

CONTRIBUTION TO THE THEORY OF ELECTRIC CONDUCTIVITY OF METALS WITH NONMAGNETIC IMPURITIES

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A theory of electric conductivity of a metal with impurities is developed which consistently takes into account deformation of the phonon spectrum due to introduction of impurity atoms and also the arbitrary variation of the amplitude of electron scattering by a separate ion. The impurity part of the resistance is found for the entire temperature interval. It is shown that in the low-temperature range electron scattering by an oscillating impurity ion leads to the appearance of a term proportional to T^2 , interference between scattering by an impurity ion and by a perturbed phonon spectrum to a term proportional to T^4 , and scattering by a deformed phonon spectrum to a term proportional to T^5 . (At low impurity concentrations all of these terms are proportional to the concentration.) The further temperature variation of the impurity resistance exhibits a number of anomalies, especially in the case of heavy impurity atoms when a quasilocal level appears. At high temperatures the impurity part of the resistance varies linearly with the temperature, the sign of the derivative being positive or negative. It is demonstrated that a simple relation holds approximately between the sign of the derivative and the relative positions of the impurity and matrix atoms in the periodic system. Comparison with the experimental data yields qualitative agreement with the theory.

1. INTRODUCTION

IN the usual analysis of the electric conductivity of metals, the impurity atoms are regarded as static defects. This leads to a temperature-independent residual resistance and, in first approximation, to the well known Mathiessen rule. Such a picture, however, is in the general case far from the truth. Actually, the impurity atoms oscillate. Furthermore, the character of their oscillations may differ greatly from the oscillations of the atoms of the host lattice. The electrons will then experience additional inelastic scattering not only from the impurity atom itself, but also from a noticeable number of atoms that surround the impurity atom and whose oscillations are perturbed.

Thus, incoherent inelastic scattering of the electrons by randomly located perturbation regions takes place when the impurity atom concentration is low. As a result, the impurity part of the resistance (which is proportional to the concentration) will depend essentially on the temperature, and this leads to violation of the Mathiessen rule; it will be shown in this paper that this violation is appreciable and of arbitrary sign. In the low-temperature region this should become particularly strongly manifest in the case of heavy impurity

atoms, when strong deformation of the vibrational spectrum takes place in the region of low frequencies and a quasilocal frequency appears (see [1] and also [2-4]). This deformation of the spectrum is clearly manifest in the very strong anomaly of the lattice specific heat, [5] which was recently observed experimentally [6] (see also [7]).

It has been known from experiment for a long time that the Mathiessen rule is violated in weak solid solutions and the temperature dependence of the impurity resistance, and in any case also of the total resistance, has an anomalous character (see [8] and also the recent papers [9-11]). All the more-or-less effective attempts at explaining the deviations from this rule pertained only to transition-element impurities and were associated with the presence of an uncompensated spin. However, the anomalous behavior of the resistance is clearly manifest also in the case of nontransition-element impurities. In the present paper we are interested only in this latter case. We shall show that a consistent allowance for the deformation of the vibrational spectrum and for the true picture of the inelastic scattering makes it possible to predict and explain a number of anomalies in the temperature behavior of the resistance, especially its impurity part.

In order to present all the results in very lucid

form, we confine ourselves to the free-electron approximation and neglect the electron-spectrum variation which can arise when impurity atoms are introduced. In addition, we assume the "rigid ion" model for the electron-ion interaction and confine ourselves in the analysis of the electron scattering to the Born approximation. In the case of an alloy we assume that we are dealing with a substitutional solution and that we can thus neglect the variation of the force constants in the dynamic matrix of the oscillations. As is well known (see, for example [12, 13]), measurements of the Mossbauer-effect probability have shown that the latter assumption is well satisfied in metals. Finally, the crystal lattice is assumed to be monatomic and cubic.

We note that almost all the assumptions made are not critical and do not change the qualitative picture. Only the change of the electron spectrum with introduction of the impurity component can become significant in certain cases, especially when the concentration is insufficiently small.

Within the framework of the assumptions made, the problems of determining the probability of electron and neutron scattering in crystals of the same type become similar. For neutrons this problem was solved in [14], the results of which could be used in principle. However, bearing in mind the averaging of the final results of the kinetic problem over the positions of the impurity atoms, it is more convenient to use the relations obtained with the aid of the Green's function formalism in the coordinate representation for a fixed impurity configuration. Two-time Green's functions in the coordinate representation were first used for analysis of problems connected with oscillations of impurity atoms in [15-16] (see also [17]).

2. DETERMINATION OF THE TRANSITION PROBABILITY

A. The solution of the kinetic equation leads to the following general expression for the resistance:

$$\rho = \left[\frac{1}{2T} \int \int dk dk' (\varphi_k - \varphi_{k'})^2 f_k^0 (1 - f_{k'}^0) W_{kk'}(\mathbf{q}, \omega) \right] \times \left| \int e \mathbf{v}_k \varphi_k (\partial f_k / \partial \epsilon_k) dk \right|^{-2}. \quad (2.1)$$

Here φ_k is the nonequilibrium correction to the electron distribution function f_k , defined by the relation

$$f_k = f_k^0 - (\partial f_k / \partial \epsilon_k) \varphi_k;$$

$W_{kk'}$ is the probability that scattering causes the

transition of the electron from a state with wave vector \mathbf{k} into a state with wave vector \mathbf{k}' ;

$$\mathbf{q} = \mathbf{k} - \mathbf{k}'; \quad \omega = \epsilon_k - \epsilon_{k'}; \quad (2.2)$$

T is the temperature in energy units.

Within the framework of the assumptions made, the probability $W_{kk'}$ is uniquely related with the scattering correlation function $S(\mathbf{q}, \omega)$, first introduced by Van Hove: [18]

$$W_{kk'} = \frac{(2\pi)^3}{m_*^2 V_0} S(\mathbf{q}, \omega), \quad (2.3a)$$

$$S(\mathbf{q}, \omega) = \frac{1}{N} \int_{-\infty}^{+\infty} dt e^{i\omega t} \left\langle \sum_{nn'} a_n(\mathbf{q}) a_{n'}(\mathbf{q}) \times \exp[-i\mathbf{q}\mathbf{R}_n(t)] \exp[+i\mathbf{q}\mathbf{R}_{n'}(0)] \right\rangle, \quad (2.3b)$$

where m_* is the effective mass of the electron, $\mathbf{R}_n = \mathbf{R}_n^0 + \mathbf{u}_n$ is the radius vector of the n -th ion, \mathbf{u}_n is the operator of displacement from the equilibrium position, $a_n(\mathbf{q})$ is the amplitude of the scattering of the electron by the n -th ion, N is the number of ions in the crystal, and V_0 the unit-cell volume. The symbol $\langle \rangle$ denotes statistical averaging with a Hamiltonian describing the system of the ions.

