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The Influence of the Electron-Phonon Interaction on the Electroconductivity of Disordered Metallic Alloys

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The aim of the present note is to develop a theory of the electroconductivity in disordered transition metal alloys with a proper microscopic treatment of the electron-phonon interaction (cf. /1 to 3/).

For a given configuration of atoms the total Hamiltonian of the electron-ion system in the substitutionally disordered alloy is written in the form

$$H = \sum_i \varepsilon_i a_i^+ a_i + \sum_{ij} t_{ij} a_i^+ a_j + \sum_{\vec{q}} \omega_{\vec{q}} b_{\vec{q}}^+ b_{\vec{q}} + H_{ep}, \tag{1}$$

where the electron-phonon interaction term in (1) is taken as

$$H_{ep} = \sum_{\vec{q}} \sum_{ij} \lambda_{\vec{q}}(j-i) \exp(i\vec{q}\vec{R}_i) (b_{\vec{q}} + b_{-\vec{q}}^+) a_i^+ a_j \; . \tag{2}$$

The electrical conductivity will be calculated starting with the Kubo expression for the dc conductivity:

$$\sigma = - \ll \vec{J} \mid \vec{P} \gg_{i\eta} \qquad (\eta \to 0^+) \; , \tag{3}$$

where $\vec{P} = e \sum_i \vec{R}_i a_i^+ a_i$ and $\vec{R}_i$ is the position vector. $\frac{m}{e}\vec{J} = \frac{m}{e}\dot{\vec{P}}$ is the operator of the total momentum of the electrons. It has the form

$$\vec{J} = - ie \sum_{ij} (\vec{R}_i - \vec{R}_j) t_{ij} a_i^+ a_j \; ; \tag{4}$$

In the following we restrict ourselves to a diagonal disorder, i.e.

$$t_{ij} = \frac{1}{N} \sum_{\vec{k}} \varepsilon_{\vec{k}} \exp\left[i \vec{k} (\vec{R}_i - \vec{R}_j) \right] . \tag{5}$$

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We are interested in the Green function $G_{ij,lm} = \ll a_i^+ a_j \mid a_l^+ a_m \gg_{i\eta}$ that can be calculated by the equation of motion method. Using the Hamiltonian (1) we find by a differentiation with respect to the l.h.s.

$$\sum_{nr} (\langle a_s^+ a_n \rangle \delta_{rt} - \langle a_r^+ a_t \rangle \delta_{sn}) G_{nr,lm} = \sum_{ij} (\langle a_i^+ a_m \rangle \delta_{lj} - \langle a_l^+ a_j \rangle \delta_{mi}) G^o_{st,ji} + \sum_{ijn} \sum_{\vec{q}} \Big[\lambda_{\vec{q}} (j - n) \exp(i\vec{q}\vec{R}_j) \times \ll a_i^+ a_n (b_{\vec{q}} + b_{-\vec{q}}^+) \mid a_l^+ a_m \gg_{i\eta} - \lambda_{\vec{q}} (n - i) \exp(i\vec{q}\vec{R}_n) \times \ll a_n^+ a_j (b_{\vec{q}} + b_{-\vec{q}}^+) \mid a_l^+ a_m \gg_{i\eta} \Big] G^o_{st,ji} , \quad (6)$$

where the zeroth-order Green functions $G^o_{ij,lm}$ describing the potential scattering are defined by

$$\sum_{nr} H_{ij,nr} G^o_{nr,lm} = \langle a_i^+ a_m \rangle \delta_{lj} - \langle a_l^+ a_j \rangle \delta_{mi} , \quad (7a)$$

$$\sum_{nr} H_{rn,lm} G^o_{ij,nr} = \langle a_i^+ a_m \rangle \delta_{lj} - \langle a_l^+ a_j \rangle \delta_{mi} , \quad (7b)$$

with

$$H_{ij,rn} = (i\eta - \varepsilon_n + \varepsilon_r) \delta_{ni} \delta_{rj} - t_{jr} \delta_{ni} + t_{ni} \delta_{rj} . \quad (8)$$

The r.h.s. higher order Green functions can be calculated in a similar way.

