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On the Changes of Electrical Properties in Cold-Worked Metal*

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Synopsis

The increase in electrical resistance of metals due to cold-work was discussed taking into account the perturbing potential due to the edge dislocation caused by the said mechanical treatment. The method of calculating the electric conductivity was based on Peterson and Nordheim's assumption for the perturbing potential. An estimation of thermoelectric power due to cold-work was made from the same point of view. A criticism was given for the theories by Koehler and Mackenzie-Sondheimer. The results obtained showed somewhat smaller value than the results of the above-mentioned authors.

I. Introduction

It has been found experimentally that, when a metal undergoes a severe cold-work, its electrical resistance and thermo-electric power will change several per cent.¹⁾ According to a recent experiment by Rutter and Reekie²⁾ in copper and aluminium, these increments of resistance $\Delta\rho$ consist of two parts, namely, temperature independency $\Delta\rho_0$ (residual resistance), and temperature dependency $\Delta\rho_T$.

$$\Delta\rho = \Delta\rho_0 + \Delta\rho_T \quad (1)$$

Let us consider only the part $\Delta\rho_0$. The causes of this residual resistance may be considered to be due to the formation of dislocations, lattice defects and cracks and changes in grain boundaries in the metals by cold-work. This problem was treated by Koehler³⁾ and Mackenzie and Sondheimer⁴⁾ by assuming that the important change during cold-work would be caused by the formation of a large number of edge dislocations. The method of treatment by Mackenzie and Sond-

* The 645th report of the Research Institute for Iron, Steel and Other Metals.

- (1) E. Schmid and W. Boas, "*Kristallplastizität*" (Verlag Julius Springer p. 214.
- (2) J. W. Rutter and J. Reekie, *Phys. Rev.* **78** (1950), 70.
- (3) J. S. Koehler, *Phys. Rev.* **75** (1949) 106.
- (4) J. K. Mackenzie and E. H. Sondheimer, *Phys. Rev.* **77** (1950) 264.

heimer was based on the assumption of rigid sphere ion, but they did not take into account the field due to the change in the charge distribution of valence electron, which would neutralize the potential field of each lattice ion in distorted crystal, and hence, it may be expected that the actual change of electrical resistance due to the introduction of dislocation will actually become several tenth smaller in value, than the Mackenzie and Sondheimer's result. Recently Landauer⁵⁾ estimated this value by using a method which took into account the conduction band structure.

Here, using the Peterson and Nordheim's assumption which takes into account⁶⁾ the change in distribution of valence electron, we could obtain theoretically the increments of resistance and thermo-electric power, the results being shown in the following pages. Since the increment of resistance due to the edge dislocation introduced by cold-working depends on the number of dislocations per unit area N , the numerical result will be controlled by the estimated values of N .

II. Evaluation of $\Delta\rho_0$

The metallic crystal lattice will undergo a kind of distortion when it suffers cold-working. For the calculation of electric conductivity of the distorted metallic crystal, the same model as those of reference (3)–(5) is used. If the wave function of conduction electron with wave vector \mathbf{k} in distorted crystal is denoted by $\Psi_{\mathbf{k}}(\mathbf{r})$ then it satisfies the following Schrödinger's equation :

$$-\frac{\hbar^2}{2m} \nabla^2 \Psi_{\mathbf{k}}(\mathbf{r}) + (V_0 + \Delta V_i + \Delta V_\rho) \Psi_{\mathbf{k}}(\mathbf{r}) = E_{\mathbf{k}} \Psi_{\mathbf{k}}(\mathbf{r}) \quad (2)$$

where V_0 is the periodic potential in undistorted crystal and $\Delta V = \Delta V_i + \Delta V_\rho$ is the perturbing potential in distorted crystal. ΔV_i is the perturbing potential due to the displacement of lattice ion from its equilibrium position and ΔV_ρ is that due to the change in charge density of conduction electron, which must be obtained in self-consistent way with $\Psi_{\mathbf{k}}(\mathbf{r})$.⁷⁾

Now, according to the consideration of Peterson and Nordheim, in metallic case, the charge density of conduction electron in each unit cell of distorted crystal is so distributed as to cancel the charge of one positive ion, and the volume of the cell changes by $\Omega = \Omega_0(1 + \text{div } \mathbf{u})$ due to the displacement \mathbf{u} of lattice point, so it is assumed that this charge density will be represented approximately by $\rho = \rho_0(1 + \text{div } \mathbf{u})^{-1}$, where Ω_0 and ρ_0 are the Volume of unit cell and the mean charge density per unit volume in undistorted crystal, respectively. If the wave function of conduction electron in distorted crystal is denoted by $U_{\mathbf{a}} \exp(i\mathbf{k}\mathbf{r})$, then ρ is proportional to $|U_{\mathbf{a}}|^2$: consequently, $U_{\mathbf{a}}$ is given approximately by

(5) R. Landauer, Phys. Rev. **82** (1951) 520.