Considering the problem of crystal oscillations in the harmonic approximation and confining ourselves to single-quantum transitions in the inelastic scattering of the electrons, we obtain for the scattering function (2.3b) the following expression:

$$S(\mathbf{q}, \omega) = \frac{1}{N} \sum_{n,n'} \exp[i\mathbf{q}(\mathbf{R}_n^0 - \mathbf{R}_{n'}^0)] a_n(\mathbf{q}) a_{n'}(\mathbf{q}) \times \exp\left(-\frac{W_n}{2} - \frac{W_{n'}}{2}\right) \{2\pi\delta(\omega) + \langle (\mathbf{q}\mathbf{u}_n(t)) (\mathbf{q}\mathbf{u}_{n'}(0)) \rangle_\omega\}, \quad (2.4)$$

$$W_n(\mathbf{q}) = \langle (\mathbf{q}\mathbf{u}_n(0))^2 \rangle. \quad (2.5)$$

Here W_n is the Debye-Waller factor and the index ω denotes the Fourier component of the corresponding correlation function.

The expression for the resistance (2.1) should be averaged over all possible configurations of the impurity atoms (the corresponding operation will be denoted by the symbol $\langle \rangle_{\mathbf{C}}$). If we choose φ_k in a form which is standard for the first approximation

$$\varphi_k = \boldsymbol{\kappa} \quad (2.6)$$

($\boldsymbol{\kappa}$ is a unit vector), then the operation of averaging is entirely transferred to $W_{kk'}$, and by the same token to the scattering function.

We shall denote by the indices 0 and 1 quantities pertaining respectively to the atoms of the host lattice and to the impurity atoms. In this case

$$a_n = a_0 + \Delta a c_n, \quad \Delta a = a_1 - a_0, \quad (2.7)$$

c_n takes the value 1 at the impurity lattice points and 0 in the remaining points.

We substitute (2.7) in (2.4) and carry out the averaging, retaining only the terms that are linear in the concentration c . Using the fact that W_n for the electrons in the metal is practically always noticeably smaller than unity, we obtain after calculations

$$\begin{aligned} \langle S(\mathbf{q}, \omega) \rangle_c &= 2\pi c (\Delta b(\mathbf{q}))^2 \delta(\omega) + (b_0(\mathbf{q}))^2 \\ &\times \frac{1}{N} \left\langle \sum_{nn'} \exp[i\mathbf{q}(\mathbf{R}_n^0 - \mathbf{R}_{n'}^0)] \langle (\mathbf{q}u_n(t)) (\mathbf{q}u_{n'}(0)) \rangle_\omega \right\rangle_c \\ &+ c (\Delta b(\mathbf{q}))^2 \langle (\mathbf{q}u_1(t)) (\mathbf{q}u_1(0)) \rangle_\omega + 2b_0(\mathbf{q}) \Delta b(\mathbf{q}) \\ &\times \frac{1}{N} \left\langle \sum_{nn'} c_n \exp[i\mathbf{q}(\mathbf{R}_n^0 - \mathbf{R}_{n'}^0)] \right. \\ &\left. \times \langle (\mathbf{q}u_n(t)) (\mathbf{q}u_{n'}(0)) \rangle_\omega \right\rangle_c. \end{aligned} \quad (2.8)$$

In this expression we use the notation

$$b_{0,1} = a_{0,1} \exp(-W_{0,1}/2), \quad \Delta b = b_1 - b_0; \quad (2.9)$$

W_0 and W_1 are the mean values of the factor (2.5) in the approximation that is linear in the concentration.

In expression (2.8), the first term describes the elastic scattering and gives rise to the residual resistance. The remaining terms describe the inelastic scattering. The second term represents scattering by the deformed phonon spectrum of the lattice, the third direct scattering by the impurity atoms, and finally the fourth the interference scattering (in (2.8) we have left out a term proportional to $\delta(\mathbf{q})$, since it does not lead to scattering).

B. The correlation functions in (2.8) can be connected with retarded (or advanced) Green's functions of the form

$$G_{nn'}^{\alpha\beta}(t-t') = -i\theta(t-t') \langle u_n^\alpha(t) u_{n'}^\beta(t') - u_{n'}^\beta(t') u_n^\alpha(t) \rangle. \quad (2.10)$$

Indeed, in accordance with the well known relations for the Green's functions (see, for example, [19]), we have

$$\langle u_n^\alpha(t) u_{n'}^\beta(t') \rangle_\omega = - \frac{2 \operatorname{Im} G_{nn'}^{\alpha\beta}(\omega + i\varepsilon)}{1 - e^{-\omega/T}} \quad (2.11)$$

(henceforth $\hbar = 1$).

The expressions for the Fourier components of the Green's function $G_{nn'}^{\alpha\beta}(\omega)$ and the corresponding correlators are derived in the Appendix. Using the results obtained there for the determination of (2.8), we write out the final relations for the transition probability $W_{kk'}$ (see (2.3) and (2.8)):

$$W_{kk'}(\mathbf{q}, \omega) = W_{kk'}^{(0)}(\mathbf{q}, \omega) + W_{kk'}^{(1)}(\mathbf{q}, \omega), \quad (2.12)$$

$$\begin{aligned} W_{kk'}^{(0)}(\mathbf{q}, \omega) &= \frac{(2\pi)^3 (b_0(\mathbf{q}))^2}{M V_0 m_*^2} \frac{\operatorname{sign} \omega}{1 - e^{-\omega/T}} \\ &\times \sum_j (\mathbf{q}v_{qj})^2 \delta(\omega^2 - \omega_{qj}^2), \end{aligned} \quad (2.13)$$

$$\begin{aligned} W_{kk'}^{(1)}(\mathbf{q}, \omega) &= c \frac{(2\pi)^3}{m_*^2 V_0} \left\{ (\Delta b(\mathbf{q}))^2 \delta(\omega) \right. \\ &+ \frac{\operatorname{sign} \omega}{1 - e^{-\omega/T}} \sum_j \frac{(\mathbf{q}v_{qj})^2}{M} \\ &\times \left[\frac{1}{c} (b_0(\mathbf{q}))^2 \left(\frac{1}{\pi} \frac{\varepsilon c \omega^2 \gamma(\omega^2)}{[\omega^2(1 - \varepsilon c \Delta(\omega^2)) - \omega_{qj}^2]^2 + [\varepsilon c \omega^2 \gamma(\omega^2)]^2} \right. \right. \\ &\left. \left. - \delta(\omega^2 - \omega_{qj}^2) \right) + (\Delta b(\mathbf{q}))^2 \frac{g(\omega^2)}{R(\omega^2)} \right. \\ &+ 2b_0(\mathbf{q}) \Delta b(\mathbf{q}) \frac{1}{\pi} \left[\gamma(\omega^2) P \frac{1}{\omega^2 - \omega_{qj}^2} \right. \\ &\left. \left. + \pi \Delta(\omega^2) \delta(\omega^2 - \omega_{qj}^2) \right] \right\}. \end{aligned} \quad (2.14)$$

(All the symbols are defined in the Appendix.)

Expression (2.13) determines the probability of the single-phonon scattering of the electron in an ideal crystal. If we substitute (2.13) in (2.1), then we arrive at the expression for the resistance of an ideal crystal, obtained within the framework of the standard theory.^[8] Relation (2.14) describes the probability of the electron scattering due entirely to the presence of the impurity atoms. It is obvious that this part of the probability is of decisive interest for the problem in question.