Using (7b) and decoupling for a weak electron-phonon scattering as $\ll a_n^+ a_r b_{\vec{q}}^+ b_{\vec{q}} \mid B \gg \approx \nu_{\vec{q}} \ll a_n^+ a_r \mid B \gg$ we find equations for $\ll a_n^+ a_r b_{\vec{q}} \mid a_l^+ a_m \gg$ and $\ll a_n^+ a_r b_{-\vec{q}}^+ \mid a_l^+ a_m \gg$ where $\nu_{\vec{q}} = \left[\exp(\beta \omega_{\vec{q}}) - 1\right]^{-1}$.

In (6) and (7) the Green functions G and G^o as well as the mean values $\langle a_i^+ a_j \rangle$ which can be expressed by one-particle Green functions depend on the atomic configuration. For the configuration averaging we use the simplest approximation

$$\overline{G \cdot G} \sim \bar{G} \cdot \bar{G} , \quad (9)$$

i.e. in all products the configurational-dependent quantities will be averaged separately. Taking into account (7), the averaged zeroth-order Green functions $\overline{G^o_{ij,lm}}$ are given by the well-known CPA solutions for two-particle Green functions in disordered metallic alloys /4/

$$\overline{G^o_{ij,lm}} = \frac{1}{N^2} \sum_{\vec{k}_1 \vec{k}_2} \exp(i\vec{k}_1 (\vec{R}_m - \vec{R}_n)) \exp(i\vec{k}_2 (\vec{R}_j - \vec{R}_l)) F_2(\vec{k}_1, \vec{k}_2) , \quad (9)$$

where $F_2(\vec{k}_1, \vec{k}_2)$ is given by

$$F_2(\vec{k}_1, \vec{k}_2) \approx i(\varepsilon_{\vec{k}_2} - \varepsilon_{\vec{k}_1}) \int (d\omega f'(\omega) \left[\mathrm{Im} \left\{ \frac{1}{\omega - \Sigma(\omega) - \varepsilon_{\vec{k}_1}} \right\} \right]^2 \quad \text{for} \quad |\varepsilon_{\vec{k}_1} - \varepsilon_{\vec{k}_2}| \ll |\Sigma(\varepsilon_{\vec{k}_1})| \quad (10)$$

and

$$F_2(\vec{k}_1, \vec{k}_2) \approx \frac{f(\varepsilon_{\vec{k}_1}) - f(\varepsilon_{\vec{k}_2})}{\varepsilon_{\vec{k}_1} - \varepsilon_{\vec{k}_2}} \quad \text{for} \quad |\varepsilon_{\vec{k}_1} - \varepsilon_{\vec{k}_2}| \gg |\Sigma(\varepsilon_{\vec{k}_1})| . \quad (11)$$

Here $\Sigma(\omega)$ denotes the coherent potential and $f(\omega)$ is the Fermi distribution function. The configurational averaged terms $\overline{\langle a_s^+ a_n \rangle}$ are given by

$$\overline{\langle a_s^+ a_n \rangle} = \sum_{\vec{k}} \exp(i\vec{k}(\vec{R}_n - \vec{R}_s)) F_1(\vec{k}) , \quad (12)$$

$$F_1(\vec{k}) = -\frac{1}{\pi} \int d\omega f(\omega) \, \mathrm{Im} \left\{ \frac{1}{\omega - \Sigma(\omega) \varepsilon_{\vec{k}}} \right\} . \quad (13)$$

