phys. stat. sol. (b) 120, K219 (1983)

Subject classification: 14.1

Laboratory of Theoretical Physics, Joint Institute of Nuclear Research, Dubna

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

By

V. CHRISTOPH 2) and A. L. KUZEMSKII

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

$$H = \sum_i \varepsilon_i a_i^+ a_i + \sum_{ij} t_{ij} a_i^+ a_j + \sum_q \omega_q b_i^+ b_q + H_{ep},$$  \hspace{1cm} (1)

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

$$H_{ep} = \sum_q \sum_{ij} \lambda_{ijq} \exp(iq \cdot \vec{R}_i) (b_{i q}^+ b_{q}^+) a_i^+ a_j^+.$$  \hspace{1cm} (2)

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

$$\sigma = - \langle \vec{J} \cdot \vec{P} \rangle_{\eta \to 0^+},$$  \hspace{1cm} (3)

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

$$\vec{J} = -ie \sum_{ij} (\vec{R}_i - \vec{R}_j) t_{ij} a_i^+ a_j;$$  \hspace{1cm} (4)

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

$$t_{ij} = \frac{1}{N} \sum_k \varepsilon_k \exp\left[ i \frac{\vec{k} \cdot (\vec{R}_i - \vec{R}_j) }{k^2} \right].$$  \hspace{1cm} (5)

1) P.O.B. 79, 101000 Moscow, USSR.

2) Permanent address: Wissenschaftsbereich Physik, Hochschule für Verkehrswesen "Friedrich List", D SF 103, DDR-8072 Dresden, GDR.
We are interested in the Green function $G_{ij,lm} = \langle a_{1}^{\dagger} a_{j} | a_{1}^{\dagger} a_{m} \rangle_{1 \gamma}$ 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.

$$\sum_{n} \left( \langle a_{1}^{\dagger} a_{n} \rangle \sigma_{rt} - \langle a_{1}^{\dagger} a_{r} \rangle \sigma_{sn} \right) C_{nr,lm} = \sum_{ij} \left( \langle a_{1}^{\dagger} a_{m} \rangle \sigma_{lj} \right) - \langle a_{1}^{\dagger} a_{j} \rangle \sigma_{ml} \right) G_{ij,lm}^{0} + \sum_{ijn} \sum_{q} \left[ \lambda_{q} (j - n) \exp (i q \vec{k}_{j}) \times \langle a_{1}^{\dagger} a_{n} (b_{q}^{+} + b_{-q}^{+}) | a_{1}^{\dagger} a_{m} \rangle \right] i q \lambda_{q} (n - i) \exp (i q \vec{k}_{n}) \times$$

$$\times \langle a_{1}^{\dagger} a_{j} (b_{q}^{+} + b_{-q}^{+}) | a_{1}^{\dagger} a_{m} \rangle \right) G_{st,ji}^{0} ,$$

(6)

where the zeroth-order Green functions $G_{ij,lm}^{0}$ describing the potential scattering are defined by

$$\sum_{i} H_{ij,lm} G_{ij,lm}^{0} = \langle a_{1}^{\dagger} a_{m} \rangle \delta_{ij} - \langle a_{1}^{\dagger} a_{j} \rangle \delta_{mi} ,$$

(7a)

$$\sum_{i} H_{lm,ir} G_{ij,lm}^{0} = \langle a_{1}^{\dagger} a_{m} \rangle \delta_{ij} - \langle a_{1}^{\dagger} a_{j} \rangle \delta_{mi} ,$$

(7b)

with

$$H_{ij,rm} = (1 - \epsilon_{n} + \epsilon_{r}) \delta_{ni} \delta_{rj} - i \epsilon_{n} \delta_{ni} + \epsilon_{r} \delta_{rj} .$$

(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

$$\langle a_{1}^{\dagger} a_{n} b_{q}^{+} | B \rangle \approx \nu_{q} \langle a_{1}^{\dagger} a_{n} | B \rangle$$

and

$$\langle a_{1}^{\dagger} a_{n} b_{q}^{+} | a_{1}^{\dagger} a_{m} \rangle$$

where $\nu_{q} = \left[ \exp (\beta \omega_{q}) - 1 \right]^{-1}$.

In (6) and (7) the Green functions $G$ and $G^{0}$ as well as the mean values $\langle a_{1}^{\dagger} a_{j} \rangle$ which can be expressed by one-particle Green functions depend on the atomic configuration. For the configuration averaging we use the simplest approximation

$$\overline{G} \cdot G \approx \overline{G} \cdot \overline{G} ,$$

(9)

i.e. in all products the configurational-dependent quantities will be averaged separately. Taking into account (7), the averaged zeroth-order Green functions $\overline{G_{ij,lm}}^{0}$ are given by the well-known CPA solutions for two-particle Green functions in disordered metallic alloys /4/

$$\overline{G_{ij,lm}}^{0} = \frac{1}{N} \sum_{k_{1} k_{2}} \exp (i \vec{k}_{1} \cdot (\vec{R}_{m} - \vec{R}_{n})) \exp (i \vec{k}_{2} \cdot (\vec{R}_{j} - \vec{R}_{i})) F_{2}(\vec{k}_{1}, \vec{k}_{2}) ,$$

(9)

where $F_{2}(\vec{k}_{1}, \vec{k}_{2})$ is given by

$$F_{2}(\vec{k}_{1}, \vec{k}_{2}) \approx \exp (i f(\epsilon_{k_{2}} - \epsilon_{k_{1}})) \int d \omega f(\omega) \left[ \frac{1}{\omega - \Sigma(\omega, \epsilon_{k_{1}})} \right]^{2}$$