3. RESISTANCE OF A METAL IN THE PRESENCE OF IMPURITY ATOMS. DISCUSSION OF RESULTS

A. We proceed to determine the resistance, to which end we substitute (2.12)–(2.14) in (2.1). In the direct calculations we make assumptions that are not critical for the qualitative results (and are the same as in Bloch's classical theory of electric conductivity^[8]). Namely, we assume that the dispersion law is isotropic in all those cases when the explicit connection between ω and \mathbf{q} is essential for the phonon spectrum. In addition, for simplicity in determining the upper limit of integration with respect to $d\mathbf{q}$, we assume that $2k_F$ and $k_{\max}(=q_0)$ are nearly equal and make no distinction between these parameters.

Recognizing that the amplitudes $b_{0,1}(\mathbf{q})$ depend only on the modulus $|\mathbf{q}|$, we arrive after direct calculations at the relation

$$\rho = \rho_0 + \rho^1, \quad \rho^1 = \rho_1 + \rho_2 + \rho_3 + \rho_4 \equiv \Delta\rho + \rho_1, \quad (3.1)$$

$$\rho_0 = \frac{\eta}{2T} \int_0^{q_0} dq q^5 (b_0(q))^2 n(q) (n(q) + 1), \quad (3.2)$$

$$\rho_1 = c \frac{M\eta}{2} \int_0^{q_0} dq q^3 (\Delta b(q))^2, \quad (3.3)$$

$$\rho_2 = c \frac{\eta}{T} \int_0^{q_0} dq q^5 (b_0(q))^2 \int_0^{\infty} d\omega \omega n(\omega) (n(\omega) + 1) \times \frac{1}{c} \left(\frac{1}{\pi} \frac{\varepsilon c \omega^2 \gamma(\omega^2)}{[\omega^2(1 - \varepsilon c \Delta(\omega^2)) - \omega_q^2]^2 + [\varepsilon c \omega^2 \gamma(\omega^2)]^2} - \delta(\omega^2 - \omega_q^2) \right) \quad (3.4)$$

$$\rho_3 = c \frac{\eta}{T} \int_0^{q_0} dq q^3 [\Delta b(q)]^2 \int_0^{\infty} d\omega \omega n(\omega) [n(\omega) + 1] \frac{g(\omega^2)}{R(\omega^2)}, \quad (3.5)$$

$$\rho_4 = c \frac{2\eta}{T} \int_0^{q_0} dq q^5 [b_0(q) \Delta b(q)] \int_0^{\infty} d\omega \omega n(\omega) [n(\omega) + 1] \times \frac{1}{\pi} \left[\gamma(\omega^2) P \frac{1}{\omega^2 - \omega_q^2} + \pi \Delta(\omega^2) \delta(\omega^2 - \omega_q^2) \right], \quad (3.6)$$

where $n(\omega) = (\exp[\omega/T] - 1)^{-1}$; by η we denote

$$\eta = \left(\frac{2\pi}{m_*^2} \right)^2 \frac{3\pi}{2e^2 v_F^2 k_F^4 M V_0},$$

(v_F is the velocity of the electron on the Fermi surface). We note that ρ_0 and ρ_1 determine respectively the resistance of the ideal lattice and the impurity resistance.

If we replace $b_0(q)$ in (3.2) by $a_0(0)$, then the expressions obtained coincide with the well-known Bloch-Gruneisen formula.

Let us consider the part of the resistance ρ_1 which is due to the elastic scattering (Eq. (3.3)). As $T \rightarrow 0$ the quantity ρ_1 determines the residual resistance, since all the remaining terms in (3.1) vanish. It is interesting that when $T \rightarrow 0$ the resistance ρ_1 begins to depend on the temperature via the Debye-Waller factors (see (2.9)), which in our case are

$$W_0(q) = \frac{q^2}{2M} \int_0^{\infty} d\omega^2 \frac{g(\omega^2)}{\omega} [2n(\omega) + 1]$$

$$W_1(q) = \frac{q^2}{2M} \int_0^{\infty} d\omega^2 \frac{g(\omega^2)}{\omega R(\omega^2)} (2n(\omega) + 1). \quad (3.7)$$

This dependence is due to the decrease of the amplitude of pure elastic scattering with increasing temperature, that is, scattering without emission or absorption of phonons, and can lead to either a decrease or an increase of ρ_1 with increasing T . The magnitude itself of this change, however, is as a rule small and may manifest itself only in the region of very low temperatures by virtue of the fact that it leads to a quadratic temperature dependence (as in the case of ρ_3 —see below).

We note that the presence of zero-point oscillations may cause the residual resistance to differ from zero, even if the impurity atoms have the same scattering amplitude as the atoms of the host lattice.

B. Let us proceed to consider $\Delta\rho$ —the impurity resistance due to inelastic processes. We consider the region of low temperatures. We assume further not only that $\Theta/T \gg 1$ but also $\omega_*/T \gg 1$, where $\Theta = v_{ac}q_0$ and

$$\omega_* = [|\varepsilon| \langle 1/\omega^2 \rangle]^{-1/2} \quad (3.8)$$

is the frequency of the quasilocal level occurring when $|\varepsilon| \gg 1$ (see [11]); $\langle \rangle$ denotes averaging over the phonon spectrum of the matrix.

After calculating (3.4)–(3.6) in this limit and retaining the fundamental terms, we obtain directly

$$\rho_2 = c J_5 \rho_{\Theta} (-2\varepsilon) (T/\Theta)^5, \\ \rho_3 = 2cd J_2 \rho_{\Theta} (T/\Theta)^2 g_1 [1 - 2\langle 1/\omega^2 \rangle \Theta^2 (J_4/J_2) \varepsilon (T/\Theta)^2], \\ \rho_4 = 4cd J_4 g_3 \rho_{\Theta} (-\varepsilon) (T/\Theta)^4 + 2c J_5 \rho_{\Theta} g_2 (T/\Theta)^5. \quad (3.9)$$

For comparison we present the value of ρ_0 in this limit:

$$\rho_0 = J_5 (T/\Theta)^5 \rho_{\Theta}. \quad (3.10)$$

In these expressions

$$\rho_{\Theta} = \eta (a_0(0))^2 q_0^6 / 2\Theta, \quad J_v = v! \zeta(v),$$

where ζ is the Riemann zeta function. In addition, d is a numerical coefficient in the low-frequency representation for the distribution function of the squared frequencies of the phonon spectrum of the matrix: $g(\omega^2) = d\omega/\Theta^3$. We have introduced also the following symbols:

$$g_1 = \frac{1}{q_0^6 (a_0(0))^2} \int_0^{q_0} dq q^5 (\Delta b(q))^2, \quad g_2 = \frac{\Delta a(0)}{a_0(0)}, \\ g_3 = \frac{\Theta^2}{q_0^6 (a_0(0))^2} \int_0^{q_0} dq q^5 \frac{\Delta b(q) b_0(q)}{\omega_q^2}. \quad (3.11)$$

It is important that in the region of low temperatures ρ_2 , just like ρ_0 , is determined in terms of the scattering amplitudes corresponding to $q \rightarrow 0$, whereas ρ_3 and ρ_4 depend on the behavior of the scattering amplitudes in the entire momentum-transfer interval. To estimate g_1 , g_2 , and g_3 we can use the value of the scattering amplitudes in the Born approximation, assuming an electron-ion interaction in the form obtained when a pseudopotential is employed (see, for example [20]), or in some more traditional form (see [8]).