After the configurational averaging equation (6) can be solved by Fourier transformation and we find

$$G(\vec{k}_1 \vec{k}_2; \vec{k}_3 \vec{k}_4) \equiv G(\vec{k}_1, \vec{k}_2) = F_2(\vec{k}_1, \vec{k}_2) \delta(\vec{k}_4, \vec{k}_1) \delta(\vec{k}_3, \vec{k}_2) - \frac{F_2(\vec{k}_1, \vec{k}_2)}{F_1(\vec{k}_1) - F_1(\vec{k}_2)} \times \sum_{\vec{q}} \Big[\lambda(\vec{q}, \vec{k}_2 - \vec{q}) \lambda(-\vec{q}, \vec{k}_2) (F_1(\vec{k}_2 - \vec{q}) - 1 - \nu_{\vec{q}}) G(\vec{k}_1, \vec{k}_2) - \lambda(\vec{q}, \vec{k}_2 - \vec{q}) \lambda(-\vec{q}, \vec{k}_1) \times (F_1(\vec{k}_1) + \nu_{\vec{q}}) G(\vec{k}_1 - \vec{q}, \vec{k}_2 - \vec{q}) \Big] / \Big[F_1(\vec{k}_1) - F_1(\vec{k}_2 - \vec{q}) - \omega_{\vec{q}} F_2(\vec{k}_1, \vec{k}_2 - \vec{q}) \Big] F_2^{-1}(\vec{k}_1, \vec{k}_2 - \vec{q}) +$$

$$+\lambda(\vec{q},\vec{k}_1)\lambda(-\vec{q},\vec{k}_2-\vec{q})(1+\nu_{\vec{q}}-F_1(\vec{k}_2))G(\vec{k}_1-\vec{q},\vec{k}_2-\vec{q})-\lambda(\vec{q},\vec{k}_1)\lambda(-\vec{q},\vec{k}_1-\vec{q})(F_1(\vec{k}_1-\vec{q})+\nu_{\vec{q}})\times$$

$$\times G(\vec{k}_1,\vec{k}_2)\,/\left[F_1(\vec{k}_1-\vec{q})-F_1(\vec{k}_2)-\omega_{\vec{q}}F_2(\vec{k}_1-\vec{q},\vec{k}_2)\right]F_2^{-1}(\vec{k}_1-\vec{q},\vec{k}_2) \; -$$

$$-\ 2 \text{ terms with } \omega_{\vec{q}} \to -\omega_{\vec{q}} \text{ and } \nu_{\vec{q}} \to (-1-\nu_{\vec{q}})\Big], \qquad (14)$$

where $\lambda(\vec{q},\vec{k}) = \frac{1}{N}\sum_{\vec{k}} \exp(i\vec{k}(\vec{R}_i - \vec{R}_j))\,\lambda_{\vec{q}}(i-j)$. Equation (14) is an integral equation for the Green function $G(\vec{k}_1,\vec{k}_2)$ to be determined. In the weak-scattering limit the CPA Green function (10) is given by (cf. /4/)

$$F_2(\vec{k}_1,\vec{k}_2) = i(\varepsilon_{\vec{k}_2} - \varepsilon_{\vec{k}_1})\,f'_{\vec{k}_1}\,\frac{1}{\Sigma(\varepsilon_{\vec{k}_1})} \quad \text{for } |\varepsilon_{\vec{k}_2} - \varepsilon_{\vec{k}_1}| \ll |\Sigma(\varepsilon_{\vec{k}_1})|\ , \qquad (15)$$

where $f'_{\vec{k}} = df/d\varepsilon_{\vec{k}}$. Corresponding to (15) the following solution ansatz for the Green function $G(\vec{k},\vec{k}+\vec{k}')$ can be used

$$G(\vec{k},\vec{k}+\vec{k}') = i\left(\frac{\partial\varepsilon}{\partial\vec{k}}\cdot\vec{k}'\right) f'_{\vec{k}}\,\frac{1}{\Sigma(\varepsilon_{\vec{k}}) + \gamma(\varepsilon_{\vec{k}})}\ , \qquad (16)$$

where γ describes the contribution of the electron-phonon scattering to the coherent potential. Taking into account that in the weakscattering limit $|\Sigma| \ll \omega_q$, the terms $F_2(\vec{k},\ \vec{k}-\vec{q})$ in the r.h.s. denominators of (14) can be replaced by (11) we find