(6) E. L. Peterson and L. W. Nordheim, Phys. Rev. **51** (1937) 335.

(7) J. Bardeen, Phys. Rev. **52** (1937) 688.

$$U_{a\infty} (1 + \text{div } \mathbf{u})^{-1/2} \cong 1 - \frac{1}{2} \text{div } \mathbf{u}. \quad (3)$$

Multiplying the both side of wave equation above mentioned by $\Psi_{\mathbf{k}}^*(\mathbf{r})$, integrating over the whole volume of crystal and using the orthogonality of $\Psi_{\mathbf{k}}$, the matrix element is obtained as follows :

$$(\mathbf{k}' | \Delta V | \mathbf{k}) = - \frac{\hbar^2}{2m} \frac{1}{V} \int \rho^{1/2} e^{-i\mathbf{k}'\mathbf{r}} \nabla^2 [\rho^{1/2} e^{i\mathbf{k}\mathbf{r}}] d\mathbf{r}. \quad (4)$$

Hereafter, quite the same treatment as Mackenzie and Sondheimer is made : the conductivity in each direction is given by the following integral forms :

$$\begin{cases} \sigma_x = \sigma_0 + \frac{3N\hbar\epsilon n\Lambda^2\tau}{8\pi^2 m^2 V^{2/3}} \int_0^\pi d\theta \int_0^{2\pi} d\phi \int_0^{2\pi} d\phi' K_x \frac{k^4 K_y^2}{(k_x^2 + k_y^2)^2} \sin\theta \cos\phi, \\ \sigma_y = \sigma_0 + \frac{3N\hbar\epsilon n\Lambda^2\tau}{8\pi^2 m^2 V^{2/3}} \int_0^\pi d\theta \int_0^{2\pi} d\phi \int_0^{2\pi} d\phi' K_y \frac{k^4 k_y^2}{(k_x^2 + k_y^2)^2} \sin\theta \sin\phi, \\ \sigma_z = \sigma_0 = n\epsilon^2\tau/m, \end{cases} \quad (5)$$

where m , ϵ , n , τ , V and Λ are the mass of electron, the charge of electron, the number of electrons per unit volume, the relaxation time, the total crystal volume and the quantities which is determined by elastic properties, respectively, and \mathbf{K} is used instead of $\mathbf{k}' - \mathbf{k}$. The coordinates θ and ϕ are the polar and azimuth angle of wave vector \mathbf{k} . Based on eq. (5) and assuming Matthiessen's rule, the mean increment of resistance for all crystallographic direction is given by

$$\Delta\rho_0 = \frac{N\hbar\lambda^2}{5k_0\epsilon^2 V^{2/3}} \left(\frac{2-\nu}{\nu-1} \right)^2, \quad (6)$$

where λ , ν and k_0 are the unit slip distance, reciprocal of Poisson's ratio and the absolute value of wave vector on the Fermi-surface, respectively.

For copper, the relative change of resistance at room temperature is obtained by putting proper numerical values in parameters of eq. (6). The result is given by

$$\Delta\rho_0/\rho = 0.5 \times 10^{-5} N. \quad (7)$$

Since the increment of resistance due to edge dislocation depends upon the number of dislocations per unit area, N , the numerical result is governed by the estimated value of N . Based on the estimation of this number in severely cold-worked material by Koehler, let N be 2.9×10^{11} per cm^2 , then the expected change of resistance becomes 0.014%, which is exceedingly small as compared with an experimental result by Rutter and Reckie. Now, the accuracy of the value of N estimated by Koehler on the energy stored during the work-hardening is somewhat questionable, as the method of estimation was based on the elastic continuum theory. If the result of present theory is correct, one must introduce as a value of N much larger

value than that previously given.

On the other hand, if the value of N estimated by Koehler is correct, the induced dislocation is not responsible for the changes of resistance due to the cold work, and the cause may be reduced to the change in grain boundary or origination of other kinds of lattice imperfections and so forth during the cold-working. Using the value obtained by the elastic theory, we can see that eq. (7) shows only one eighth of the value of Mackenzie and Sondheimer. The theoretical and experimental results are summarized in Table I and Table II.

Table I. Theoretical results of increment of resistance in cold-worked copper, $\Delta\rho_0/\rho$, at temperature 20°C.

