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INFLUENCE OF CRYSTAL DEFECTS ON THE CRITICAL SUPERCONDUCTIVITY TRANSITION TEMPERATURE

E. G. MAKSIMOV

Institute of High Pressure Physics, USSR Academy of Sciences

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The superconductivity equations for an imperfect crystal is obtained on the basis of the complete electron-ion Hamiltonian. It is shown that the critical temperature T_c for a superconductor of this type can be expressed by means of the correlation scattering function $S(q, \omega)$ previously employed for calculating the resistance of a normal metal. The change in T_c due to impurities and disordering is calculated. The relation between changes in T_c and changes in the linear resistivity coefficient of a metal at high temperature is established.

1. INTRODUCTION

As is well known, crystal lattice defects influence very strongly most physical properties of a crystal. The presence of defects in the crystal, particularly in the presence of local or quasilocal oscillations connected with impurities or extended defects (dislocations, boundaries of the sample, etc.), leads to an appreciable change in the dynamics of the lattice, and this in turn greatly influences the specific heat of the crystal, the probability of the Mössbauer effect, and the scattering of x-rays and slow neutrons, and leads to violation of the Matthiessen rules for the residual resistance of metal[1-5].

It is also known that the presence of impurities or other static defects in the crystal leads to an appreciable change of the electromagnetic properties of superconductors, particularly to an appreciable increase of the critical magnetic fields[6]. As shown by the calculation[6-8], the influence of the static nonmagnetic impurities on the thermodynamic characteristics of superconductors is exceedingly small, and reduces to a certain decrease of the critical temperature T_c, owing to the isotropization of the energy gap. Calculations of the thermodynamic characteristics of superconductors, based on a Hamiltonian with electron-phonon interaction, has shown[9-12] that these characteristics depend significantly on the lattice dynamics, particularly on the density of the phonon states. However, the calculations performed in[9-12] actually pertain only to ideal crystals, and a consistent account of the dynamic properties of defects within the framework of the formalism developed there is quite difficult. This is connected, if with nothing else, with the fact that in[9-12] the ion displacement operator is expanded in terms of plane phonons, which is rather ineffective in non-ideal crystals[1].

It is of considerable interest to generalize the results of[9-12] and to write the complete equations of superconductivity with the aid of the correlation functions of the displacements of the ions, which are widely used in investigations of the properties of non-ideal crystals. Such a reformulation of the equations of superconductivity makes it possible, first, to take consistent account of the influence of the dynamic character of the defects on the properties of the superconductor and, second, to relate the change of the superconducting characteristics of the metals with the changes of a number of other experimentally observed quantities, particularly with the change of the resistance at high temperatures[13].

This is all the more interesting because recently a number of experiments have been reported, indicating the possibility of an appreciable change of the thermodynamic characteristics of superconductors, particularly T_c, resulting apparently from structural realignment of the lattice or from the appearance of extended defects in the lattice. The most considerable change of T_c is observed in thin amorphous films of metal[14-17], where a significant change takes place in the entire dynamics of the crystal lattice. A less radical but noticeable change of T_c is observed in bulky samples following the appearance in them of dislocations and other extended defects[18]. A change was observed also in the energy gap, owing to the appearance of local impurity oscillations in the lattice[19,20].

It should be noted that the superconductivity equation obtained in this paper, and also the concrete estimates of the change of T_c, are applicable only to non-transition metals and their alloys, while the electron-ion interaction can be described by a small pseudopotential[21].

2. DERIVATION OF GENERAL EQUATIONS OF SUPERCONDUCTIVITY THEORY FOR CRYSTALS WITH DEFECTS

Let us consider a system of interacting electrons and ions in a metal. We assume for simplicity that the crystal lattice is monoatomic and cubic, that the interaction between the electron and the ion in simple metals is described with the aid of a pseudopotential $v_n(\mathbf{r})$. Then it is convenient to use for our purposes the following Hamiltonian of this system:

$$H = H_i + H_e + H_{e,\,i}, \tag{1}$$

$$H_i = \sum_n \frac{\mathbf{p}_n{}^2}{2M_n} + \frac{1}{2} \sum_{n,n'} \Phi^{\alpha\beta}_{n,n'} u_n{}^\alpha u_{n'}{}^\beta, \tag{2}$$

$$H_e + H_{e,i} = \sum_{\mathbf{k}} \varepsilon_{\mathbf{k}} \psi_{\mathbf{k}}{}^+ \tau_3 \psi_{\mathbf{k}} + \sum_{\mathbf{k},\mathbf{k}'} \Delta v(\mathbf{k}' - \mathbf{k}) \psi_{\mathbf{k}'}{}^+ \tau_3 \psi_{\mathbf{k}}$$

$$+\sum_{\mathbf{k},\mathbf{k}',n} V_n{}^{\alpha}(\mathbf{k}'-\mathbf{k})\psi_{\mathbf{k}'}{}^{+}\tau_3\psi_{\mathbf{k}}u_n{}^{\alpha}+\frac{1}{2}\sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} V_c(\mathbf{q})\psi_{\mathbf{k}'+\mathbf{q}}\tau_3\psi_{\mathbf{k}'}\overset{+}{\psi}_{\mathbf{k}-\mathbf{q}}\tau_3\psi_{\mathbf{k}}. \quad (3)$$

