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ELECTRICAL RESISTIVITY FOR DISLOCATION

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The object of the paper is to find the electrical resistivity in a crystal containing a dislocation. The scattering of an electron by an exponential dislocation potential has been calculated by using the eikonal and first Born approximations. The theoretical curve of the increase in electrical resistivity in copper has been calculated at different temperatures. The present results are found to be physically meaningful.

ЭЛЕКТРИЧЕСКОЕ УДЕЛЬНОЕ СОПРОТИВЛЕНИЕ ПРИ НАЛИЧИИ ДИСЛОКАЦИЙ

Цель статьи состоит в определении электрического удельного сопротивления кристалла с дислокациями. Приведен расчет рассеяния электрона на экспоненциальном потенциале дислокации при использовании эйконального и борновского приближений. Кроме того, рассчитана теоретическая кривая роста электрического удельного сопротивления меди для различных температур. Обнаружено, что полученные результаты имеют глубокий физический смысл.

I. INTRODUCTION

Interest has been focused recently on the calculations of the electrical and the thermal resistivity due to dislocations from the scattering of conduction electrons [1—3].

The effect of plastic deformation on residual resistivity has been demonstrated. The resistivity of a deformed specimen is greater than that of a well-annealed single crystal [4]. An appreciable fraction of this increase (approximately 10%) [5] in resistivity is presumably the contribution of scattering of the conduction electrons. This contribution of electrical resistivity to dislocation has been calculated by many workers [1—4], [6—10] by the use of different methods (Born approximation, partial wave method, phase shift approach, perturbation theory, umklapp process) and with different types of pseudopotential [4, 6—10]. It is now accepted that the

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use of low order perturbation theory (i.e. Born or Born type theory) is not suitable for the scattering of conduction electrons by dislocation [4, 11, 12]. It has been suggested by Brown [1—3] that one should use a nonperturbative approach. In the present work we have used the eikonal method to study the problem. The eikonal method is a nonperturbative one and is used in various scattering problems in different branches of physics. In the eikonal approximation, the incident wave is replaced by the eikonal wave function, which takes into account the distortion of the incident wave due to the presence of a perturbing potential. This approximation is found to be valid for the exponential, the Yukawa, the Coulomb potential and for a screened Coulomb potential [13]. Therefore we expect in the present case the use of this method may be helpful in determining the contribution to resistivity due to the presence of dislocations in metals. An ionic type of dislocation potential is generally used for the study of this type of problem. Koehler has used the ionic type of dislocation potential for studying electrical resistivity. We have used the ionic type of exponential dislocation potential.

II. SOLUTION OF THE PROBLEM

The Schrödinger equation for the conduction electron is given by

$$(\mathcal{H}_0+\mathcal{V})\,\Psi(\mathbf{r})=E\Psi(\mathbf{r})\,, \qquad (1)$$

where $\mathcal{H}_0$ is the unperturbed Hamiltonian, $\mathcal{V}$ the scattering potential as seen by the conduction electron and E is the total energy of the system. In the framework of the eikonal approximation one expresses the wave function of the particle in the form

$$\Psi(\mathbf{r})=e^{i\mathbf{K}\cdot\mathbf{r}}\,\eta(\mathbf{r})\,, \qquad (2)$$

where $\eta(\mathbf{r})$ varies slowly over the particle wavelength. This constraint necessarily implies that the incident energy greatly exceeds the magnitude of the potentional energy and the particle wave length is much smaller than the potential width. With these assumptions, one can obtain the particle wave function [13] as

$$\Psi(\mathbf{r})=e^{i\mathbf{K}\cdot\mathbf{r}}\,e^{-i/\theta}\exp\left(\int_{-\infty}^{z}\mathcal{V}(\mathbf{b}+\hat{k}z')\,dz'\right), \qquad (3)$$

wirth $\mathbf{r}=\mathbf{b}+\hat{k}z$. Here $\mathbf{b}$ is the impact parameter perpendicular to the wave vector $\mathbf{k}$, which is along the z-axis.

