% of impurity) of transition metal residual electrical resistivity (RR), ρ is linear with impurity concentration $\mathbf{c}$.[1–3] The specific contribution of impurity atoms to RR ($\rho_{\mathbf{c}} = d\rho/d\mathbf{c}$) value essentially depends not only on the solvent type but also on the type of impurity. One can see that within classical Linde's and Friedel's rules, the calculation of these contributions leads to unreasonably high values of RR.[4,5] The reasons are the single-band conductivity model and the *weak interaction* limit used in RR calculations.

It was shown[5] that the conductivity in transition metals and their alloys is realized mainly via highly mobile *s* electrons, which scatter not only within the *s* band, but transit to a partially filled *d* band as well. This process results in immobilization of some fraction of *s* electrons into the *d* band and according to Mott it is the main mechanism explaining the high resistivity of transition metals.[5] The probability of this interband scattering process is proportional to *d*-band density of states (DOS) at the Fermi level and consequently the resistivity is proportional to the ratio of *d*-band DOS to *s*-band DOS. The correlation between the *d*-band DOS value and resistivity values is evidence pointing to the validity of Mott's two-band conductivity model application. Experimental data on transition metals and their alloys resistivity demonstrate such a correlation: (i) the temperature resistivity coefficients are proportional to the *d*-band DOS in pure transition metals;[6] (ii) RR maxima in concentration dependence in transition metal continuous solid solutions are shifted toward the metal having a higher *d*-electron DOS.[7,8] Also, the correlation between $\rho_{\mathbf{c}}$ and the solvent *d*-electron DOS is seen in dilute alloys as well (Fig. 1).

On the other hand, Mott's two-band conductivity model experimental confirmations follows, for example, from high-frequency conductivity data extrapolated to zero frequency: the ratio of *s* to *d* conductivities is about 10 (Ref. 9); therefore the conductivity in transition metals and their alloys is realized mainly via highly mobile *s* electrons. The contribution of *d* electrons to total conductivity is very low and thus might be neglected. Consequently, our opinion is that Mott's two-band conductivity model may well be applied to the transition metals dilute alloys RR calculation.

At the present time *ab initio* (KKR-CPA, LMTO, and others) methods are used for transition metal alloys kinetic properties calculations by some authors.[10,11] These methods demonstrate excellent results of energy spectrum and DOS in metallic alloys calculations but may be applied to calculation of conductivity only in a simple case of the single-band model. The use of this model in the case of the multiple bands conductivity model is rather complicated and have a lot of unsolved problems up until now. The most moot point is an equivalence between the electron transport time and the one-electron level relaxation time. If using this approach one has to introduce a number of relaxation times in accordance with possible scattering processes, the definition of this value is a fairly difficult problem by itself and has no solution within the approaches of *ab initio* methods at the present time. The opportunity to take into account the interband transitions was discussed in the pioneer Butler's work.[10] Indeed, Butler and the authors following him put into operation a complementary approximation for taking into account an interband transition that allows a rather rough estimation only.

Moreover, some principal things cannot be found within the relaxation time approximation. For example, one cannot postulate *ab initio* the rule for the summation of several relation relaxation times. According to the commonly used rule, one has to summarize independently conductivities in several bands in analog to the parallel connection of several isolated conductors. Actually these conductors (*s* and *d*

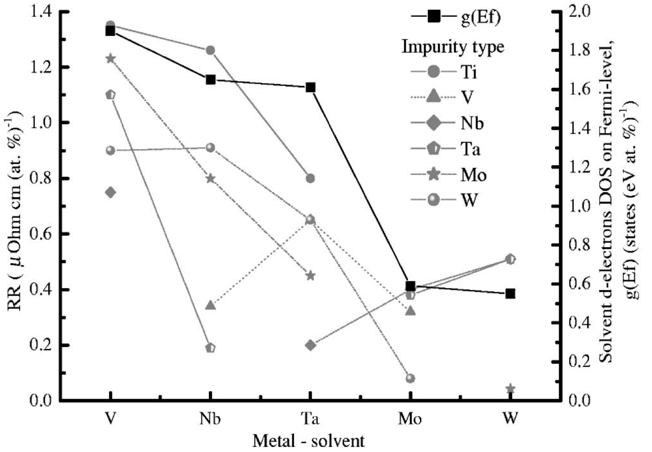

FIG. 1. The correlation between the specific contribution of impurity atoms to RR and solvent *d*-electron DOS on the Fermi level.