$$\gamma = \beta\frac{\Omega}{2\pi N}\ \frac{\lambda^2\, m^*}{2(2\,m^*\,\varepsilon_f)^{3/2}}\int q^4\, dq\, \omega_{\vec{q}}\,\nu_{\vec{q}}\,(1+\nu_{\vec{q}}) \qquad (17)$$

corresponding to the Bloch-Grüneisen law. For a binary alloy with concentrations of the constituents c_A, c_B and the corresponding atomic energies ε_A, ε_B, in the weak-scattering limit the coherent potential is given by /3/:

$$\Sigma = c_A\, c_B\,(\varepsilon_A - \varepsilon_B)^2\, N_o(\varepsilon_f)\ , \qquad (18)$$

where $N_o(\varepsilon_f)$ is the density of states at the Fermi energy. Then the conductivity becomes

$$\sigma = -\frac{e^2}{3(2\pi)^3}\int d\vec{k}\left(\frac{\partial\varepsilon}{\partial\vec{k}}\right)^2 f'_k\,\tau\ , \qquad (19)$$

where

$$\tau^{-1} = \Sigma + \gamma \qquad (20)$$

in correspondence with the Matthiessen, Nordheim, and Bloch-Grüneisen rules.

For a strongly disordered alloy the electron-phonon interaction can be considered as a small perturbation and the Green functions $G(\vec{k},\vec{k}')$ on the r.h.s. of (14) can be replaced by CPA Green functions $F(\vec{k},\vec{k}')$. For simplicity, on the r.h.s. of (14) we take into consideration only terms proportional to the Bose distribution function giving the main contribution to the temperature dependence of the conductivity.

Then for small temperatures the conductivity becomes

$$\sigma = \sigma_{CPA} + \Delta\sigma(T)\ , \qquad (21)$$

where

$$\sigma_{CPA} = \frac{e^2}{\Omega}\sum_{\vec{k}}\left(\frac{\partial\varepsilon}{\partial\vec{k}}\right)^2\left[\mathrm{Im}\left\{\frac{1}{\varepsilon_f - \Sigma(\varepsilon_f) - \varepsilon_{\vec{k}-\vec{q}}}\right\}\right]^2 \qquad (22)$$

is the well-known CPA result for the conductivity and

$$\Delta\sigma(T) = \frac{2e^2\lambda^2}{\Omega}\sum_{\vec{k}}\left(\frac{\partial\varepsilon}{\partial\vec{k}}\right)^2\sum_{\vec{q}} q\nu_{\vec{q}}\left[\mathrm{Im}\left\{\frac{1}{\varepsilon_f - \Sigma(\varepsilon_f) - \varepsilon_{\vec{k}-\vec{q}}}\right\}\right]^2 -$$

$$-\left[\mathrm{Im}\left\{\frac{1}{\varepsilon_f - \Sigma(\varepsilon_f) - \varepsilon_{\vec{k}}}\right\}\right]^2 . \qquad (23)$$

Introducing the effective mass of the electrons with $\varepsilon_{\vec{k}} \approx \varepsilon_f$ the temperature-dependent correction to the conductivity reads

$$\Delta\sigma(T) = \frac{2e^2\lambda^2}{\Omega}\ \frac{1}{m^{*2}}\sum_{\vec{k}}\sum_{\vec{q}}\ q^3\ \nu_{\vec{q}}\left[\mathrm{Im}\left\{\frac{1}{\varepsilon_f - \Sigma(\varepsilon_f) - \varepsilon_{\vec{k}}}\right\}\right]^4 . \qquad (24)$$

$\Delta\sigma(T)$ is positive definite and increases with temperature, hence, in strongly disordered alloys where the electron-phonon scattering is weak as com-

pared with the disorder scattering the temperature coefficient of the resistivity is negative /5/. It should be mentioned, however, that the concrete temperature dependence of the correction term (24) cannot be taken too seriously because in the derivation of (24) the influence of the disorder on the lattice vibrations has been neglected.

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