We have introduced here standard symbols for the momenta and coordinates, $\Phi^{\alpha\beta}_{nn'}$ is the dynamic ion interaction matrix in a nonideal crystal, for which concrete expressions, with account taken of the presence of disordering or impurities, will be presented later. We have retained the coordinate representation for the ion system, the electron system is written in the second-quantization representation, and for convenience in the calculations of the superconducting properties the electron Hamiltonian is written with the aid of the two-component spinor

$$\psi_{\mathbf{k}}=\begin{vmatrix} a_{\mathbf{k}} \\ \overset{+}{a}_{-\mathbf{k}} \end{vmatrix}, \qquad \psi_{\mathbf{k}}{}^{+}=|\,a_{\mathbf{k}}{}^{+}a_{-\mathbf{k}}\,|, \quad (4)$$

$$\tau_1=\begin{vmatrix} 0 & 1 \\ 1 & 0 \end{vmatrix}, \quad \tau_2=\begin{vmatrix} 0 & -i \\ i & 0 \end{vmatrix}, \quad \tau_3=\begin{vmatrix} 1 & 0 \\ 0 & -1 \end{vmatrix}, \quad \tau_4=\begin{vmatrix} 1 & 0 \\ 0 & 1 \end{vmatrix}. \quad (5)$$

The second term in (3) corresponds to the interaction of the electrons with static deviation of the potential of the non-ideal lattice from the periodic potential of the ideal crystal. As will be shown later, we shall not need a concrete expression for $\Delta v(\mathbf{k}'-\mathbf{k})$, and we shall therefore not write it out.

The third term in (3) is the interaction of the electrons with the dynamic vibrations of the atoms:

$$V_n{}^{\alpha}(\mathbf{k}'-\mathbf{k})=\frac{i}{V}(\mathbf{k}'-\mathbf{k})^{\alpha}v_n(\mathbf{k}'-\mathbf{k})\exp\{i(\mathbf{k}'-\mathbf{k})\mathbf{R}_n\}, \quad (6)$$

where V is the volume of the system, v_n is the pseudopotential of the interaction of the electron with the ion, $\mathbf{R}_n = \mathbf{R}_n^0 + \delta\mathbf{R}_n$ is the position of the mass center of the ion in the non-ideal lattice, $\mathbf{R}_n^0$ is the position of the ion in the ideal lattice. The fourth term is the direct Coulomb repulsion of the electrons.

It is assumed that all the interactions that enter in the Hamiltonian (1) have been calculated with allowance for the static screening. A Hamiltonian similar to ours but without allowance for the interaction with the static deviation from the ideal conductivity, and using the phonon representation for ions, was already employed in[10]. The possibility of using such a Hamiltonian with screened interaction is justified in that reference, and will not be discussed here.

To derive equations describing the superconductor properties of an electron-ion system, we shall use the technique of temperature Green's function[6]. To this end, we introduce the following Green's functions describing the behavior of the electron and ion systems:

$$G_{\mathbf{k}\mathbf{k}'}(\tau) = -\langle T_\tau(\psi_{\mathbf{k}}(\tau)\psi_{\mathbf{k}'}{}^{+}(0))\rangle, \quad (7)$$

$$D^{\alpha\beta}_{nn'}(\tau) = -\langle T_\tau(u_n{}^{\alpha}(\tau)u_{n'}{}^{\beta}(0))\rangle. \quad (8)$$

For the spatially homogeneous distribution of the defects the Fourier component of the Green's function (7) can be written, after averaging over these defects, in the form

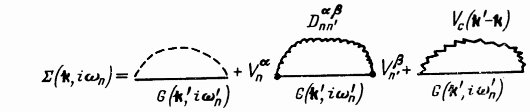
$$G_{\mathbf{k}\mathbf{k}'}(i\omega_n) = G(\mathbf{k},\, i\omega_n)\delta_{\mathbf{k}\mathbf{k}'}. \quad (9)$$

In the Born approximation, accurate to $1/p_F l$, where p_F is the Fermi momentum of the electron and l is the mean free path, the function $G(\mathbf{k}, i\omega_n)$ takes the form[6,8]

$$G^{-1}(\mathbf{k},\, i\omega_n) = G_0{}^{-1}(\mathbf{k},\, i\omega_n) - \Sigma(\mathbf{k},\, i\omega_n), \quad (10)$$

where

$$G_0{}^{-1}(\mathbf{k},\, i\omega_n) = i\omega_n - \varepsilon_{\mathbf{k}}\tau_3. \quad (11)$$



The self-energy part $\Sigma(\mathbf{k}, i\omega_n)$ is determined by the diagrams shown in the figure. This leads us to the following integral equation, which determines the thermodynamic characteristics of the superconductor

$$\Sigma(\mathbf{k}, i\omega_n) = -\sum_{\mathbf{k}'}\overline{|\Delta v(\mathbf{k}'-\mathbf{k})|^2}\tau_3G(\mathbf{k}', i\omega_n)\tau_3 - T\sum_{\omega'}\sum_{\mathbf{k}'}\tau_3G(\mathbf{k}', i\omega_n{}')\tau_3$$
$$\times\Big[\sum_{n,n'}V_n{}^{\alpha}(\mathbf{k}'-\mathbf{k})V_{n'}{}^{\beta}(\mathbf{k}-\mathbf{k}')D^{\alpha\beta}_{nn'}(i\omega_n-i\omega_n{}')+V_c(\mathbf{k}'-\mathbf{k})\Big]. \quad (12)$$

A superior bar denotes averaging over the position of the defect or the disorder. The need for such averaging and its meaning are discussed in detail in[1,2,6], and some examples of such mean values will be considered in the succeeding sections in the calculation of the critical temperature of concrete systems.