Now the scattering amplitude in the atomic unit is given by

$$f(\Theta)=-\frac{1}{2\pi}\int d\mathbf{r}\,e^{i\mathbf{k}_f\cdot\mathbf{r}}\mathcal{V}(\mathbf{r})e^{i\mathbf{k}_f}\,e^{-i/\theta}\exp\left(\int_{-\infty}^{z}\mathcal{V}(\mathbf{b}+kz')\,dz'\right), \qquad (4)$$

where $\mathbf{k}_i$ and $\mathbf{k}_f$ are the incident and final momenta of the system.

Assuming the momentum transfer vector $\mathbf{k}_i-\mathbf{k}_f$ to be perpendicular to $\mathbf{k}_i$ we can perform the integration over z immediately. Thus we have

$$f(\Theta)=-\frac{\mathbf{k}_i}{2\pi i}\int e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{b}}\,e^{-i/\theta}\exp\left(\int_{-\infty}^{\infty}\mathcal{V}(\mathbf{b}+\mathbf{k}z')dz'\right)d^2b\,, \qquad (5)$$

where $d^2b=b^2db\,d\varphi$. The eikonal approximation due to the above assumption is supposed to hold good for the small scattering angle. As the potential has azimuthal symmetry we may also perform the integration over Φ. Thus we have

$$f(\Theta)=-iK\int_0^{\infty}J_0(qb)\,[e^{i\chi(b)}-1]\,b\,db\,, \qquad (6)$$

where $\chi(b)$ is the phase shift function and can be expressed as

$$\chi(b)=\frac{K}{2E}\int_{-\infty}^{\infty}\mathcal{V}(\mathbf{r})\,dz\,, \qquad (7)$$

where the position vector $\mathbf{r}$ has the magnitude $(b^2+z^2)^{1/2}$.

The energy $E(T)$ of the electrons can be obtained from the Fermi–Dirac distribution of energy [14] as

$$E(T)=E_F\left[1-\frac{\pi^2}{12}\left(\frac{KT}{E_F}\right)^2\right], \qquad (8)$$

where E_F is the Fermi energy, K is Boltzmann's constant and T is the absolute temperature.

The momentum k can be expressed as

$$k^2=2m^*.E(T)\,, \qquad (9)$$

where m^* is the effective mass of the electron.

We have chosen the ionic type of dislocation potential as

$$\mathcal{V}(\mathbf{r})=-V_0(1+|r|)\exp(-|r|)\,. \qquad (10)$$

Employing the equation (10) in equation (7) and after performing integration over dz one obtains

$$\chi(b)=-\frac{KV_0b}{E(T)}[2k_1(b)+b^2k_0(b)]\,, \qquad (11)$$

where $k_0(b)$ and $k_1(b)$ are modified Bessel functions of the second kind of order zero and one.

With the help of equations (9) and (11), the scattering amplitude $f(\Theta)$ in equation (6) can be evaluated numerically for different temperatures.

We have also computed the scattering amplitude of the electrons in a crystal by using the first Born approximation. The scattering amplitude in the first Born approximation takes the form

$$f^B(\Theta)=\frac{1}{2\pi}\int_0^\infty e^{i\mathbf{q}\cdot\mathbf{r}}V(\mathbf{r})\,d\mathbf{r}\,, \tag{12}$$

where $\mathbf{q}=\mathbf{k}_i-\mathbf{k}_f$. Making use of equation (10) in equation (6) one gets

$$f^B(\Theta)=\frac{1}{2\pi}[I_1+I_2]\,, \tag{13}$$

where

$$I_1=\int \exp(i\mathbf{q}.\mathbf{r})\exp(-r)\,d\mathbf{r} \tag{14a}$$

and

$$I_2=\int r\exp(i\mathbf{q}.\mathbf{r})\exp(-r)\,d\mathbf{r}\,. \tag{14b}$$

The integration over $d\mathbf{r}$ can be easily carried out and equations (14) reduce to

$$f^B(\Theta)=\frac{16\,V_0}{(q^2+1)^3}\,. \tag{15}$$

The electrical resistivity ϱ due to the dislocation can be related to the momentum cross section, i.e. the diffusion cross section can be obtained as [15]

$$\varrho\alpha 2\pi\int_0^\infty |f(\Theta)|^2(1-\cos\Theta)\sin\Theta\,d\Theta\,. \tag{16}$$

The electrical resistivity has been calculated for copper at different temperatures from equation (16). The value of E_F in expression (8) is taken to be 5 eV.