We now analyze expression (3.9). We consider first the case when the scattering amplitudes b_0 and b_1 are practically equal to each other, and by

the same token $\Delta\rho$ is determined entirely by the value of ρ_2 . As seen from (3.9), the inelastic impurity resistance $\Delta\rho$ has at sufficiently low temperatures the same temperature dependence as ρ_0 , a positive sign if the impurity atom is heavier than the atom of the matrix ($\epsilon < 0$), and a negative sign in the opposite case ($\epsilon > 0$). This result has a clear-cut physical meaning. Indeed, when $M_1 > M_0$ the deformation of the vibrational spectrum leads to an increase in the density of the frequencies in the region of low ω , and by the same token increases the probability of scattering at low temperatures. When $M_1 < M_0$, the density of the frequencies in the region of low ω decreases, and we have the opposite picture. (We note that the appearance of a local frequency does not change anything qualitatively.) In the limit as $T \rightarrow 0$ we have

$$\Delta\rho / \rho_0 \rightarrow -2\epsilon c. \quad (3.12)$$

Thus, the relative change in the resistance for heavy impurity atoms turns out to be $2|\epsilon|$ times larger than the concentration.

With increasing temperature, this ratio begins to increase rapidly when $|\epsilon| \gg 1$. In order to trace this result in explicit form, we assume for simplicity strong screening ($b_0(q) \approx b_0(0)$) and a linear dispersion for the phonons. Expression (3.4) is then transformed at low temperatures into

$$\rho_2 = cJ_5\rho_0(-2\epsilon) \left(1 + (-\epsilon) \frac{9}{8} \frac{J_6}{J_5} \frac{T}{\Theta} \right) \left(\frac{T}{\Theta} \right)^5, \quad (3.13)$$

and when $-\epsilon \gg 1$ there is actually a strong increase in the ratio $\Delta\rho/\rho_0$.

With further increase in temperature, the strong deformation of the vibrational spectrum, due to the presence of the quasilocal level, causes $\Delta\rho(T)/\rho_0(T)$ to go through a maximum at $T < \omega$, and then to start decreasing relatively rapidly. It is easy to find the value of ρ_2 at a temperature of the order of ω_* . To this end it is sufficient to use in the calculation of (2.4) the resonant character of the behavior of the function $\gamma(\omega^2)$ (A.8) (see, for example, [11]). As a result we find

$$\Delta\rho = \rho_2 \approx \frac{1}{6}\rho_0 c (T/\Theta). \quad (3.14)$$

For purpose of illustration, Fig. 1 shows a plot of $\Delta\rho(T)/c\rho_0(T)$ against T/Θ , calculated for $|\epsilon| = 7$. For comparison we present also the curve for $|\epsilon| = 3$.

We now consider the general case, when $\Delta b \neq 0$. Then contributions are made to $\Delta\rho$ not only by ρ_2 but also by ρ_3 and ρ_4 which in accord with (3.9) have an entirely different temperature de-

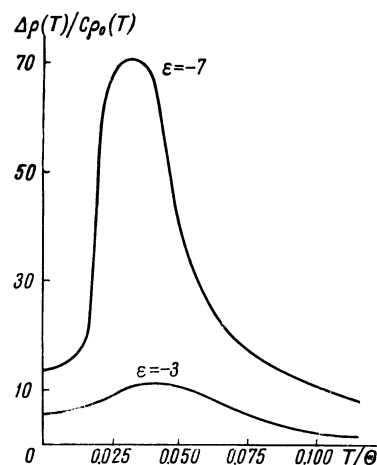


FIG. 1

pendence. At extremely low temperature the predominant role will be played in $\Delta\rho$ by ρ_3 —the resistance due to inelastic scattering by the impurity atoms themselves. Nonconservation of the momentum in such collisions causes a quadratic temperature dependence. ρ_3 always makes a positive contribution to $\Delta\rho$, i.e., it increases the resistance and differs from zero even in the absence of phonon-spectrum deformation, i.e., as $\epsilon \rightarrow 0$ (it is precisely the latter case which was the subject of a relatively recent discussion [21, 22]).

The region of temperatures where ρ_3 plays the main role in the general temperature-dependent part of the resistance (including ρ_0) is usually relatively small and amounts to several degrees at a concentration of the order of 1%. (With regard to the impurity part of the resistance, this temperature interval turns out to be, naturally, much larger and independent of the concentration.) This is connected to a decisive degree with the fact that ρ_3 contains a factor g_1 , which according to the customary rough estimates is of the order of several times 10^{-2} . It must be emphasized, however, that the specific behavior of the Fourier component of the pseudopotential at large momentum transfers can in some cases lead to large values of g_1 , thus increasing the temperature interval in which the quadratic temperature dependence predominates in the total resistance.

It must be noted that it is actually necessary to consider simultaneously with ρ_3 also the resistance ρ_1 (3.3) which, as already noted, depends on the temperature via the Debye-Waller factors (3.7). We separate in (3.3) the resistance component ρ_1' which depends on the vibrational spectrum. Using expression (2.9) and assuming, as usual, that $W_{0,1}$ are small compared with unity, we get

$$\rho_1' = c \frac{M\eta}{2} \int_0^{q_0} dq q^3 \{ -(\Delta a(q))^2 W_1 - a_0(q) \Delta a(q) (W_1 - W_0) \}. \quad (3.15)$$

It is easy to find the first temperature term in the expansion of ρ_1' at low temperatures. In accord with (3.7), it is equal to

$$\rho_1'(T \rightarrow 0) = -cdJ_2g_1(T/\Theta^2)\rho_0. \quad (3.15')$$

Thus, allowance for this term decreases ρ_3 (3.9) by one half.

We note that when $|\epsilon| \gg 1$ the appearance of the quasilocal level leads, as in the case of ρ_2 , to a strong increase of $\rho_3 + \rho_1'$, and the ratio $(\rho_0 + \rho_1')/(T/\Theta)^2$ passes through a sharp maximum at temperatures lower than ω_* given by (3.8).

Finally, let us consider the interference term ρ_4 . As follows from (3.6), ρ_4 is the sum of two terms, the first of which is connected simultaneously with the difference in the scattering amplitudes and with the deformation of the vibrational spectrum (the first term in the square brackets). It vanishes both when $\Delta b \rightarrow 0$ and when $\epsilon \rightarrow 0$. The second term, on the other hand, which is due to the interference between the scattering by the impurity atom and by the unperturbed phonon spectrum, differs from zero even when $\epsilon \rightarrow 0$. This situation is reflected also in the low-temperature representation for ρ_4 (3.9).

The expansion of ρ_4 begins with a term proportional to T^4 . This term contains a factor g_3 (3.11) which, like g_1 , is usually much smaller than unity. If this is so, then this term has the same order of magnitude as the second term in the expansion of ρ_3 (see (3.9)), and at low temperatures it will actually play the role of a correction to ρ_3 (compare ρ_3 and ρ_4 in (3.9)).