	Koehler	Mackenzie and Sondheimer	Landauer	Present method
$\Delta\rho_0/\rho$	$2.72 \times 10^{-14}N$ (0.79%)	$4 \times 10^{-15}N$ (0.116%)	$5 \times 10^{-14}N$ (1.45%)	$0.5 \times 10^{-15}N$ (0.014%)

Table II. Experimental results of increment of resistance in cold-worked metals and the change of thermo-electric power at room temperature

Increment of resistance ($\Delta\rho_0/\rho$)		Thermo-electric power ($\Delta s/s$)	
Schmid and Boas ⁽¹⁾ (severely cold-worked)		Rutter and Reekie ⁽²⁾ (50% reduction)	
Cu :	2%	Cu :	$\Delta\rho_0=0.4\%$ $\Delta\rho_\tau=0.9\%$
AG :	3%		
Ni :	8%		
Mo :	18%	Al :	$\Delta\phi_0=0.2\%$ $\Delta\rho_\tau=0.5\%$
W :	50%		
			Borelius and Thiele*
			Cu : +1.2% 1.6%
			Au : +1.4%
			Ag : +8%

* G. Borelius, Ann. d. Physik, **60** 381 (1919)

J. Thiele, Ann. d. Physik **72** 549 (1925).

It is also to be remarked here that the adopted perturbing potential was based upon the elastic continuum theory and will not reproduce the correct form of potential in the vicinity of the dislocation centre. The adopted potential overestimates the deviation from periodic potential and hence, the change of resistance will become slightly less than that given by eq. (6).

It is also remarked here that the screw dislocation is of no importance in the change of resistance by this theory, because the displacement around the screw dislocation is given by⁽⁸⁾ $u_x=0$, $u_y=0$ and $u_z=(b/2\pi) \tan^{-1}(y/x)$, where b is the z -component of the slip vector. Hence, in this case, the relation $div \mathbf{u}=0$ holds, and consequently no volume change will occur: then the change of resistance will not be caused by the dislocation of this type.

III. Thermo-electric power

(8) W. T. Read and W. Schockey, Phys Rev. **78** 275, Appendix D (1950).

With the same model as in the previous section, we can formulate the change of thermo-electric power produced by cold-work for the case in which the temperature gradient lies along the x -direction.

Thermo-electric power is given by Mott as follows: ⁹⁾

$$S_i = \frac{\pi^2}{3} \frac{kT}{\epsilon} \left\{ \frac{\partial (\log \sigma_i(E))}{\partial E} \right\}_{E=\zeta} \quad (i = x, y \text{ and } z), \quad (8)$$

where k is Boltzmann constant. Assuming the Matthiessen's rule ($\rho_i = \rho_0 + \Delta\rho_i$), the conductivities in each direction is given by

$$\sigma_i(E) = \sigma_0(E) - [\sigma_0(E)]^2 / \sigma_i'(E), \quad \sigma_z = \sigma_0. \quad (9)$$

Since $\rho_0 \gg \Delta\rho_i$, that is $\sigma_0 \ll \sigma_i'$, it turns out to be

$$S \simeq S_0 + \frac{\pi^2}{3} \frac{kT}{\epsilon} \left[\frac{\partial}{\partial E} \left(\frac{\sigma_0(E)}{\sigma_i'(E)} \right) \right]_{E=\zeta},$$

where S_0 is the thermo-electric power in a metal with no lattice defect. According to Mott's treatment, the form $\sigma_0(E) = C \times E^x$ is assumed to hold in the vicinity of Fermi energy. Hence, the real conductivity $\sigma_0(\zeta)$ is expressed by $\sigma_0(\zeta) = C \times \zeta^x$ (ζ is Fermi energy and C is a constant). From these relations, we obtain the change of thermo-electric power as follows:

$$\Delta S_i \equiv S_0 - S_i = \frac{\pi^2 kT}{3\epsilon} \left\{ \frac{x}{\rho} \frac{\Delta\rho_i}{\rho_0} - \frac{\Delta\rho_i}{\rho_0^2} \left[\frac{\partial}{\partial E} \sigma_i'(E) \right]_{E=\zeta} \right\}. \quad (16)$$

Since $\rho_0 \gg \Delta\rho_i$, the second term will be negligibly small compared with the first term, and then we will obtain the relation

$$\Delta S_i / S_0 \simeq \Delta\rho_i / \rho_0. \quad (17)$$

It is expected from the present theory that the relative change in absolute thermo-electric power due to cold-work is equal to the relative change in electric resistance. As the Table II shows, the relative change in thermo-electric power in copper does not coincide exactly with that in electric resistance. These two data were, however, referred to different samples by different authors. A new measurement of both quantities in respect to the same sample is desirable from the present point of view.

(9) N. F. Mott and H. Jones "The Theory of the Properties of Metals and Alloys" (Oxford University Press, New York, (1936) p. 310.