For a normal metal at $T > T_c$, the approximation used by us for $\Sigma(\mathbf{k}, i\omega_n)$ leads directly to the result obtained in[6], namely that the analytic continuation of the self-energy part $\Sigma(\mathbf{k}, \omega)$, connected with scattering by the impurities, is of the form

$$\Sigma(\mathbf{k}, \omega) = -i\tau^{-1}\,\mathrm{sign}\,\omega, \quad (13)$$

where

$$\frac{1}{\tau} = \pi n N(0)\int\overline{|\Delta v(\mathbf{k}'-\mathbf{k})|^2}\frac{d\Omega}{4\pi}, \quad (14)$$

n is the impurity concentration N(0) is the density of states of the electrons on the Fermi surface, and Ω is the solid angle made up by the vectors $\mathbf{k}$ and $\mathbf{k}'$. For a superconducting metal, the expression for $\Sigma(\mathbf{k}, i\omega_n)$ in the form (12) signifies, besides neglecting the corrections of order $1/p_F l$, which result from the crossing diagrams, also that there is no spatial correlation between the changes of the energy gap. Allowance for such correlations is essential in the calculation of T_c if the average distance between the impurities is smaller than the correlation length ξ_0. Taking $\xi_0 = 10^{-4}$ cm, we find that the corresponding impurity concentration amounts to a fraction of one per cent, and calculations of their influence at lower concentrations are of no practical interest.

For the function $D^{\alpha\beta}_{nn'}(i\nu)$ we can write the spectral representation

$$D^{\alpha\beta}_{nn'}(i\nu) = \int_0^{\infty}\rho^{\alpha\beta}_{nn'}(\omega')\left[\frac{1}{i\nu-\omega'}-\frac{1}{i\nu+\omega'}\right]d\omega', \quad (15)$$

$$\rho^{\alpha\beta}_{nn'}(\omega) = \frac{1-e^{-\omega/T}}{\mathrm{Sp}\,e^{-H/T}}\sum_{m,m'}e^{-E_m/T}\langle m|u_n{}^{\alpha}|m'\rangle\langle m'|u_{n'}{}^{\beta}|m\rangle, \quad (16)$$

$$H_i|m\rangle = E_m|m\rangle.$$

Using this spectral representation for $D^{\alpha\beta}_{nn'}(i\nu)$, and also the analytic properties of the functions $G(\mathbf{k}, i\omega_n)$, we can go over in Eq. (12) from summation over the discrete frequencies to integration with respect to the complex frequency ω. Then, continuing analytically the functions $G(\mathbf{k}, i\omega_n)$ and $\Sigma(\mathbf{k}, i\omega_n)$ to real frequencies, we can change over to an integral equation for the function $\Sigma(\mathbf{k}, \omega)$. These calculations are perfectly analogous to those given in[8,10], so that we shall write down immediately the resultant integral equation for $\Sigma(\mathbf{k}, \omega)$:

$$\Sigma(\mathbf{k},\omega)=-\sum_{\mathbf{k}'}\overline{|\Delta v(\mathbf{k}'-\mathbf{k})|^2}\tau_3 G(\mathbf{k}',\omega)\tau_3$$

$$-\frac{1}{\pi}\frac{1}{V}\sum_{\mathbf{k}'}\int\limits_{-\infty}^{+\infty}d\omega'\,\mathrm{Im}[\tau_3 G(\mathbf{k}',\omega')\tau_3]\left\{\int\limits_0^\infty d\omega''S(\mathbf{k},\mathbf{k}',\omega'')\right.$$

$$\left.\times\left[\frac{f(-\omega')+N(\omega'')}{\omega-\omega'+\omega''}+\frac{f(\omega')+N(\omega'')}{\omega-\omega'-\omega''}\right]+\frac{1}{2}V_c(\mathbf{k}'-\mathbf{k})\,\mathrm{th}\frac{\omega'}{2T}\right\} \quad (17)$$

where

$$f(\omega)=(e^{\omega/T}+1)^{-1},\quad N(\omega)=(e^{\omega/T}-1)^{-1},$$

$$S(\mathbf{k},\mathbf{k}',\omega)=\frac{1}{N}\sum_{n,n'}\exp\{i(\mathbf{k}'-\mathbf{k})(\mathbf{R}_n-\mathbf{R}_{n'}\}\,V_n{}^\alpha(\mathbf{k}'-\mathbf{k})$$

$$\times V_{n'}{}^\beta(\mathbf{k}-\mathbf{k}')\rho_{nn'}^{\alpha\beta}(\omega). \quad (18)$$

Recognizing that in the summation over k′ the significant region is near the Fermi surface and has a thickness of the order of the Debye energy, we can make the substitution

$$\frac{1}{V}\sum_{\mathbf{k}'}\to N(0)\int\frac{d\Omega}{4\pi}\int d\zeta,$$

where ζ is the deviation of the energy from the Fermi surface. We write $\Sigma(\mathbf{k},\omega)$ and $G(\mathbf{k},\omega)$ in the form

$$\Sigma(\mathbf{k},\omega)=[1-Z(\mathbf{k}\ \ \omega)]\omega\tau_4+Z(\mathbf{k},\omega)\Delta(\mathbf{k},\omega)\tau_1+\chi(\mathbf{k},\omega)\tau_3, \quad (19)$$

$$G(\mathbf{k},\omega)=\frac{\omega Z(\mathbf{k},\omega)\tau_4+\bar{\varepsilon}(\mathbf{k},\omega)\tau_3+Z(\mathbf{k},\omega)\Delta(\mathbf{k},\omega)\tau_1}{\omega^2Z^2(\mathbf{k},\omega)-\bar{\varepsilon}^2(\mathbf{k},\omega)-Z^2(\mathbf{k},\omega)\Delta^2(\mathbf{k},\omega)}, \quad (20)$$

where

$$\bar{\varepsilon}(\mathbf{k},\omega)=\varepsilon_{\mathbf{k}}+\chi(\mathbf{k},\omega),$$

and $\chi(\mathbf{k},\omega)$ are the Hartree-Fock corrections to the particle energy of the results of the interaction with the static potential, $Z(\mathbf{k},\omega)$ is the renormalization due to the interaction with the dynamic oscillations of the ions, and $\Delta(\mathbf{k},\omega)$ is the energy gap in the spectrum of excitations of the superconductor.