The first term in ρ_4 , which is proportional to T^5 , depends only on the scattering amplitude as $q \rightarrow 0$, and therefore contains no small parameter whatever. In the general case it is of the same order as ρ_2 . It is very important that for fixed ϵ this term can have an arbitrary sign, depending on the sign of Δb . Thus, if g_1 and g_3 are really small, then we have approximately for the impurity resistance in the low-temperature region

$$\widetilde{\Delta\rho} \approx cdJ_2\rho_0g_1\left(\frac{T}{\Theta}\right)^2 + 2cJ_5\rho_0\left(-\epsilon + \frac{Z_1 - Z_0}{Z_0}\right)\left(\frac{T}{\Theta}\right)^5. \quad (3.16)$$

We use here the result obtained for electron-ion interaction in metals in the framework of the usual theories:

$$\Delta a(0) / a_0(0) = (Z_1 - Z_0) / Z_0$$

(Z_0 and Z_1 is the charge of the ion in the matrix

and the charge of the impurity ion in the given matrix); and in addition, we took into account ρ_1' , so that $\widetilde{\Delta\rho} = \Delta\rho + \rho_1'$.

The first term in (3.16) is always positive, and the sign of the second is determined simply by the sign of the quantity

$$S = -\epsilon + \frac{Z_1 - Z_0}{Z_0} = \frac{M_1 - M_0}{M_0} + \frac{Z_1 - Z_0}{Z_0}. \quad (3.17)$$

Thus, if $S < 0$, then the impurity resistance as a function of the temperature passes through a maximum. The position of this maximum can be readily obtained from (3.16):

$$T_{max} = \left(\frac{dJ_2g_1}{5J_5(-S)}\right)^{1/5} \Theta. \quad (3.18)$$

Here

$$\widetilde{\Delta\rho}(T_{max}) = 3c(-S)\rho_0(T_{max}). \quad (3.19)$$

When $S > 0$ the quantity $\widetilde{\Delta\rho}$ increases monotonically with the temperature.

We note that the change in the electron spectrum can lead also to an additional term in $\Delta\rho$, proportional to $(T/\Theta)^5$, and consequently, to a change of S . This change, however, is apparently small, and qualitatively the entire picture should remain the same. (Thus, in the approximation of the quasifree electrons, if we assume that k_F^3 is proportional to the overall density of the electrons and $a_0(0) \sim \epsilon_F$,^[8] then a coefficient $^{2/3}$ appears in the second term of (3.17).)

The described picture can experience appreciable changes if it turns out in some cases that g_1 and g_2 , although smaller than unity, are still appreciable. This will particularly come into play when $|\epsilon| \gg 1$, since, as seen from (3.9) and (3.13), the discarded terms contain the factor ϵ . It turns out that this may even give rise to a minimum in the dependence of the total resistance on the temperature. To demonstrate this, let us consider the temperature region $T \gtrsim \omega_*/2$ (see (3.8)). In this region, the sum of ρ_3 and of the first term in (3.15)

$$\frac{c\eta}{T} \int_0^{q_0} dq q^5 (\Delta a(q))^2 \int_0^\infty d\omega \omega \frac{g(\omega^2)}{R(\omega^2)} \left\{ n(\omega)[n(\omega) + 1] - \frac{T}{2\omega} [2n(\omega) + 1] \right\} \quad (3.20)$$

vanishes if we take into account the sharply resonant character of the function g/R near the quasilocal frequency ω_* . The second term in (3.15), on the other hand, differs from zero, for in the temperature region under consideration the classical

limit sets in only for the function W_1 . As a result we obtain

$$\rho_3 + \rho_1' = -c\rho_0 g_4 \Theta^2 \langle 1/\omega^2 \rangle (T/\Theta),$$

$$g_4 = \frac{1}{a_0^6 (a_0(0))^2} \int_0^{q_0} dq q^5 a_0(q) \Delta a(q). \quad (3.21)$$

Under the conditions in question, the main contribution to ρ_4 is made by the first term in (3.6). The resonant behavior of $\gamma(\omega^2)$ (A.8) makes it possible to obtain immediately the explicit form of the expression for the resistance:

$$\rho_4 = 2c\rho_0 g_3 T / \Theta. \quad (3.22)$$

With regard to ρ_2 , we have already obtained earlier the corresponding expression (3.14). This expression should really contain a certain numerical factor $\beta < 1$ by virtue of the fact that it was assumed in its derivation that $b_0(q) \approx b_0(0)$. Thus, taking (3.21), (3.22), (3.14), and expression (3.10) for ρ_0 into account, we have for the temperature-dependent part of the total resistance:

$$\rho / \rho_0 = J_5 (T/\Theta)^5 + c\delta (T/\Theta),$$

$$\delta = 2g_3 - \Theta^2 \langle 1/\omega^2 \rangle g_4 + \beta / 6. \quad (3.23)$$

If $\delta < 0$, then it follows immediately from (3.23) that the total resistance can pass through a minimum, the position of which is determined in trivial manner:

$$T_{min} = \Theta (|\delta| / 5J_5)^{1/4} c^{1/4}. \quad (3.24)$$

It must be noted that inasmuch as it was assumed in the derivation of (3.24) that T is at least of the order of $\omega_*/2$, the obtained results can be really valid when $c \gtrsim 1\%$. However, at lower temperatures all three terms which make up the part of ρ that depends linearly on T begin to increase rapidly in approximately the same temperature interval, when the discarded term (3.20) is still small. As a result the minimum of the total resistance may appear also at noticeably smaller values of concentration and temperature.

C. Let us consider now the region of high temperatures. As is well known (see [11]), we have

$$\int_0^\infty d\omega^2 \frac{g(\omega^2)}{\omega^2 R(\omega^2)} = \int_0^\infty d\omega^2 \frac{g(\omega^2)}{\omega^2}$$

and in the classical limit with respect to temperature we have $W_0 = W_1$. Hence, taking into consideration (3.5), (3.15), and (3.20), we readily obtain

$$\rho_3 + \rho_1' \rightarrow 0. \quad (3.25)$$

Thus, in the region of high temperatures part of

the impurity resistance, due to scattering by the impurity atoms themselves, ceases to depend on the temperature at all (a similar result was obtained by Taylor [22], who neglected the difference between the masses M_0 and M_1 and the deformation of the vibrational spectrum).