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bands) cannot be considered as isolated and it will be shown in the present paper that the resulting conductivity of a transition metal alloy is not identical to the conductivity of connected in parallel “isolated” electron conductive bands. It is impossible to obtain this principal result in the framework of the relaxation time approximation.

In this paper we will formulate an approach and obtain the kinetic equation within the two-band conductivity model for the case of an *arbitrary* electron-impurity interaction and perform results of RR calculations for a number of transition metal dilute alloys in the simple model-Thomas-Fermi screened potential approximation.

II. THE MODEL

Let us consider a one-electron Hamiltonian describing scattering of s and d electrons by a Coulomb field of randomly distributed A- and B-type ions in a binary alloy. Intra- and interband transitions of conduction electrons are the result of scattering of the type

$$\hat{H} = \sum_{l} E_l a_l^{+} a_l + \frac{1}{N}\sum_{n,l,l'} \exp(-i(\vec{k}-\vec{k}',\vec{r}_n))B_{l,l'}(n)a_l^{+}a_{l'}, \tag{1}$$

where E_l is the energy of electron with quantum number l, which includes band index j $(j=s,d)$ and wave vector $\vec{k}$; $\vec{r}_n$ is a radius vector of a crystal lattice site with the number n. The $B_{l,l'}(n)$ is the configurationally dependent part of electron energy:

$$B_{l,l'}(n) = \nu(n)[\lambda_{ll'}\delta_{j,j'} + \lambda_{ll'}(1-\delta_{j,j'})], \tag{2}$$

where coefficient $\nu(n)=\alpha_A(n)c_B-\alpha_B(n)c_A$ describes the random distribution of ions at crystal lattice sites: $\alpha_{A(B)}(n)=1$, if an ion at site n is of the $A(B)$ type and 0 in the other case. Matrix elements λ_{ll} and $\lambda_{ll'}$ characterize the intensities of intra- and interband electron transitions, respectively,

$$\lambda_{ll'} = \frac{1}{\Omega_0}\int d\vec{r}\,\psi_l^{*}\Delta U(\vec{r})\psi_{l'}, \tag{3}$$

where ψ_l are the solvent electron wave functions, Ω_0 is unit cell volume, and $\Delta U(\vec{r})=U^A(\vec{r})-U^B(\vec{r})$ is an interaction energy.

One can include an expression defining s-d hybridization, but it is well known that it only means a renormalization of *nonperturbed* one-electron energy level values, i.e., does not contribute to perturbation and can be incorporated with E_l. It is seen that by accounting for the hybridization the initial s and d bands transform into new s_1 and d_1 bands. But for the sake of simplicity let us use previous symbols, i.e., s and d.

It has been shown[6] that a system of kinetic equations defining the nonequilibrium additions f_l to equilibrium Fermi distribution functions f_l^0 in the linear to external electrical field approximation for two-band conductivity model can be deduced without using the relaxation time limit. The Swenson’s identity law[12] for the generalized scattering probability $W_{ll'}$ in time units,