Substituting (19) and (20) in (17) and integrating with respect to ζ, we obtain the following integral equations for the energy gap $\Delta(\Omega,\omega)$ and for the renormalization $Z(\Omega,\omega)$:

$$[1-Z(\Omega,\omega)]\omega$$

$$=i\pi N'(0)\int\frac{d\Omega'}{4\pi}\overline{|\Delta v(\mathbf{k}'-\mathbf{k})|^2}\frac{\omega}{[\omega^2-\Delta^2(\Omega',\omega)]^{1/2}}$$

$$+N'(0)\int\limits_0^{\omega_0}d\omega'\int\frac{d\Omega'}{4\pi}\mathrm{Re}\left(\frac{\omega'}{[\omega'^2-\Delta^2(\Omega',\omega')]^{1/2}}\right)$$

$$\times\left\{\int\limits_0^\infty d\omega''S(\mathbf{k},\mathbf{k}',\omega'')[(f(-\omega')+N(\omega''))K_-(\omega,\omega',\omega'')\right. \quad (21)$$

$$\left.+(f(\omega')+N(\omega''))K_-(\omega,-\omega',\omega'')]\right\},$$

$$Z(\Omega,\omega)\Delta(\Omega,\omega)=$$

$$=-i\pi N'(0)\int\frac{d\Omega'}{4\pi}\overline{|\Delta v(\mathbf{k}'-\mathbf{k})|^2}\frac{\Delta(\Omega',\omega)}{[\omega^2-\Delta^2(\Omega',\omega)]^{1/3}}$$

$$+N'(0)\int\limits_0^{\omega_0}d\omega'\int\frac{d\Omega'}{4\pi}\mathrm{Re}\left(\frac{\Delta(\Omega',\omega')}{[\omega'^2-\Delta^2(\Omega',\omega')]^{1/2}}\right).$$

$$\times\left\{\int\limits_0^\infty d\omega''S(\mathbf{k},\mathbf{k}',\omega'')[(f(-\omega')+N(\omega''))K_+(\omega,\omega',\omega'')\right.$$

$$\left.-(f(\omega')+N(\omega''))K_+(\omega,-\omega',\omega'')]-U_c\,\mathrm{th}\frac{\omega'}{2T}\right\}, \quad (22)$$

where

$$K_\pm(\omega,\omega',\omega'')=\frac{1}{\omega'+\omega+\omega''+i\delta}\pm\frac{1}{\omega'-\omega+\omega''-i\delta},$$

$N'(0)$ is the density of states of the electrons, renormalized as a result of the interaction with the static potential. It can be determined by writing the equation for $\chi(\Omega,\omega)$, but in simple metals all the corrections for the crystal field are small and will henceforth be disregarded.

In the derivation of (21) and (22) we have used the fact that in a narrow layer near the Fermi surface, of the order of the Debye energy, $\Delta(\mathbf{k},\omega)$ and $Z(\mathbf{k},\omega)$ do not depend on the modulus of the vector k, but only on its direction. We have also introduced in the usual manner (see[10]), in place of the Coulomb potential $V_c(\mathbf{k}'-\mathbf{k})$, the pseudopotential U_c

$$U_c=\frac{N(0)V_c}{1+N(0)V_c\ln(\varepsilon_F/\omega_0)}.$$

It is seen from (21) and (22) that in the isotropic case, when Δ and Z do not depend on the angle, substitution of the expression for Z from (21) in (22) leads to a cancellation of the terms connected with the static interaction. However, if defects are present in the crystals, the dynamic interaction connected with the function $S(\mathbf{k},\mathbf{k}',\omega)$ also changes. The influence of the anisotropy can be accounted for in complete analogy with[8], but for simplicity we confine ourselves to the case of an isotropic superconductor, and this enables us to separate more clearly the influence of the dynamic properties of the defect on T_c.

In view of the formal similarity of our Eqs. (21) and (22) with the equations of[11,12], we can use the results obtained there and write the expressions for T_c of superconductors with weak coupling in the form

$$T_c=\omega_0\exp\left\{-\frac{1}{\lambda-U_c}\right\} \quad (23)$$

where

$$\lambda=\frac{N(0)(2\pi)^2}{m^2}\int\limits_0^{2k_F}\frac{q\,dq}{k_F{}^2}\int\limits_0^\infty\frac{S(q,\omega)\,d\omega}{\omega} \quad (24)$$

$$S(q,\omega)=\frac{1}{N}\int\limits_{-\infty}^{+\infty}dt\,e^{i\omega t}\sum_{n,n'}\exp\{i\mathbf{q}(\mathbf{R}_n-\mathbf{R}_{n'})\}\,a_n(q).\ a_{n'}(q)\langle\mathbf{q}\mathbf{u}_n(t)\,\mathbf{q}\mathbf{u}_{n'}(0)\rangle. \quad (25)$$

In writing down (24) and (25), we have introduced, in place of the pseudopotential $v_n(g)$, the scattering amplitudes in the Born approximation

$$a_n(q)=\frac{m}{2\pi}v_n(q),$$

where m is the electron mass; we have also rewritten the spectral density $\rho_{nn}^{\alpha\beta}(\omega)$ in terms of the Fourier component of the displacement correlator. Since we confine ourselves to the case of superconductors with weak coupling, we have neglected the quantity $e^{-\omega/T}$ compared with unity, which introduces a small error of the order of T_c/ω_0[9].