We show now that ρ_2 also vanishes at high temperatures. To this end we consider the first term in (3.4) and transform the integral into

$$I_1 = -\frac{1}{4\pi i} \int_0^\infty d\omega^2 \frac{1}{\omega^2} \left\{ \frac{1}{\omega^2 (1 - \epsilon c \Delta(\omega^2)) - \omega_q^2 + i\epsilon \omega^2 c \gamma(\omega^2)} - \text{c.c.} \right\} = -\frac{1}{4\pi i} \int_0^\infty \frac{dx}{x} \left\{ \frac{1}{x - \omega_q^2 - F(x)} - \text{c.c.} \right\},$$

$$F(x) = \epsilon c x \left[1 - \epsilon x \int_0^1 dx' \frac{g(x')}{x - x' + i\delta} \right]^{-1} \equiv \epsilon c x \psi(x). \quad (3.26)$$

We consider first the case when there is no local level. Then this integral can be represented in the form of an integral in the complex domain, along a contour C consisting of two horizontal lines from $\xi + i\delta$ to $\infty + i\delta$ in the upper half plane and from $\infty - i\delta$ to $\xi - i\delta$ in the lower half-plane ($\xi, \delta \rightarrow +0$):

$$I_1 = -\frac{1}{4\pi i} \int_C \frac{dz}{z} \Phi(z), \quad \Phi(z) = \frac{1}{z - \omega_q^2 - F(z)}$$

It is easy to verify that the function $\Phi(z)$ outside the segment of the real axis from 0 to 1 is an analytic function. Therefore the integration can be carried out along the contour C_1 shown in Fig. 2a by the continuous line.

Closing the contour with a circle of radius ξ around the point $x = 0$ (dashed contour C_ξ), we have

$$I_1 = -\frac{1}{4\pi i} \int_{C_R + C_1 + C_\xi} \frac{dz}{z} \Phi(z) + \frac{1}{4\pi i} \int_{C_R + C_\xi} \frac{dz}{z} \Phi(z),$$

where C_R is a circle of radius $R \rightarrow \infty$ traced in a counterclockwise direction. The first integral obviously vanishes. We easily see that the integral along the contour C_R is also equal to zero. As a result we are left only with the integral along C_ξ , and we readily obtain

$$I_1 = 1 / 2\omega_q^2. \quad (3.27)$$

Substituting this result in (3.4), we find directly that ρ_2 actually vanishes. This result remains unchanged also in the presence of a local level. Indeed, in this case $\gamma(x)$ and $F(x)$ have a singularity on the real axis at the point where x coincides with the local frequency. But this point is bypassed automatically when the initial contour C is chosen

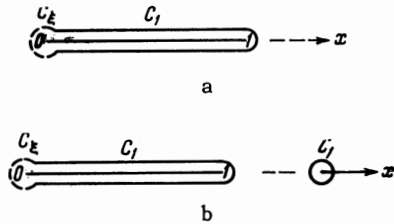


FIG. 2

(see Fig. 2b). We note that the transition from (A.9) to (A.10) in the presence of a local level actually presupposes the existence of a small but finite smearing of this level, which always exists, if for no other reason than anharmonicity. In this case there would appear in place of the circular contour on Fig. 2b a closed contour which surrounds a finite segment of the real axis x , corresponding to the smeared local level, but the result (3.27) would remain the same.

We now proceed to ρ_4 . We consider the first term in (3.6), and rewrite, using (3.26), the integral with respect to frequency in the form

$$I_2 = \frac{1}{2\pi} \int_0^{\infty} \frac{d\omega^2}{\omega^2} \frac{1}{\pi} \frac{\gamma(\omega^2)}{\omega^2 - \omega_q^2}$$

$$= -\frac{1}{4\pi i} \int_0^{\infty} \frac{dx}{x} \frac{1}{x - \omega_q^2} (\psi(x) - \psi^*(x)).$$

Going over to integration in the complex domain, similar to that used in the calculation of I_1 , we obtain immediately

$$I_2 = -\frac{1}{4\pi i} \int_{C_1} \frac{dx}{x} \frac{1}{x - \omega_q^2} \psi(x) - \frac{\text{Re } \psi(\omega_q^2)}{2\omega_q^2},$$

where the contour C_1 coincides with the continuous contour on Fig. 2b. After similar calculations, we obtain

$$I_2 = [1 - \Delta(\omega_q^2)] / 2\omega_q^2.$$

Substituting this result in (3.6), we obtain the value of ρ_4 , and at the same time also the temperature-dependent part of the impurity resistance in the classical temperature region $T > \Theta/2$:

$$\rho_4(T) = (\Delta\rho)_T = 2c\eta T \int_0^{q_0} dq q^5 b_0(q) \Delta b(q) \frac{1}{2\omega_q^2}$$

$$= 2cg_3\rho_0 \frac{T}{\Theta} \quad (3.28)$$

(see the notation in (3.11)).

Thus, at high temperatures the impurity resistance tends to a constant limit only when $\Delta a \rightarrow 0$ (in the classical limit $\Delta b(q) = \exp[-W_0(q)/2]\Delta a(q)$). If $\Delta a \neq 0$, then the impurity resistance, just as

the resistance of a pure metal, depends linearly on the temperature, and $(\Delta\rho)_T$ can have an arbitrary sign, depending on the sign of Δa or, more rigorously, on the sign of g_3 . We note that the deformation of the electron spectrum can in some cases complicate this result.

4. COMPARISON WITH EXPERIMENT

The results obtained in the preceding section enable us to analyze the character of the dependence

$$(\Delta\rho)_T = \Delta\rho(T) - \Delta\rho(0)$$

on T in the entire interval of temperatures for arbitrary values of ϵ and Δa . It should be noted here that whereas the sign of $\Delta a(q)$ as $q \rightarrow 0$ is determined essentially by the difference in the charges of the ions, the same cannot be said concerning the region of large q . Indeed, the features of the behavior of the pseudopotential in this region are such that one cannot exclude the possibility of reversal of the sign of $\Delta a(q)$ at large q in the case of atoms belonging to different periods of the periodic system. Bearing this in mind, we shall speak during the analysis of the results simply to the sign of Δa , but refer in this case essentially to the sign of the quantity g_3 (3.11), which determines the asymptotic temperature behavior of $(\Delta\rho)_T$. In comparison with experiment, on the other hand, we shall always assume that the signs of Δa and of g_3 are determined when $Z_1 \neq Z_0$ by the sign of the difference $Z_1 - Z_0$, that is, they coincide with the sign of Δa when $q \rightarrow 0$.

A. $\Delta a < 0$. As follows from the results of the preceding section, when $\Delta a \rightarrow 0$ the impurity resistance always increases with increasing T in the initial temperature region; on the other hand, in the high-temperature region the condition $\Delta a < 0$ leads to negative $(\Delta\rho)_T$, which decreases linearly with the temperature (see (3.28)). Thus, $(\Delta\rho)_T$ as a function of the temperature will always go through a maximum, and then through zero at a certain temperature, retaining a negative sign at high temperatures. This result is clearly illustrated in Fig. 3, where we present for purposes of illustration plots of $(\Delta\rho)_T = f(T)$ calculated under the assumption of strong screening and for $a_1(0) = (\frac{1}{2})a_0(0)$ at three values of ϵ : -7 , -3 , and 0.7 . For the phonon spectrum of the matrix, we assumed the Debye approximation. A similar temperature dependence of the impurity resistance was recently observed experimentally with Mg alloys with small contents of Ag ($Z_1 - Z_0 = 1$).¹⁹⁻²⁰ An analogous result was obtained also for an alloy

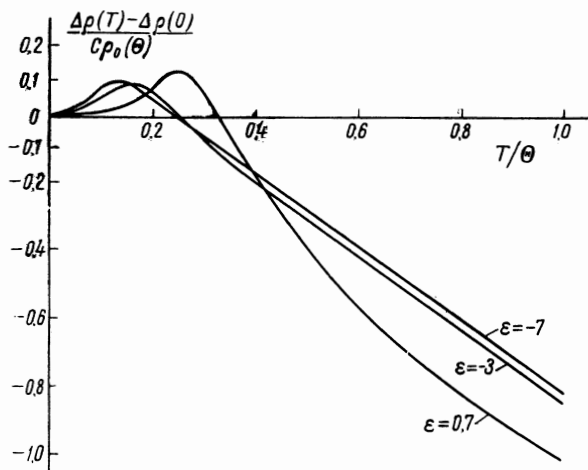


FIG. 3

of Mg with Li ($Z_1 - Z_0 = 1$).^[10] The fact that an entirely different result was obtained in^[9] for a similar alloy is due, in all probability, to the large content of Li (4.4 at. %).