III. RESULTS AND DISCUSSIONS

We have to perform numerically the one dimensional integration over db to obtain the scattering amplitude (Eq. 6). The presence of a Bessel function in the expression of the scattering amplitude in equation (6) makes the integrand oscillating. One has to be very careful at the time of integration. We have found the zeros of the Bessel function and the integration has been performed between the two consecutive zeros using the Gauss–Lagendre quadrature points and the integration proceeds similarly. The convergence of the results has been tested.

The magnitude of the first Born momentum transfer cross section, which is proportional to electrical resistivity, is greater (10^{10}) than that of the eikonal method. In the given interval of temperature the Born results are almost constant. In Fig. 1 we have plotted the ratio of the change of electrical resistivity (i.e. $(\varrho_T-\varrho_{10})/\varrho_{10}$) against temperature. The rations of the eikonal value are much greater than those of FBA. One can conclude from the Born results that the electrical resistivity does not depend on temperature. The results of the eikonal method do necessarily suggest that the temperature has a small but not negligible effect on electrical resistivity by the dislocation mechanism.

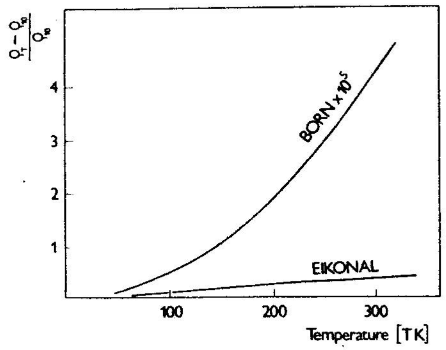

Fig. 1.

It is well known that the first Born approximation is not at all valid in the temperature region considered in the present investigation. It has also been noticed by earlier workers that the first Born approximation always predicts the higher values. It is interesting to note that if one expands the exponential function containing the phase shift function $\chi(b)$ in the expression of the scattering amplitude $f(\Theta)$ (Eg. (6)), the first term gives the first Born approximation. Therefore the eikonal method is an improvement over the first Born approximation. Our variation of electrical resistivity due to the scattering is about 5%. Therefore the effect of the scattering on the electrical resistivity due to dislocation is small. This is in confirmity with the earlier prediction [5]. Recently Brown [16—18] has calculated the scattering phase shifts and has predicted resonances and subsequently the effect of the conduction electron scattering by dislocation on the electrical resistivity may be greater than that suggested here. This warrants further investigations.

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REFERENCES

[1] Brown, R. A.: J. Phys. F *7* (1977), L 155.
[2] Brown, R. A.: J. Phys. F *7* (1977), 1269.
[3] Brown, R. A.: J. Phys. F *7* (1977), 1283.
[4] Sosin, A., Koehler, J. S.: Phys. Rev. *101* (1956), 972.
[5] Hull, R. D.: *Introduction to Dislocation.* Pergamon. New York 1975.
[6] Harrison, W. A.: *Pseudopotentials in the Theory of Metals.* Bengamin 1966.
[7] Koehler, J. S.: Phys. Rev. *75* (1949), 109.
[8] Dexter, D. S.: Phys. Rev. *85* (1952), 939.
[9] Dexter, D. S.: Phys. Rev. *86* (1952), 770.
[10] Stehle, H., Seeger, A.: Z. Phys. *146* (1956), 242.
[11] Seeger, A., Bross, H.: Z. Naturf. *15 a* (1960), 663.
[12] Blatt, J. F.: *Solid State Physics,* Vol. 4. Ed. by F. Seitz and Turnbull. Academic Press, New York 1972.
[13] Glauber, R. J.: *Lectures in Theoretical Physics.* Ed. by W. E. Britten et al. Interscience Publ. New York 1972.
[14] Busch, G., Schade, H.: *Lectures on Solid State Physics.* Pergamon, Oxford 1975.
[15] Nabarro, R. R. N.: *Theory of Crystal Dislocation.* Pergamon, Oxford 1967.
[16] Brown, R. A.: J. Phys. F *8* (1978), 825.
[17] Brown, R. A.: J. Phys. F *8* (1978), 1467.
[18] Brown, R. A.: J. Phys. F *9* (1979), L 241.

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