For an ideal crystal, our formulas coincide completely with the usual formulas for the electron-phonon coupling constant, obtained in[12], with λ expressed in terms of the density of states of the phonons and the matrix element of the electron-phonon interaction, while the structure factor

$$S(\mathbf{k}'-\mathbf{k}-\mathbf{q})=\frac{1}{N}\sum_{n,n'}\exp\{i(\mathbf{k}'-\mathbf{k}-\mathbf{q})(\mathbf{R}_n-\mathbf{R}_{n'})\}=\Delta(\mathbf{k}'-\mathbf{k}-\mathbf{q})$$

leads to the presence of momentum conservation laws accurate to the reciprocal-lattice vector

$$\mathbf{k}' - \mathbf{k} - \mathbf{q} = \mathbf{K}_n.$$

On the other hand, for a non-ideal crystal, the formulas obtained by us are more general, since they include the changes connected with the density of states of the phonons, as well as the changes of T_c due to structural realignment of the lattice. The change of the structure factor can lead to violation of the momentum conservation laws and to the appearance of diffused scattering of the electrons, something not taken into account in the previously obtained results[12]. Moreover, since the correlation function can be sufficiently well measured with the aid of scattering of slow neutrons, the formulas (23)—(25) obtained by us make it possible, in principle, to estimate more accurately, for a single-component metal, the value of the Coulomb pseudopotential.

3. CHANGE OF CRITICAL TEMPERATURE. INFLUENCE OF IMPURITIES

Using the formulas (23)—(25) obtained in the preceding section, we can calculate the critical-temperature change resulting from the presence of impurities in the crystal. When impurities are added to the crystal, generally speaking, the critical temperature changes as a result of isotropization of the energy gap, of changes in the density of states of the electrons of the Fermi surface, and of the change of the Coulomb pseudopotential. For an exact comparison with the experimental data it is necessary to calculate all these effects. In simple metals, however, all these effects are small[12,21], whereas the change of the lattice dynamics resulting from the appearance of local and quasilocal impurity oscillations may be much stronger[2,4,5]. Therefore, in order to estimate qualitatively the influence of the changes in the lattice dynamics on the magnitude of the critical temperature, we confine ourselves to the simplest assumptions. We consider the free-electron approximation and neglect the influence of the Coulomb pseudopotential. Since the presence of impurities leads to a change of the constant λ in the argument of the exponential, we shall henceforth disregard the change of the pre-exponential factor ω_0.

In first order in the concentration of the impurities, we can write

$$S(q, \omega) = S_0(q, \omega) + \Delta S(q, \omega), \quad \lambda = \lambda_0 + \delta\lambda, \tag{26}$$

where λ_0 is the electron-phonon coupling constant in the ideal crystal, and $\delta\lambda$ are the changes connected with the presence of the impurity

$$\delta\lambda = \frac{N(0)\,(2\pi)^2}{m^2} \int_0^{2k_F} \frac{q\,dq}{k_F^2} \int_0^\infty \frac{\Delta S(q, \omega)}{\omega}\, d\omega. \tag{27}$$

The calculation of the averaged correlation function $S(q, \omega)$ in the presence of impurities was carried out in[4,5], where it was shown that corrections of three types appear in $S(q, \omega)$:

$$\Delta S(q, \omega) = \Delta S_1(q, \omega) + \Delta S_2(q, \omega) + \Delta S_3(q, \omega),$$

where $\Delta S_1(q, \omega)$ is connected with the scattering of the electrons by the modified phonon spectrum, $\Delta S_2(q, \omega)$ with diffuse scattering directly by the impurity atoms, and $\Delta S_3(q, \omega)$ with the interference of the first two corrections. It is important that all these corrections, generally speaking, are of the same order, and therefore the change of T_c following the occurrence of local and quasilocal oscillations in the crystals is not connected with the change of the density of states of the phonons only, as was assumed in[22]. An even greater difference between our results and those of[22] is that in accordance with the calculations of[22] the presence of local and quasilocal oscillations leads to a change of the constant λ regardless of the cause of these oscillations, simply as a result of the change of the density of states of the phonons. In particular, this change would result from the presence in the crystal of oscillations connected with an isotopic impurity, thereby contradicting the existence of the isotopic effect in superconductors. In fact, however, as shown in[4,5], for the isotopic impurity we have

$$\Delta S(q) = \int_0^\infty \frac{\Delta S(q, \omega)}{\omega}\, d\omega = 0\ ,$$

and consequently $\delta\lambda = 0$. Moreover, even if the impurity is not isotopic, and there exists a change in the scattering amplitude and of the force constants, then the value of the impurity mass does not enter at all in the expression for $\Delta S(q)$, and consequently also in $\delta\lambda$.

In the simplest model of a metal with nearest-neighbor interaction $\Delta S(q)$ was calculated in[5] and can be written in the form

$$\Delta S(q) = n\left[\frac{q^2 a_0(q)\,\Delta a(q)}{M\omega_0^2(q)} + \frac{\tau q^2 a_0(q)\, a_1(q)}{M\omega_D^2} + \frac{\tau q^2 a_0^2(q)}{M\omega_D^2}\right] \tag{28}$$

where M is the mass of the ion of the ideal crystal, $\omega_0(q)$ is the spectrum of the oscillations of the ideal crystal, ω_D is the Debye frequency of the ideal crystal, $a_0(q)$ and $a_1(q)$ is the amplitude of scattering of the electron by the main crystal and by the impurity respectively, $\Delta a(q) = a_1(q) - a_0(q)$, τ is the relative change of the force constants, and n is the impurity concentration.

Experimental studies of the Mössbauer effect and of the resistance of metals shows[5] that in metals the change of the scattering amplitudes and of the force constants is small. This explains the experimentally observed fact that the change of T_c following the introduction of the impurities is small, although the impurity itself can lead to an appreciable change of the specific heat of the crystal or of the Mössbauer-effect probability, owing to the considerable difference between the mass of the impurity and the mass of the ions of the host lattice. Using (28), we can calculate $\delta\lambda$ and find the change of T_c resulting from the influence of the impurities; the results are in qualitative agreement with experiment, in particular, T_c increases if the impurity has a larger valence $\Delta a > 0$. It must be recognized, however, that the changes of the electron state density and of the Coulomb pseudopotential are in this case of the same order, and they must be taken into account in order to obtain quantitative agreement with the experimental data.