$$W_{ll'} = |T_{ll'}|^2 - \sum_{l''} W_{ll''}|G_{l''}|^2|T_{l''l'}|^2, \tag{4}$$

to the first order in concentration $\mathbf{c}$ written as $W_{ll'}(n)=|T_{ll'}|^2$ (in the *weak interaction* limit $W_{ll'}\approx|B_{ll'}|^2$). $T_{ll'}$ is the matrix element of the total T-scattering matrix and $G_l=(z-E_l)^{-1}$ does the diagonal part of resolvent operator of Hamiltonian $\hat{H}$, Eq. (1). Since the configuration averaging of the one site T-matrix elements in a dilute alloy is $<|t_{ll'}(n)|^2>_{\mathbf{c}}=\mathbf{c}\cdot|T_{ll'}|^2$ (Ref. 13), in single-electron and one-site approximations one obtains the following expression for kinetic equations in the framework of the two-band conductivity model:

$$2\mathbf{c}\pi\left\{\sum_{\vec{k}'}\delta(E_{\vec{k}s}-E_{\vec{k}'s})|T_{\vec{k}s,\vec{k}'s}|^2(f_{\vec{k}s}-f_{\vec{k}'s}) + \delta(E_{\vec{k}s}-E_{\vec{k}'d}) \times|T_{\vec{k}s,\vec{k}'d}|^2(f_{\vec{k}s}-f_{\vec{k}'d})\right\} = e\hbar(\vec{F},\vec{v}_{\vec{k}s})\frac{\partial f_{\vec{k}s}^0}{\partial E_{\vec{k}s}}, \tag{5}$$

where e is the electron charge, $\vec{F}$ is an external electric field, and $\vec{v}_l$ is an electron velocity with quantum number l. The equation for d-band electrons can be obtained by simple index replacement $s\leftrightarrow d$ in (5). The problem can be solved by putting the nonquilibrium additions f_l in the form of the right-hand side part of (5):

$$f_l = e\hbar(\vec{F},\vec{v}_l)C_l\frac{\partial f_l^0}{\partial E_l}, \tag{6}$$

where C_l are the coefficients to be found. Such substitution transforms kinetic Eq. (5) into a system of algebraic equations for C_l coefficients:

$$\begin{bmatrix} C_{\vec{k}s} \\ C_{\vec{k}d}\end{bmatrix} = \begin{bmatrix} I_{\vec{k}ss}+J_{\vec{k}sd} & L_{\vec{k}sd} \\ L_{\vec{k}ds} & I_{\vec{k}dd}+J_{\vec{k}ds}\end{bmatrix}^{-1}\begin{bmatrix}1\\1\end{bmatrix}, \tag{7}$$

where $[C_l]$ is a matrix column of C_l coefficients and

$$I_{\vec{k}jj} = \mathbf{c}\frac{\Omega_0}{(2\pi)^3}\int d\vec{k}'\,\delta(E_{\vec{k}j}-E_{\vec{k}'j})|T_{\vec{k}j,\vec{k}'j}|^2(1-\cos(\vec{v}_{\vec{k}j},\vec{v}_{\vec{k}'j})),$$

$$J_{\vec{k}jj'} = \mathbf{c}\frac{\Omega_0}{(2\pi)^3}\int d\vec{k}'\,\delta(E_{\vec{k}j}-E_{\vec{k}'j'})|T_{\vec{k}j,\vec{k}'j'}|^2,$$

$$L_{\vec{k}jj'} = -\mathbf{c}\frac{\Omega_0}{(2\pi)^3}\int d\vec{k}'\,\delta(E_{\vec{k}j}-E_{\vec{k}'j'}) \times|T_{\vec{k}j,\vec{k}'j'}|^2\left|\frac{\vec{v}_{\vec{k}'j'}}{\vec{v}_{\vec{k}j}}\right|\cos(\vec{v}_{\vec{k}j},\vec{v}_{\vec{k}'j'}). \tag{8}$$

The first integral describes intraband electron scattering within a j band. The second and third integrals refer to interband scattering processes, $j\rightarrow j'$ and $j'\rightarrow j$, respectively. System (7) yields

$$C_{\vec{k}s} = \frac{I_{\vec{k}dd}+J_{\vec{k}ds}+L_{\vec{k}sd}}{(I_{\vec{k}ss}+J_{\vec{k}sd})(I_{\vec{k}dd}+J_{\vec{k}ds})-L_{\vec{k}sd}L_{\vec{k}ds}}. \tag{9}$$

Coefficient $C_{\vec{k}d}$ is obtained by the $s\leftrightarrow d$ index replacement.

