cipitate oriented along certain crystallographic directions. Bozorth, Tilden, and Williams have suggested that the presence of such an oriented precipitate in cobalt ferrite may explain their results obtained by heat treatment of this material in a magnetic field. More recently Williams, Nesbitt, and Heidenreich[4] have found more direct experimental evidence for this idea by the use of torque curves and electron diffraction. It is possible that this view could be confirmed by a study of the diffuse scattering of x-rays from single crystals of these substances.

[4] Williams, Nesbitt, and Heidenreich (to be published).

ACKNOWLEDGMENTS

The author is indebted to R. T. Walsh for technical assistance, to R. D. Heidenreich, F. J. Schnettler, E. A. Nesbitt, H. J. Williams, and several others for interesting discussions of this problem, to R. M. Bozorth and A. J. Williams for heat treatment of samples, and to Brookhaven National Laboratory for the provision of neutron diffraction facilities.

PHYSICAL REVIEW VOLUME 102, NUMBER 3 MAY 1, 1956

Resistivity of Interstitial Atoms and Vacancies in Copper*

A. W. OVERHAUSER AND R. L. GORMAN†
Department of Physics, Cornell University, Ithaca, New York
(Received January 30, 1956)

The residual resistivity associated with the presence of interstitial atoms or vacancies in copper is studied with particular attention devoted to the scattering of conduction electrons resulting from lattice distortions surrounding the imperfections. For interstitials this scattering is found to be an order of magnitude larger than that from the defect itself. For vacancies it is smaller but still important. Interference between scattering from the defect and the surrounding lattice distortion is computed and found to be very small. The calculated resistivity associated with one atomic percent of interstitial atoms is 10.5 μohm cm. The corresponding value for vacancies is 1.5 μohm cm. Using nominal values for the energy of formation of these defects, the stored energy to resistivity ratios associated with interstitials, vacancies, and interstitial-vacancy pairs are 1.4, 3.4, and 1.6 cal/g per μohm cm, respectively.

I. INTRODUCTION

THE increase in the residual resistivity of copper arising from the presence of interstitial atoms or vacancies has been studied by several workers. Dexter[1] approximated the scattering potential associated with the imperfections by a shielded Coulomb interaction, $(e^2/r)\exp(-\mu r)$, and computed electronic transition matrix elements by the Born approximation. The shielding constant μ was adjusted so that the computation yielded experimental values when applied to the analogous problem of substitutional impurities having adjacent atomic number. The estimated resistivity change for 1% of interstitials was 0.6 μohm cm, and for 1% of vacancies was 0.4μ ohm cm. Dexter also investigated the scattering arising from the elastic distortion of the lattice surrounding the imperfections. He concluded that such effects probably contribute less than 10% to the scattering cross sections for both types of imperfection. In making this estimate the discrete positive ion lattice was approximated by a smeared-out positively charged continuum.

In treating the same problem, Jongenburger[2] used for the scattering potential of a lattice vacancy a shielded Coulomb interaction with constants adjusted so as to fit as closely as possible the Hartree field of a copper atom. The scattering cross section was computed by the partial wave method. Jongenburger obtained a resistivity of 1.8 μohm cm per atomic percent of vacancies. (Jongenburger gives a value of 1.3, but apparently a numerical error was made in converting phase shifts to resistivity.) He estimated the contribution arising from elastic distortions by comparing the displacement of nearest neighbors of the vacancy with the root mean square atomic displacements caused by lattice vibrations, which are responsible for the temperature dependent electrical resistivity. A value of 0.04 μohm cm was obtained. Jongenburger[3] has also estimated by the same method the extra resistivity caused by interstitial atoms. For the contribution of the interstitial scattering potential alone a value of 1 to 2 μohm cm was found, and an additional 3.5 μohm cm resulting from nearest neighbor displacements was obtained.

More recently, Blatt[4] has computed the resistivity associated with one atomic percent of interstitial atoms, assuming that the scattering effects of elastic strains can be neglected. An appropriately screened Hartree

* This work was supported in part by the Office of Naval Research.
† Present address: Gulf Research and Development Company, Pittsburgh, Pennsylvania.
[1] D. L. Dexter, Phys. Rev. **87**, 768 (1952).
[2] P. Jongenburger, Appl. Sci. Research **B4**, 237 (1953).
[3] P. Jongenburger, Nature **175**, 545 (1955).
[4] F. J. Blatt, Phys. Rev. **99**, 1708 (1955).

field for a Cu^+ ion was used in conjunction with a partial wave analysis of the scattering. The calculation yielded 1.4 μohm cm. The method was applied also to the problem of substitutional impurities having adjacent atomic number. The results were generally larger, by about a factor of two, than experimentally determined resistivities. Blatt concluded that systematic errors (arising perhaps from the use of the free electron approximation) were being made, and suggested that the computed resistivity associated with either interstitial atoms or vacancies should be divided by a factor of two. This conclusion indicates that the contribution of one atomic percent of interstitial defects or vacancy defects to the resistivity is about 0.7 and 0.9 μohm cm, respectively.