It should be noted that by writing the expressions for T_c and λ in the form (23)—(25) we can establish a significant correlation between the change of T_c due to the presence of defects in the crystal and the change of the linear coefficients of resistance at high temperatures due to the same defects. Indeed, the resistance of the metal at high temperatures, due to single-phonon scattering, can be written in the form

$$\rho = \eta T \int_0^{2k} q^3\, dq \int_0 \frac{S(q,\omega)\, d\omega}{\omega}, \tag{29}$$

where

$$\eta = \left(\frac{2\pi}{m}\right)^2 \frac{3\pi}{2e^2 v_F{}^2 k_F{}^4}.$$

Using (26), this can be written in the form

$$\rho = \rho_0 + \delta\rho,$$

where

$$\delta\rho = \eta T \int_0^{2k_F} q^3\, dq\, \Delta S(q).$$

Concrete calculations with $\Delta S(q)$ in the form (28) show that there exists a relation

$$\delta\lambda / \lambda_0 \approx \delta\rho / \rho_0. \tag{30}$$

The presence of such a connection between the changes of the constant λ and of the resistance make it possible to measure the change of T_c, even without resorting to the low-temperature technique, using the fact that expression (23) for T_c leads to

$$\frac{\delta T}{T_c{}^0} \approx \frac{\delta\lambda}{\lambda_0} \ln\frac{\omega_0}{T_c{}^0} \approx \frac{\delta\rho}{\rho_0} \ln\frac{\omega_0}{T_c{}^0}.$$

Of course, relation (30) may turn out to be incorrect for such defects that lead to the appearance in $\Delta S(q)$ of a sharp peak at certain values of q, owing to the presence in (29) of the factor q^3, as against q in formula (24). It would therefore be extremely interesting to verify the presence of the connection noted by us between T_c and the resistance experimentally for different defects.

4. SINGLE-COMPONENT METAL. INFLUENCE OF DISORDER ON T_c

As already noted in the Introduction, the greatest change of the critical temperature in comparison with its value in the ideal bulky sample is observed in thin amorphous metal films. This phenomenon is apparently connected with the appreciable change of the lattice dynamics in such a system, and also with a change of the character of the electron-ion interaction—the increase of the contribution of the diffuse scattering of the electrons. Estimates of the change of the critical temperature of superconductors of small dimensions, based on an allowance for changes of only on the phonon spectrum, were presented in[23,24]; they lead to a reasonable qualitative agreement with the experimental data[14,15]. It should be noted that in these calculations the influence of the structural changes on the character of the electron-ion interaction is patently underestimated. In this section we confine ourselves to calculation of the corrections to the critical temperature of a bulky sample, resulting from its structural disordering, while the influence of the finite dimensions of the sample will be considered somewhere else. As in the preceding section, we confine ourselves to the approximation of the isotropic superconductor, and will disregard the influence of the small Coulomb pseudopotential, which is practically independent of the structure of the crystal. Then the correlation function $S(q, \omega)$ can be written in the following form:

$$S(k,\omega) = \frac{a^2(k)}{N} \sum_{n,n'} \exp\{i\mathbf{k}(\mathbf{R}_n{}^0 - \mathbf{R}_{n'}{}^0) \tag{31}$$

$$+ i\mathbf{k}(\delta\mathbf{R}_n - \delta\mathbf{R}_{n'})\}\langle \mathbf{k}\mathbf{u}_n(t)\mathbf{k}\mathbf{u}_{n'}(0)\rangle_\omega,$$

where we have introduced the following notation: $\mathbf{R}_n^0$ is the position of the ion in an ideal lattice and $\delta\mathbf{R}_n$ is the static deviation of the ion from its position in the ideal lattice.

To obtain the corrections to the critical temperature we need to calculate the correlator $\langle u_n^\alpha(t) u_{n'}^\beta(0)\rangle$ for the disordered crystal, and to average $S(q, \omega)$ over the disorder, assuming that the mean-squared deviation of the ion from its position in the ideal lattice, $\overline{\delta R_n^2} = \overline{\delta R^2}$, is specified, with

$$\overline{\delta\mathbf{R}^2 / \mathbf{R}^2} < 1, \quad \overline{\delta\mathbf{R}} = 0.$$

In calculating the displacement correlator we shall use the following form of the ionic Hamiltonian for the disordered lattice, where account is taken of the presence of the effective anharmonicity:

$$H_i = \sum_n \frac{\mathbf{p}_n{}^2}{2M} + \frac{1}{2}\sum_{n,n'} \Phi_{nn'}^{\alpha\beta} u_n{}^\alpha u_{n'}{}^\beta + \frac{1}{2}\sum_{n,n'n''} \Phi_{nn'n''}^{\alpha\beta\gamma}\, \delta R_{n''}^\gamma u_n{}^\alpha u_{n'}{}^\beta, \tag{32}$$

where $\Phi_{nn'}^{\alpha\beta}$ are the force constants of the ideal lattice, and $\Phi_{nn'n''}^{\alpha\beta\gamma}$ are the anharmonicity constants of the ideal lattice. Assuming the deviations $\delta\mathbf{R}$ of the atoms to be small, expanding them in terms of the static displacement waves:

$$\delta\mathbf{R}_n = i \sum_{\mathbf{k}} \mathbf{R}_{\mathbf{k}} \exp\{i\mathbf{k}\mathbf{R}_n{}^0\} \quad \mathbf{R}_{-\mathbf{k}} = -\mathbf{R}_{\mathbf{k}}{}^*, \tag{33}$$

and expanding the dynamic displacements of the ions in terms of plane phonons

$$\mathbf{u}_n = \sum_{\mathbf{q},\lambda} \frac{1}{(NM)^{1/2}} \mathbf{e}_{\mathbf{q}\lambda} Q_{\mathbf{q}\lambda} \exp\{i\mathbf{q}\mathbf{R}_n{}^0\}, \tag{34}$$

where $\mathbf{e}_{q\lambda}$ is the polarization vector of the ions, we can write down, accurate to second order in $\delta\mathbf{R}$, the following expression:

$$S(k,\ \omega) = S_0(k,\ \omega) + \Delta S_1(k,\ \omega) + \Delta S_2(k,\ \omega) + \Delta S_3(k,\ \omega) \tag{35}$$