B. $\Delta a > 0$. In this case $(\Delta\rho)_T$ has the same (positive) sign both at low and at high temperatures. In the intermediate temperature region the curve may be quite complicated, with one or more inflection points, and even with loss of monotonicity in some cases. Common to all cases is the linear increase of the impurity resistance in the classical region of temperatures.

There are quite many experimental results that confirm the described picture. Mention should be made first of the classical work of Linde^[23] (see also^[24], which contains part of Linde's unpublished results), in which the linear growth of $(\Delta\rho)_T$ with temperature was observed for alloys of Au with Sn and In, for alloys of Cu with In, Sb, and Sn,^[23] and also alloys of Cu with Ga, Ge, As, and Be, Al, Si, P^[24] (in all cases $Z_1 - Z_0 > 0$). Similar results were obtained recently^[11] for alloys of Au with Zn and of Au with Al ($Z_1 - Z_0 > 0$). It must be stated that in all the results even satisfy the following approximate condition: the greater the difference $Z_1 - Z_0$ the larger the slope of $\Delta\rho(T)/c$ in the classical region.

Alloys of Mg with different contents of Sn impurity were investigated in^[10]. The observed picture varied strongly with the concentration. The assumptions on which the present paper is based are satisfied all the better, the lower the concentration of the impurity component. Indeed, for the alloy with minimum content of Sn (~ 0.1 at. %) the obtained dependence of $(\Delta\rho)_T$ on T does not contradict the theoretical results.

The only case which cannot be explained in these investigations, assuming that the signs of g_3

and $Z_1 - Z_0$ coincide, is the case of the alloy of Mg with Al.^[9] The observed picture is close to that obtained when $g_3 < 0$. Whether this is the consequence of the specific nature of the pseudopotential for large q or whether the initial premises are violated cannot be decided readily without additional experimental information.

C. $Z_1 = Z_0$. This case is quite complicated to analyze, since it is not clear how to determine consistently the signs of Δa and g_3 for two elements pertaining to the same group but to different periods of the periodic system. The opposite is more likely to occur, and this sign may be determined from an analysis of the behavior of $\Delta\rho$ at high temperatures.

If Δa turns out to be very small, then $(\Delta\rho)_T$ will assume in the classical temperature limit a constant value. In the intermediate region $(\Delta\rho)_T$ will then go through a maximum or a minimum, depending on the sign of ϵ , as is clearly demonstrated the curves of Fig. 4, calculated under the same assumptions as in the case of Fig. 3 but for $A_1 = A_0$. In the general case the picture will be much more complicated, since one cannot neglect the difference Δa of the scattering amplitudes.

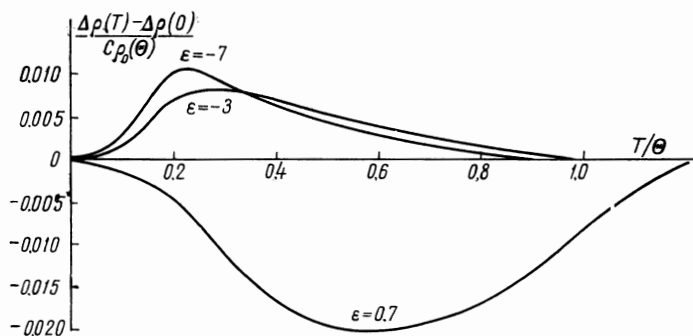


FIG. 4

The fact that $(\Delta\rho)_T$ is approximately constant at high temperatures was observed experimentally for an alloy of Au with Cu in^[11] and in less pronounced form in^[23]. A similar result was obtained for alloys of Au containing small amounts of Ag (and vice versa) in^[25], and also in^[23]. The behavior of $(\Delta\rho)_T$ in the transition region of temperatures is difficult to analyze without exact knowledge of $\Delta a(q)$.

In addition to these alloys, an alloy of Mg and Cd ($Z_1 = Z_0$) was also investigated.^[9, 10] This alloy exhibited clearly a temperature dependence of $(\Delta\rho)_T$ perfectly analogous to the case when $\Delta a < 0$. This possibly leads to conclusions concerning the sign of $\Delta a(q)$ in the main part of the phase space, characteristic of the integral (3.11).

Thus, the results obtained in the present paper explain qualitatively most known experimental data pertaining principally to the regions of high and intermediate temperatures. Unfortunately, the lack of precise measurements of the impurity resistance in the region of low temperatures prevents a comparison with the theoretical results obtained for this temperature region. It is also very important to obtain experimental results with particular attention to the nontrivial character of the temperature dependence of $(\Delta\rho)_T$ and its sensitivity to the parameters of the alloy.

APPENDIX

In the case under consideration the Hamiltonian of the system can be represented in the form

$$H = \sum_{\mathbf{n}\alpha} \frac{(p_{\mathbf{n}}^{\alpha})^2}{2M_{\mathbf{n}}} + \frac{1}{2} \sum_{\mathbf{n}, \mathbf{n}'; \alpha\beta} \Phi_{\mathbf{nn}'}^{\alpha\beta} u_{\mathbf{n}}^{\alpha} u_{\mathbf{n}'}^{\beta}, \quad (\text{A.1})$$

where $M_{\mathbf{n}} = (1 - \epsilon c_{\mathbf{n}})M$, M is the mass of the ideal-lattice atom, $\mathbf{p}_{\mathbf{n}}$ and $\mathbf{u}_{\mathbf{n}}$ are the momentum and displacement operators of the \mathbf{n} -th nucleus, and $\Phi_{\mathbf{nn}'}^{\alpha\beta}$ is the dynamic matrix of interaction of the alloy atoms.