The purpose of the present paper is to examine in greater detail the contribution of the elastic displacement of atoms near the imperfections to the increase in the residual resistivity. We shall find that such effects are not so small as has been supposed. In fact, for the case of interstitial atoms, we shall find that the scattering from the strained regions of the lattice is an order of magnitude larger than the scattering from the interstitial atoms themselves. The treatment of the problem to be given has several virtues: the free electron approximation is not made, and unknown parameters such as the effective mass and the electron-lattice interaction constant are eliminated by comparing the final formula with the theoretical resistivity associated with lattice vibrations, in which the unknown parameters appear identically. The experimental lattice resistivity is then used, due account being taken of the role of umklapp processes, to obtain the residual resistivity resulting from the strained lattice.

II. SCATTERING CROSS SECTION OF INTERSTITIAL STRAINS

In treating the interaction between the conduction electrons and the lattice distortion we shall make use of the rigid-ion model,[5] so as to be specific. We could employ instead the deformable-ion model, but the results will not depend upon the particular model chosen so long as the same approach is used in computing the scattering associated with lattice vibrations.

Let $U(\mathbf{r}-\mathbf{L})$ be the effective potential energy of an electron arising from the atom located at the lattice point $\mathbf{L}$ of the crystal. The wave functions of the conduction electrons for the undistorted lattice will be Bloch waves,

$$\psi_k = u_k e^{i\mathbf{k}\cdot\mathbf{r}}/N^{\frac{1}{2}},$$

where N is the number of atoms in the lattice. If an atom is displaced from its normal position, the perturbation is

$$U(\mathbf{r}-\mathbf{L}-\mathbf{u}_L)-U(\mathbf{r}-\mathbf{L})\approx-\mathbf{u}_L\cdot\nabla U(\mathbf{r}-\mathbf{L}),$$

where $\mathbf{u}_L$ is the displacement vector of the atom. The total scattering potential is, then,

$$V=-\textstyle\sum_L \mathbf{u}_L\cdot\nabla U(\mathbf{r}-\mathbf{L}). \tag{1}$$

The matrix element for the scattering of an electron from ψ_k to $\psi_{k'}$ is

$$V_{kk'}=-N^{-1}\textstyle\sum_L \mathbf{u}_L\cdot\int u_{k'}{}^* u_k e^{-i\mathbf{q}\cdot\mathbf{r}}\nabla U(\mathbf{r}-\mathbf{L})d\tau,$$

where $\mathbf{q}=\mathbf{k}'-\mathbf{k}$. This expression can be written

$$V_{kk'}=-N^{-1}\textstyle\sum_L \mathbf{u}_L\cdot e^{-i\mathbf{q}\cdot\mathbf{L}}\int u_{k'}{}^* u_k e^{-i\mathbf{q}\cdot(\mathbf{r}-\mathbf{L})}\nabla U(\mathbf{r}-\mathbf{L})d\tau.$$

The integral extends over the entire crystal, but it has contributions only from the lattice cell $\mathbf{L}$, since $U(\mathbf{r}-\mathbf{L})$ is zero outside of the cell. The integral is independent of $\mathbf{L}$ and, when evaluated approximately,[5] yields $iC\mathbf{q}$, so that

$$V_{kk'}=-iCN^{-1}\textstyle\sum_L \mathbf{q}\cdot\mathbf{u}_L e^{-i\mathbf{q}\cdot\mathbf{L}}, \tag{2}$$

where C, the electron-lattice interaction constant, generally has a magnitude of several electron volts (and is negative for the rigid-ion model).

The differential scattering cross section, $\sigma(\mathbf{k},\mathbf{k}')$, for scattering from the state whose wave vector is $\mathbf{k}$ to states in the solid angle $d\Omega(\mathbf{k}')$, is given by

$$\sigma(\mathbf{k},\mathbf{k}')=\frac{m^2|V_{kk'}|^2}{4\pi^2\hbar^4}=\gamma A, \tag{3}$$

where $\gamma=m^2C^2/4\pi^2N^2\hbar^4$ and

$$A=|\textstyle\sum_L \mathbf{q}\cdot\mathbf{u}_L e^{-i\mathbf{q}\cdot\mathbf{L}}|^2. \tag{4}$$

We must now calculate A for the set of lattice displacements $\mathbf{u}_L$ associated with an interstitial configuration.