Here

$$\Delta S_1(k,\omega) = a^2(k) \sum_\lambda \frac{(\mathbf{k}\mathbf{e}_{\mathbf{q}\lambda})^2}{M} [\langle Q_{\mathbf{q}\lambda}(t) Q_{-\mathbf{q}\lambda}(0)\rangle_\omega - \delta(\omega^2 - \omega_{q\lambda}{}^2)],$$

$$\Delta S_2(k,\omega) = 2a^2(k) \sum_{\mathbf{q}'\lambda',\lambda} \frac{(\mathbf{k}\mathbf{e}_{\mathbf{q}\lambda})(\mathbf{k}\mathbf{e}_{\mathbf{q}'\lambda'})}{M} \tag{36}$$

$$\times \mathrm{Re}\, [\mathbf{k}\mathbf{R}^*_{\mathbf{q}+\mathbf{q}'} \langle Q_{\mathbf{q}'\lambda'}(t) Q_{\mathbf{q}\lambda}(0)\rangle_\omega],$$

$$\Delta S_3(k,\omega) = a^2(k) \sum_{\mathbf{q}'\lambda',\mathbf{q}''\lambda''} \frac{(\mathbf{k}\mathbf{e}_{\mathbf{q}'\lambda'})(\mathbf{k}\mathbf{e}_{\mathbf{q}''\lambda''})}{M} \tag{37}$$

$$\times (\mathbf{k}\mathbf{R}^*_{\mathbf{q}+\mathbf{q}'}) (\mathbf{k}\mathbf{R}_{\mathbf{q}+\mathbf{q}'}) \langle Q_{\mathbf{q}'\lambda}(t) Q_{\mathbf{q}''\lambda''}(0)\rangle_\omega. \tag{38}$$

In formulas (36)—(38), the vector q is determined from the condition of momentum conservation

$$\mathbf{k} - \mathbf{q} = \mathbf{K}_n,$$

and the vectors q′ and q″ are arbitrary phonon vectors, over which the summation is carried out. The function ΔS_1 is connected with the scattering of the electrons with the changes of the phonons spectrum, $\Delta S_3(k, \omega)$ is connected with the diffuse scattering by the displacement fluctuations, and ΔS_2 is the interference scattering.

Since the initial Hamiltonian (32) is quadratic in the dynamic displacements of the ions, the calculation of the correlators is best carried out with the equal-time Green's function[25]:

$$D_{\mathbf{q}\lambda\mathbf{q}'\lambda'}(t) = -i\Theta(t)\langle[Q_{\mathbf{q}'\lambda'}(t) Q_{\mathbf{q}\lambda}(0)]\rangle, \tag{39}$$

where the correlators needed for our calculations are connected with the Fourier components $D_{q\lambda q'\lambda'}(\omega)$ by the simple relation

$$\langle Q_{\mathbf{q}'\lambda'}(t)Q_{\mathbf{q}\lambda}(0)\rangle_\omega = -\frac{i}{1-e^{-\omega/T}}[D_{\mathbf{q}'\lambda'\mathbf{q}\lambda}(\omega+i\delta) - D_{\mathbf{q}'\lambda'\mathbf{q}\lambda}(\omega-i\delta)]. \tag{40}$$

The calculation of the Green's functions and of the correlators is given in the Appendix. Substituting the expressions obtained there into (36)—(38) and averaging over $\mathbf{R}_k$, which in the case of a random disorder can be represented in the form

$$\overline{\mathbf{R}_\mathbf{k}{}^*\mathbf{R}_{\mathbf{k}'}} = \overline{|\mathbf{R}_\mathbf{k}|^2}\delta_{\mathbf{k}\,\mathbf{k}'} = N^{-1}\overline{\delta\mathbf{R}^2}\delta_{\mathbf{k}\mathbf{k}'}, \tag{41}$$

$$\overline{\mathbf{R}_\mathbf{k}{}^*\mathbf{R}_{\mathbf{k}'}{}^*} = N^{-1}\overline{\delta\mathbf{R}^2}\delta_{\mathbf{k},\,-\mathbf{k}'}, \tag{42}$$

we obtain a final expression for the coupling constant

$$\lambda = \lambda_0 + \delta\lambda,$$

$$\delta\lambda = \frac{N(0)\,(2\pi)^2}{m^2}\int_0^{q_0}\frac{k\,dk}{2k_F{}^2}a^2(k)\sum_\lambda\frac{(\mathbf{k}\mathbf{e}_{\mathbf{q}\lambda})^2}{M}\int_0^\infty\frac{d\omega^2}{\omega^2}$$

$$\times\left\{\frac{1}{\pi}\frac{\operatorname{Im}\Pi_{\mathbf{q}\lambda}(\omega)}{[\omega^2-\omega_{q\lambda}{}^2-\operatorname{Re}\Pi_{\mathbf{q}\lambda}(\omega)]^2+[\operatorname{Im}\Pi_{\mathbf{q}\lambda}(\omega)]^2}-\delta(\omega^2-\omega_{q\lambda}{}^2)\right\}$$

$$+\frac{N(0)\,(2\pi)^2}{m^2}\int_0^{q_0}\frac{kdk}{2k_F{}^2}a^2(k)\,k^2\overline{\delta\mathbf{R}^2}\frac{1}{N}\sum_{\mathbf{q}'\lambda'}\frac{(\mathbf{k}\mathbf{e}_{\mathbf{q}'\lambda'})^2}{M}\int_0^\infty\frac{d\omega^2}{\omega^2}\delta(\omega^2-\omega_{q\lambda}{}^2). \tag{43}$$

(All the symbols are defined in the Appendix.)