As follows from (6) and (9), the nonequilibrium additions f_l to equilibrium Fermi distribution functions for s and d electrons essentially depend on both intra- and interband transitions.

To calculate coefficients $C_{\vec{k}j}$ one has to define the squared modulus of nondiagonal elements of the scattering T matrix. It is reasonable to use the common definition of the one electron T matrix,

$$\frac{1}{N}\sum_{n,l,l'} \exp(-i(\vec{k}-\vec{k}',\vec{r}_n))T_{ll'}(n)a_l^{+}a_{l'} = \frac{1}{N}\sum_{n,l,l'} \exp(-i(\vec{k}-\vec{k}',\vec{r}_n)) \times \left[B_{l,l'}(n) + \sum_{l''} B_{l,l''}(n)G_{l''}B_{l'',l'}(n) + \cdots\right]a_l^{+}a_{l'}. \tag{10}$$

It is impossible to sum up the row (10) without simplifying assumptions, so we use the quasilocal approach[15] in the following form:

$$\int d\vec{r}\,\psi_l^{*}V\delta(\vec{r})\psi_{l'} = \frac{1}{\pi\Omega_0}\int_0^{\pi} d\Theta \int d\vec{r}\,\psi_l^{*}\Delta U(\vec{r})\psi_{l'} = \lambda_{jj'}, \tag{11}$$

where $\lambda_{jj'}$ is the quantity averaged over angles between wave vectors $\vec{k}$ and $\vec{k}'$. Then the power series in (10) can be summed up exactly, since the interaction matrix elements $B_{ll'}$ depend on the band indexes only.

Let us determine the Green's function $[F]$ and interaction matrix $[B]$ as double row matrices on band indexes, whose elements are not dependent on the wave vector:

$$[F] = \begin{bmatrix} F_s & 0 \\ 0 & F_d \end{bmatrix}, \quad [B] = \begin{bmatrix} \lambda_{ss} & \lambda_{sd} \\ \lambda_{ds} & \lambda_{dd} \end{bmatrix}, \tag{12}$$

where

$$F_j = \frac{1}{N}\sum_{\vec{k}} \frac{1}{z - E_{\vec{k},j}} \tag{13}$$

is Green's function of an electron in the j band.

Note that the power series in (10) is a geometric progression of matrices (12), which can be easily summed up:

$$[B] + [B][F][B] + [B][F][B][F][B] + \cdots = [B]([I] - [F] \times [B])^{-1}. \tag{14}$$

As a result one obtains the squared moduli of elements of the T matrix:

$$|T_{ss}|^2 = \frac{1}{A}|\lambda_{ss}(1 - F_d\lambda_{dd}) + \lambda_{sd}F_d\lambda_{ds}|^2,$$

$$|T_{sd}|^2 = \frac{1}{A}|\lambda_{sd}|^2, \quad |T_{ds}|^2 = \frac{1}{A}|\lambda_{ds}|^2$$

$$|T_{dd}|^2 = \frac{1}{A}|\lambda_{dd}(1 - F_s\lambda_{ss}) + \lambda_{ds}F_s\lambda_{sd}|^2, \tag{15}$$

where

$$A = |(1 - F_s\lambda_{ss})(1 - F_d\lambda_{dd}) - \lambda_{sd}F_s\lambda_{ds}F_d|^2. \tag{16}$$