(10)

$$\text{for} \quad \epsilon_{k_{1}} - \epsilon_{k_{2}} \ll \Sigma(\epsilon_{k_{1}}) \right) ,$$

(11)

Here $\Sigma(\omega)$ denotes the coherent potential and $f(\omega)$ is the Fermi distribution function. The configurational averaged terms $\langle a_{1}^{\dagger} a_{n} \rangle$ are given by

$$\langle a_{1}^{\dagger} a_{n} \rangle = \sum_{k} \exp (i \vec{k}_{i} \cdot (\vec{R}_{n} - \vec{R}_{i})) \overline{F}_{1}(\vec{k}) ,$$

(12)

$$\overline{F}_{1}(\vec{k}) = - \frac{1}{\pi} \int d \omega f(\omega) \text{Im} \left\{ \frac{1}{\omega - \Sigma(\omega, \epsilon_{k})} \epsilon_{k} \right\} .$$

(13)

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

$$G(\vec{k}_{1}, \vec{k}_{2}) = F_{2}(\vec{k}_{1}, \vec{k}_{2}) \delta(\vec{k}_{1} + \vec{k}_{2}) - \frac{F_{2}(\vec{k}_{1}, \vec{k}_{2})}{\overline{F}_{1}(\vec{k}_{1}) - \overline{F}_{1}(\vec{k}_{2})} \times$$

$$\times \sum_{q} \lambda_{q}(\vec{k}_{1}, \vec{k}_{2}, -\vec{k}_{1})(-\nu_{q} F_{1}(\vec{k}_{2}, -\vec{k}_{1}) - \nu_{q} G(\vec{k}_{1}, -\vec{k}_{2}) - \lambda(\vec{k}_{1}, \vec{k}_{2}, -\vec{k}_{1}) \lambda(-\vec{k}_{1}) \times$$

$$\times (\overline{F}_{1}(\vec{k}_{1}) + \nu_{q} G(\vec{k}_{1}, -\vec{k}_{2}, -\vec{k}_{1})) / \left[ \overline{F}_{1}(\vec{k}_{1}) - \overline{F}_{1}(\vec{k}_{2}, -\vec{k}_{1}) - \nu_{q} F_{2}(\vec{k}_{1}, \vec{k}_{2}, -\vec{k}_{1}) \right]^{2} .$$

(9)
\[
\sigma = \frac{e^2}{3(2\pi)^3} \int d\mathbf{q} \left( \frac{\partial \epsilon}{\partial k} \right)^2 f^d_{\mathbf{q}} \tau, \tag{19}\]
\]
where \( \tau^{-1} = \Sigma + \tau \), \( \tau \)

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 \( G(\mathbf{k}, \mathbf{k}') \) on the r.h.s. of (14) can be replaced by CPA Green functions \( F(\mathbf{k}, \mathbf{k}') \). 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

\[
\sigma = \sigma_{\text{CPA}} + \Delta \sigma(T), \tag{21}\]
\]
where

\[
\sigma_{\text{CPA}} = \frac{e^2}{\Omega} \frac{\lambda^2}{2(2m^*)^{3/2}} \sum_{\mathbf{k}} \frac{\epsilon_\mathbf{k}^*}{\epsilon_{\mathbf{k}}} \frac{1}{\epsilon_{\mathbf{k}}^* + \tau(\epsilon_{\mathbf{k}})}, \tag{22}\]

\[
\text{is the well-known CPA result for the conductivity and}
\]

\[
\Delta \sigma(T) = \frac{2e^2 \alpha^2}{\Omega} \sum_{\mathbf{k}} \frac{\epsilon_{\mathbf{k}}^*}{\epsilon_{\mathbf{k}}} \sum_{\mathbf{q}} q^3 \nu_q \left[ \frac{\text{Im} \left[ \frac{1}{\epsilon_{\mathbf{k}} - \Sigma(\epsilon^*_{\mathbf{k}})} \right]}{\epsilon_{\mathbf{k}} - \Sigma(\epsilon^*_{\mathbf{k}}) - \epsilon_{\mathbf{k}}^*} \right]^2 - \frac{\epsilon_{\mathbf{k}}^*}{\epsilon_{\mathbf{k}} - \Sigma(\epsilon^*_{\mathbf{k}}) - \epsilon_{\mathbf{k}}^*} \right]\left[ \frac{1}{\epsilon_{\mathbf{k}} - \Sigma(\epsilon^*_{\mathbf{k}}) - \epsilon_{\mathbf{k}}^*} \right]^2 \tag{23}\]

Introducing the effective mass of the electrons with \( \epsilon_{\mathbf{k}}^* \propto \epsilon_t \) the temperature-dependent correction to the conductivity reads

\[
\Delta \sigma(T) = \frac{2e^2 \alpha^2}{\Omega} \frac{1}{m^2} \sum_{\mathbf{k}} \sum_{\mathbf{q}} q^3 \nu_q \left[ \frac{\text{Im} \left[ \frac{1}{\epsilon_{\mathbf{k}} - \Sigma(\epsilon^*_{\mathbf{k}})} \right]}{\epsilon_{\mathbf{k}} - \Sigma(\epsilon^*_{\mathbf{k}}) - \epsilon_{\mathbf{k}}^*} \right]^4. \tag{24}\]

\( \Delta \sigma(T) \) 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.

References


(Received September 13, 1983)