Accurate to second order in $\delta\mathbf{R}$, the interference term $\Delta S_2(k, \omega)$ makes no contribution to the change of λ, owing to the condition (42). Integration with respect to ω in formula (43) is carried out directly with the aid of the method presented in[4,5], and estimates using the Debye spectrum for the phonons show that in this case relation (30) holds between the change of the constants λ and the resistance ρ, and in order of magnitude we have

$$\delta\lambda\,/\,\lambda_0 \approx \mathbf{R}^{-2}\overline{\delta\mathbf{R}^2}, \tag{44}$$

where R is the average interatomic distance.

It should be noted that a much more significant change in the critical temperature should be observed if extended defects are present in the crystal. These, first, lead to the appearance of static deviations of the atoms from their positions in the ideal lattice, and consequently to the appearance of diffuse scattering, and, second, they lead to the occurrence of one-dimensional (or two-dimensional) local and quasilocal oscillations. The influence of these oscillations on the constant λ may turn out to be quite appreciable, for unlike in the case of impurities, the existence of these oscillations is not due to differences between the masses of the defect and the ideal lattice (the latter, as we have verified, does not influence λ). The most effective in this case is the interaction with the "heavy" low-frequency phonons[23,26] that appear in such systems.

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APPENDIX

We calculate the correlators $\langle Q_{q'\lambda'}(t)Q_{q\lambda}(0)\rangle_0$ for a disordered crystal. To this end, we rewrite the Hamiltonian (32) in terms of the variables Q_q:

$$H_i = \frac{1}{2}\sum_{\mathbf{q}\lambda}[\dot{Q}_{\mathbf{q}\lambda}\dot{Q}_{-\mathbf{q}\lambda} + (\omega_{q\lambda}{}^0)^2Q_{\mathbf{q}\lambda}Q_{-\mathbf{q}\lambda}] + \sum_{\mathbf{q}\lambda,\ \mathbf{q}'\lambda'}V(\mathbf{q}\lambda, \mathbf{q}'\lambda')Q_{\mathbf{q}\lambda}Q_{\mathbf{q}'\lambda'}, \tag{A.1}$$

where

$$V(\mathbf{q}\lambda, \mathbf{q}'\lambda') = \frac{i}{2}\sum_\mathbf{k}\sum_{n,\,n'n''}\Phi_{nn'n''}^{\alpha\beta\gamma}\mathbf{R}_k^\gamma\exp\{i\mathbf{k}\mathbf{R}_{n''}^0\}$$

$$\times\frac{\mathbf{e}_{\mathbf{q}\lambda}{}^\alpha}{(NM)^{1/2}}\exp\{i\mathbf{q}\mathbf{R}_n{}^0\}\frac{\mathbf{e}_{\mathbf{q}'\lambda'}^\beta}{(NM)^{1/2}}\exp\{i\mathbf{q}'\mathbf{R}_{n'}\}. \tag{A.2}$$

The exact expression for $V(q\lambda, q'\lambda')$ is very complicated, but for our purposes we can use the simplest approximation for $V(\mathbf{q}\lambda, \mathbf{q}'\lambda')$[2]:

$$V(\mathbf{q}\lambda, \mathbf{q}'\lambda') = \gamma\omega_{\mathbf{q}\lambda}\omega_{\mathbf{q}'\lambda'}(\mathbf{q}'-\mathbf{q})\mathbf{R}_{\mathbf{q}'-\mathbf{q}}, \tag{A.3}$$

where γ is the Gruneisen constant.

The Fourier component of the Green's function $D_{q\lambda q'\lambda'}(\omega)$ (39) is determined in accordance with the Hamiltonian (A.1) by the following expression:

$$D_{\mathbf{q}\lambda\mathbf{q}'\lambda'}(\omega) = D_{\mathbf{q}\lambda}{}^0(\omega) + \sum_{\mathbf{q}''\lambda''}D_{\mathbf{q}\lambda}{}^0(\omega)V(-\mathbf{q}\lambda, \mathbf{q}''\lambda'')D_{\mathbf{q}''\lambda''\mathbf{q}'\lambda'}(\omega), \tag{A.4}$$

where

$$D_{\mathbf{q}\lambda}{}^0(\omega) = 1\,/\,(\omega^2-\omega_{q\lambda}{}^2), \tag{A.5}$$

and with accuracy sufficient for our purposes we obtain from (A.4)

$$D_{-\mathbf{q}'\lambda',\,\mathbf{q}\lambda}(\omega) = D_{\mathbf{q}'\lambda}^0(\omega)V(\mathbf{q}'\lambda', -\mathbf{q}\lambda)D_{\mathbf{q}\lambda}{}^0(\omega), \tag{A.6}$$

$$D_{\mathbf{q}\lambda,\,-\mathbf{q}\lambda}(\omega) = [\omega^2-\omega_{\mathbf{q}\lambda}{}^2-\Pi_{\mathbf{q}\lambda}(\omega)]^{-1}, \tag{A.7}$$

where

$$\Pi_{\mathbf{q}\lambda}(\omega) = \int\sum_{q''\lambda'}V(-\mathbf{q}\lambda, \mathbf{q}''\lambda'')V(-\mathbf{q}''\lambda'', \mathbf{q}\lambda)\delta(\omega'^2-\omega_{q''\lambda''})\frac{d\omega'}{\omega^2-\omega'^2}. \tag{A.8}$$

On the basis of formulas (A.6)—(A.8) it is easy to determine the correlators needed by us, using the relation (40).

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