Straightforward calculations using (15) and (16) are rather difficult. Since the probability of scattering in the s band is sufficiently low, i.e., $g_s(E_F) \ll g_d(E_F)$, the relationship $|\lambda_{jj'}F_s| \ll 1$ is valid and allows rewriting (15) and (16) in the simplified form:

$$|T_{ss}|^2 = \frac{1}{A}|\lambda_{ss}(1 - F_d\lambda_{dd}) + \lambda_{sd}F_d\lambda_{ds}|^2,$$

$$|T_{sd}|^2 = \frac{1}{A}|\lambda_{sd}|^2, \quad |T_{ds}|^2 = \frac{1}{A}|\lambda_{ds}|^2, \quad |T_{dd}|^2 = \frac{1}{A}|\lambda_{dd}|^2,$$

and

$$A = |1 - F_d\lambda_{dd}|^2. \tag{17}$$

One can see that elements of the T matrix in a dilute alloy are defined via Green's functions of solvent d electrons and interaction matrix elements calculated with electron wave functions assigned to the solvent.

Taking into account substitution (6), the expression for the electrical current can be written as

$$\vec{J} = 2\frac{e^2\hbar}{3}\vec{F}\sum_j n_j \int dE\, C_l v_l^2 \frac{\partial f_l^0}{\partial E_l} g_j(E), \tag{18}$$

where n_j and $g_j(E)$ are the concentration of electrons in the j band and the DOS in the j band, respectively.

One obtains that the main result for electrical conductivity after integration (18) at zero temperature is

$$\sigma = 2\frac{e^2\hbar}{3}\left[n_s v_s^2 g_s(E_F)\frac{I_{dd} + J_{ds} + L_{sd}}{(I_{ss} + J_{sd})(I_{dd} + J_{ds}) - L_{sd}L_{ds}} + n_d v_d^2 g_d(E_F)\frac{I_{ss} + J_{sd} + L_{ds}}{(I_{ss} + J_{sd})(I_{dd} + J_{ds}) - L_{sd}L_{ds}}\right]. \tag{19}$$

This result corresponds to the conductivity summation rule of connected in parallel "nonisolated" conductors (s and d bands). One can see from a later equation that the analog to parallel connection of several "isolated" conductors usually used for a resistivity calculation of the system with many-band conductivity character is not valid. It is to be noted that a similar result was derived in earlier works[6,14] for many-band conductivity models.

III. RESULTS AND DISCUSSION

It is well known that scattering probabilities are proportional to the DOS in accepting bands and $g_s(E_F) \ll g_d(E_F)$. According to Mott's model approximation, i.e., $L_{sd} = L_{ds} = 0$ (which is equivalent to a statement that the d band is a trap for s-conduction electrons) the contribution of s intraband scattering to the total scattering probability can be neglected compared with s-d scattering. Hence the main contribution to the RR in dilute alloy comes from the J_{sd} integral, which corresponds to s-electrons transfer from an s band to a d band:

$$J_{sd} = c\frac{\Omega_0}{(2\pi)^3}\int d\vec{k}\ \delta(E_{\vec{k}_F j} - E_{\vec{k}' j'})\left|\frac{\lambda}{1 - F_d\lambda}\right|^2. \qquad (20)$$

The final expression for the ρ in this approximation is the following:

$$\rho = c\frac{6\pi m}{e^2\hbar n_s E_F}\left(\frac{g_d(E_F)}{g_s(E_F)}\right)\left|\frac{\lambda}{1 - F_d\lambda}\right|^2. \qquad (21)$$

It should be emphasized that ρ_c turns out to be dependent, not only on the imaginary part of the Green's function at the solvent Fermi level but on its real part as well.

Within the *weak interaction* approach, i.e., $|T_{j,j'}|^2 \approx |\lambda_{jj'}|^2$, the $s \rightarrow d$ transitions make the dominant contribution to RR leading to the following expression, typical for classical Mott's model:

$$\rho \sim c\frac{g_d(E_F)}{g_s(E_F)}|\lambda_{sd}|^2. \qquad (22)$$

The main difference between *strong* and *weak* limits is only in the presence of the denominator $|1 - F_d\lambda|$ including the solvent Green's function.