Using this expression for the Hamiltonian, we can derive for the frequency Fourier component of the Green's function (2.10) an analog of the Dyson equation in the coordinate representation:

$$G_{\mathbf{nn}'}^{\alpha\beta}(\omega) = G_{\mathbf{nn}'}^{\alpha\beta,0}(\omega) + M\omega^2\epsilon \sum_{\mathbf{n}_1, \gamma} G_{\mathbf{nn}_1}^{\alpha\gamma}(\omega) c_{\mathbf{n}_1} G_{\mathbf{n}_1\mathbf{n}'}^{\gamma\beta}(\omega), \quad (\text{A.2})$$

$$G_{\mathbf{nn}'}^{\alpha\beta}(\omega) = \frac{1}{MN} \sum_{\mathbf{f}, j} \frac{v_{\mathbf{fj}}^{\alpha} v_{\mathbf{fj}}^{\beta} \exp\{i\mathbf{f}(\mathbf{R}_{\mathbf{n}}^0 - \mathbf{R}_{\mathbf{n}'}^0)\}}{\omega^2 - \omega_{\mathbf{fj}}^2}. \quad (\text{A.3})$$

$\omega_{\mathbf{fj}}$ and $\mathbf{v}_{\mathbf{fj}}$ denote here the natural frequency and the polarization vector for the ideal lattice, corresponding to the wave vector \mathbf{f} and to the branch number j .

We confine ourselves to a cubic crystal and rewrite Dyson's equation in the case when one of the indices (for example, \mathbf{n}) coincides with the impurity lattice point:

$$G_{\mathbf{nn}'}^{\alpha\beta}(\omega) = \mu G_{\mathbf{nn}'}^{\alpha\beta,0}(\omega) + \mu\lambda \sum_{\mathbf{n}_1, \gamma} \tilde{G}_{\mathbf{nn}_1}^{\alpha\gamma}(\omega) c_{\mathbf{n}_1} G_{\mathbf{n}_1\mathbf{n}'}^{\gamma\beta}(\omega). \quad (\text{A.4})$$

We have introduced here the notation

$$\lambda = M\omega^2\epsilon, \quad \mu = (1 - \lambda G_{\mathbf{nn},0}^{\alpha\alpha}(\omega))^{-1}, \\ \tilde{G}_{\mathbf{nn}'}^{\alpha\beta} = G_{\mathbf{nn}'}^{\alpha\beta,0} - \delta_{\mathbf{nn}'} \delta_{\alpha\beta} G_{\mathbf{nn}'}^{\alpha\beta,0}.$$

Substituting the obtained equation in the second term of (A.2), we can construct an iteration series with respect to the concentration c .

We now proceed to determine the correlation

functions in (2.8), bearing relation (2.11) in mind. We begin with the simplest case, corresponding to the third term in (2.8). Since this term is already linear in the concentration, we must determine the corresponding Green's function only in the approximation that is of zero order in the concentration, that is, it is sufficient to take into account only the first term in (A.4). Taking into account (2.11) and the explicit form of (A.3), we obtain

$$\langle\langle u_{\mathbf{n}}^{\alpha}(t) u_{\mathbf{n}'}^{\beta}(t') \rangle\rangle_{\omega} c = \frac{2\pi}{1 - e^{-\omega/T}} \frac{\delta_{\alpha\beta}}{M} \frac{\text{sign } \omega g(\omega^2)}{R(\omega^2)}, \quad (\text{A.5})$$

where

$$R(\omega^2) = (1 - \epsilon\omega^2 J(\omega^2))^2 + (\pi\epsilon\omega^2 g(\omega^2))^2, \\ J(\omega^2) = \int_0^{\infty} dz \frac{g(z)}{\omega^2 - z} \quad (\text{A.6})$$

($g(\omega^2)$ is the distribution function of the squares of the frequencies of the phonon spectrum of the matrix).

We proceed next to determine the last term in (2.8). To this end, limiting ourselves only to the approximation linear in the concentration, we again use only the first term in (A.4). Then

$$\left\langle \frac{1}{N} \sum_{\mathbf{nn}'} \exp[i\mathbf{q}(\mathbf{R}_{\mathbf{n}}^0 - \mathbf{R}_{\mathbf{n}'}^0)] c_{\mathbf{n}} \langle u_{\mathbf{n}}^{\alpha}(t) u_{\mathbf{n}'}^{\beta}(t') \rangle_{\omega} \right\rangle c \\ = \frac{2\pi c}{1 - e^{-\omega/T}} \sum_j \frac{v_{\mathbf{qj}}^{\alpha} v_{\mathbf{qj}}^{\beta}}{M} \frac{1}{\pi} \left[P \frac{\text{sign } \omega \gamma(\omega^2)}{\omega^2 - \omega_{\mathbf{qj}}^2} \right. \\ \left. + \pi \text{sign } \omega \delta(\omega^2 - \omega_{\mathbf{qj}}^2) \Delta(\omega^2) \right], \quad (\text{A.7})$$

where

$$\gamma(\omega^2) = \frac{\pi\epsilon\omega^2 g(\omega^2)}{R(\omega^2)}, \quad \Delta(\omega^2) = \frac{1 - \epsilon\omega^2 J(\omega^2)}{R(\omega^2)}. \quad (\text{A.8})$$

We consider finally the second term in (2.8). In this case the lower indices of the Green's function are arbitrary, and we should use the general equation (A.2). For the Green's function in the right side of (A.2) we use the representation (A.4). Then the zeroth and first-order terms in the concentration turn out to be expressed only in terms of the zero-order Green's functions, and the iteration series begins with terms of order c^2 . Using (A.3), we obtain in the approximation linear in the concentration

$$\left\langle \frac{1}{N} \sum_{\mathbf{n}, \mathbf{n}'} \exp[i\mathbf{q}(\mathbf{R}_{\mathbf{n}}^0 - \mathbf{R}_{\mathbf{n}'}^0)] G_{\mathbf{nn}'}^{\alpha\beta}(\omega) \right\rangle c = \frac{1}{N} \sum_{\mathbf{n}, \mathbf{n}'} \langle G_{\mathbf{nn}'}^{\alpha\beta}(\omega) \rangle c \\ \times \exp[i\mathbf{q}(\mathbf{R}_{\mathbf{n}}^0 - \mathbf{R}_{\mathbf{n}'}^0)] = \frac{1}{M} \sum_j \frac{v_{\mathbf{qj}}^{\alpha} v_{\mathbf{qj}}^{\beta}}{\omega^2 - \omega_{\mathbf{qj}}^2} \\ + \frac{\mu\lambda c}{M^2} \sum_j \frac{v_{\mathbf{qj}}^{\alpha} v_{\mathbf{qj}}^{\beta}}{(\omega^2 - \omega_{\mathbf{qj}}^2)^2} + \dots \quad (\text{A.9})$$

In the same approximation or, more rigorously, carrying out selective summation of the pole terms of the iteration series, we have

$$\begin{aligned} & \left\langle \frac{1}{N} \sum_{nn'} \exp [iq(\mathbf{R}_n^0 - \mathbf{R}_{n'}^0)] \langle u_n^\alpha(t) u_{n'}^\beta(t') \rangle_\omega \right\rangle_c \\ &= \frac{2\pi}{1 - e^{-\omega/T}} \sum_j \frac{v_{qj}^\alpha v_{qj}^\beta}{M} \frac{1}{\pi} \\ & \times \frac{\text{sign } \omega \varepsilon c \omega^2 \gamma(\omega^2)}{[\omega^2(1 - \varepsilon c \Delta(\omega^2)) - \omega_{qj}^2]^2 + [\varepsilon c \omega^2 \gamma(\omega^2)]^2}. \quad (\text{A.10}) \end{aligned}$$

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