Let us consider some of the simple cases—the Thomas-Fermi screened potential approximation of the interaction between the conduction electron and impurity atoms. According to this approach the matrix elements of the electron-impurity interaction in the plane-wave representation are

$$\Delta U(r) = \frac{e\Delta Z}{4\pi\varepsilon_0}\frac{e^{-qr}}{r}, \qquad (23)$$

where q is inverse screening length and ΔZ is the relative excess electric charge (REEC) of an impurity ion.

Moreover, one can neglect the difference between averaged interaction matrix elements of the intensities of intra- and interband electron transitions, i.e., $\lambda_{sd} \approx \lambda_{dd} = \lambda$, understanding that it is a sufficiently rough approximation. After averaging (11) over angles between $\vec{k}$ and $\vec{k}'$ one obtains

$$\lambda = \left(\frac{e^2\Delta Z}{\varepsilon_0\Omega_0}\right)\frac{1}{q\sqrt{4k_F^2 + q^2}}. \qquad (24)$$

As is seen from (24) and (21), the dependence of the ρ_c on the impurity type is described only by the REEC of the impurity ion. The other parameters of the system are determined by the solvent.

The REEC ΔZ of impurity ions in nontransition metals is commonly taken as the difference between the solute and solvent valencies.[1,4] But for transition metals the valency can be unambiguously defined only in intermetallic compounds. It has been proposed[16] to take the valency of all transition metals in simple metal solvents equal to 2. This assumption seems to be meaningless for the case of transition metal alloys. Thus it is noteworthy that ΔZ has another physical sense.

TABLE I. The calculated values of the REEC charge of different solutes in various solvent metals.

	Matrix solvent				
Impurity	V	Nb	Mo	Ta	W
Ti	0.371	−0.237			
V	×	−0.13	−0.2	−0.152	
Nb	0.13	×	−0.17	−0.067	−0.18
Mo		0.17	×	0.12	−0.041
Ta	0.2	0.067	−0.12	×	−0.161
W	0.3	0.18	0.041	0.161	×

We think that two factors may determine the REEC value in transition metal alloys. The first is solvent lattice deformation caused by impurity ion embedding and the second is network excess charge resulting from an impurity ion in a solvent cell.

One way to estimate the REEC value is the *ab initio* LDA-method,[17] which was applied to the problem in the following manner.

The first step is standard calculation of an energy structure and a DOS of pure metal solvent under the condition that the charge flow through the unit cell surface equals zero. The second step is the direct calculation of an REEC of the system under consideration. The background of the latter calculation was as follows. An impurity atom was immersed into the solvent cell consisting of 20 atoms assuming that this impurity ion cannot change the solvent wave functions and Fermi surface significantly. The effective charge of the cell, i.e., charge flow through the surface, then became nonzero due to the presence of the impurity atom and could be obtained using the solvent wave functions.

The second method to estimate the REEC value is the semi-empirical procedure described in Appendix A. This method was used to check the *ab initio* calculation results. The REEC values obtained for a number of impurities and solvents are presented in the Table I.

It is obvious that the REEC $\Delta Z < 1$ in all considered dilute alloys of transition metals. It means that the valencies of alloy components are approximately equal and this result agrees qualitatively with Harrison.[16]

In isoelectronic metal alloys, such as Nb–Ta, Ta–Nb, V–Nb, Nb–V, V–Ta, Mo–W and W–Mo, a correlation between under- (over-) size deformation effect parameters $(1/a)(da/dc)$ (where a is the alloy lattice parameter), and the REEC value could be expected. Actually, the quantities $(1/a)(da/dc)$, calculated on the basis data,[18] were found to be proportional to corresponding REEC values. However in nonisoelectronic metal alloys such a correlation cannot be found. The cause might be an essential difference between electron configuration of solvent and impurity ions. Therefore one has to take into account both factors: the lattice deformation and electronic structure modification in the matrix solvent.

Let us consider the Nb-solvent case. The obtained values of ΔZ for Ta, V, W, and Mo impurities had approximately equal absolute values but opposite signs if the mentioned

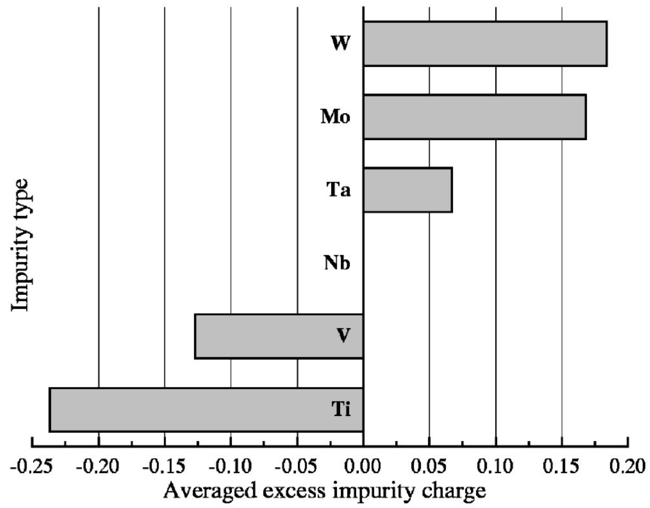

FIG. 2. The calculated REEC values for a row of impurities (Ta, V, W, and Mo) in a Nb solvent.

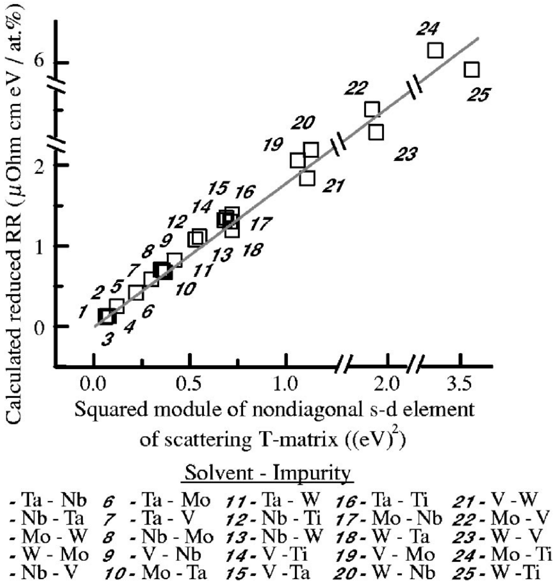

FIG. 3. The experimental data for the relationship between the specific contribution of impurity atoms to RR and the squared modulus of nondiagonal *sd* *T*-matrix elements for various 3*d* alloys (squares) and their approximation (solid line).

metals were considered in turn as a solvent or solute: $\Delta Z_{\text{Nb–Ta}} = -\Delta Z_{\text{Ta–Nb}}$ (see Table I).

This fact allowed us to assume the REEC as a universal constant for each pair of metals. Suggesting ΔZ additivity, one can obtain it for every pair of metals. For example, $\Delta Z_{\text{Mo–Ta}} = -\Delta Z_{\text{Ta–Mo}} = \Delta Z_{\text{Nb–Ta}} - \Delta Z_{\text{Nb–Mo}}$. It is easy to understand using Fig. 2.

Using the results for REEC values and (23), one can perform the RR calculation. As seen from expression (23), ρ is proportional to the squared modulus of a nondiagonal *sd* *T*-matrix element $|\lambda/(1-F_d\lambda)|^2$ and DOS *d* electrons at the Fermi level. So the linear relationship between ρ_g (ρ_g is ρ normalized to *d* electrons DOS at the Fermi level) and the squared modulus of a nondiagonal *sd* *T*-matrix element should be verified experimentally. One can see the comparison of calculation results and experimental normalized RR values for some V-, Nb-, Mo-, Ta-, and W-based alloys in Fig. 3.

In more detail, the results of calculations of RR for V-, Nb-, Mo-, Ta-, and W-based alloys were compared with experimental data in Table II.

Minimal values of RR were found in the isoelectronic Nb–Ta, Ta–Nb, Mo–W, and W–Mo alloys having the lowest values of ΔZ and the electron-impurity interaction constant ($|\lambda F| \approx 0.03-0.1$). In this case perturbation theory can be applied for the calculation of RR. In the other alloys the intensity of the electron-impurity interaction is sufficiently high ($|\lambda F| \approx 0.2-0.8$) and the latter approach is not valid. For example, $|\lambda F| = 0.27$ and 0.16 in V–Nb and Nb–V isoelectronic alloys, respectively, since the *d*-electron DOS at the Fermi level of the host metal and ΔZ have sufficiently high values.

The typical difference between RR experimental and calculated values is 10%–15% in the majority of dilute alloys. But in Mo–V and W–V alloys, the ratio of calculated (using (23)) to experimental values exceeds 4. It should be noted that in W and Mo the ratio of DOS of *d* and *s* electrons is only about 4, i.e., sufficiently low for the application of the Mott's approximation. RR calculations performed according to (19) without this approximation yields 0.26 and $0.21 \mu\Omega$ cm/at.% in Mo–V and W–V alloys, respectively. These values agree satisfactorily with the experimental data.

IV. CONCLUSION

It is demonstrated that in dilute alloys of transition metals the reduced residual electrical resistivity (RR) is a linear function of squared nondiagonal *sd* *T*-matrix elements calculated with plane wave functions.

The approximate values of relative excess electric charge (REEC) obtained by this method can be used for a prelimi-

TABLE II. Experimental data and results of calculation of RR for V-, Nb-, Mo-, Ta-, and W-based alloys ($\mu\Omega$ cm/at.%).

		Matrix solvent				
Impurity		V	Nb	Ta	Mo	W
Ti	Exp	1.35	1.26	0.80		
	Calc	1.20	1.21	1.59	2.16	2.00
V	Exp		0.34	0.65	0.32	
	Calc		0.29	0.67	1.23	1.09
Nb	Exp	0.75		0.20	0.40	0.51
	Calc	0.63		0.13	0.46	0.62
Ta	Exp	1.10	0.19		0.38	0.51
	Calc	1.23	0.14		0.26	0.40
Mo	Exp	1.23	0.80	0.45		0.04
	Calc	1.88	0.82	0.48		0.04
W	Exp	0.90	0.91	0.65	0.08	
	Calc	2.00	1.29	0.99	0.05	

TABLE III. Solvent metal parameters used in calculations: E_F is the Fermi energy; $g_d(E_F)$ is the DOS of d electrons at the Fermi level (Refs. 20 and 21); r_{kov} is the covalent radius (Ref. 22); Re(G) and Im(G) are the real and imaginary parts of the Green's function, respectively.

Parameter	V	Nb	Mo	Ta	W
E_F(eV)	10.36	9.22	10.95	9.73	12.35
$g_d(E_F)$(s/eV at.)	1.9	1.65	0.59	1.61	0.55
r_{kov}(nm^{-1})	12.11	14.06	13.15	13.64	13.01
Re(G)(eV^{-1})	0.17	0.77	−0.5	0.8	0.01
Im(G)(eV^{-1})	−3.21	−2.86	−0.78	−1.77	−0.3

nary prediction of the ρ_c values of any transition metal impurity in any transition metal solvent.

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APPENDIX

To determine ΔZ in a transition metal alloy, the following semiempirical procedure was developed. Using the experimental data for ρ_c and expressions (21) and (23), one can restore the REEC values for a number of alloys.

According to Skorcheletti[19] the inverse screening length in the rigid spheres model can be replaced by the inverse covalent radius. The latter was calculated according to the simple empirical procedure based on the solvent metal periodical table number.[22] The calculated values of the inverse covalent radius and the other band and energy parameters of the electronic structure of pure transition metal solvents[20,21] used in calculations of ρ_c are presented in Table III. The real parts of Green's functions were calculated using the Leman representation according to the known DOS functions computed from the first principles. The s-electron DOS at the Fermi level was calculated within a free electron approximation.[16]

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