Huntington[6] has considered in detail the elastic strains around an interstitial atom in copper for two types of interstitial configuration. We shall assume that the configuration of lowest energy is the one for which the interstitial atom is located at the body-centered position of a cubic cell, since the calculations yield essentially equal energies for the two configurations. The displacement of the atoms of the lattice from their normal positions were chosen as follows:

$$\begin{aligned}&\mathbf{u}_L=\epsilon\mathbf{L}, \text{ for nearest neighbors only,}\\ &\mathbf{u}_L=ga^3\mathbf{L}/L^3, \text{ for all other atoms.}\end{aligned} \tag{5}$$

The values of ϵ and g were determined by minimizing the energy associated with the elastic strains, and were found to be 0.21 and 0.04, respectively. The lattice constant is a. The displacement of second-nearest neighbors is probably not given very well by (5) since, as Huntington has pointed out, the displacement of the nearest neighbors actually reduces the outward pressure

[5] See, for example, A. H. Wilson, *The Theory of Metals* (Cambridge University Press, Cambridge, 1953), Chap. 9.

[6] H. B. Huntington, Phys. Rev. **91**, 1092 (1953); Acta Metallurgica **2**, 554 (1954).

on the second-nearest neighbors. However, the inward pressure exerted by the third-nearest neighbors is reduced by their displacement. Consequently, the magnitude of the second-nearest neighbor displacement probably lies between 0 and the value given by (5). We shall calculate the scattering cross section for both of these limiting cases.

Unfortunately it is very difficult to evaluate the sum occurring in Eq. (4) without approximation. We shall treat the problem by calculating the following cross sections: σ_1, arising from nearest neighbor displacements only; σ_2, arising from second-nearest neighbor displacements only; σ_{3+}, arising from all other displacements; and $\sigma_{1,2}$, $\sigma_{1,3+}$, $\sigma_{2,3+}$, the contributions to the total cross section associated with the interference terms. These latter terms, of course, may be negative or positive.

The six nearest neighbors are at a distance $b=\frac{1}{2}a$ from the interstitial atom and lie along the x,y,z axes passing through the interstitial site. The contribution to A, Eq. (4), from these neighbors is

$$A_1=4\epsilon^2b^2(\textstyle\sum_i q_i \sin bq_i)^2, \quad (i=x,y,z). \tag{6}$$

The corresponding cross section σ_1 is proportional to A_1, and therefore depends not only on the scattering angle but also on the orientation of the scattering event with respect to the crystallographic axes. This latter dependence can be eliminated by averaging A_1 over all orientations of the crystal axes. The maximum argument of the sine functions in (6) is approximately $3\pi/2$. In performing the averaging process it is convenient to approximate $\sin x$ as follows:

$$\sin x \approx \alpha_1 x+\alpha_2 x^3+\alpha_3 x^5, \tag{7}$$

where α_1, α_2, and α_3 are determined by minimizing the difference squared between $\sin x$ and the right-hand side of (7) throughout the interval $(0,3\pi/2)$. The appropriate values are

$$\alpha_1=0.8992, \quad \alpha_2=-0.1228, \quad \alpha_3=0.00335.$$

When this approximation is used, A_1 can be averaged easily over all orientations of the crystal axes. The calculation yields

$$A_1'=4\epsilon^2(\beta_1q^4+\beta_2q^6+\beta_3q^8+\beta_4q^{10}+\beta_5q^{12}), \tag{8}$$

where

$$\beta_1=\alpha_1^2b^4,$$
$$\beta_2=(6/5)\alpha_1\alpha_2b^6,$$
$$\beta_3=[(41/105)\alpha_2^2+(6/7)\alpha_1\alpha_3]b^8,$$
$$\beta_4=(46/77)\alpha_2\alpha_3b^{10},$$
$$\beta_5=(241/1001)\alpha_3^2b^{12}.$$

If Eq. (8) is inserted into Eq. (3), the resulting expression for the (partial) cross section depends only on the scattering angle θ, since

$$q=2k_0 \sin\tfrac{1}{2}\theta, \tag{9}$$

where k_0 is the wave number associated with the Fermi surface:

$$k_0a=(12\pi^2)^{1/3}=4.9109.$$

The appropriate average cross section that is needed in calculating the resistivity is

$$\sigma=\int \sigma(\theta)(1-\cos\theta)d\Omega. \tag{10}$$

Consequently,

$$\sigma_1=\int_0^\pi \gamma A_1'(1-\cos\theta)2\pi \sin\theta d\theta.$$

This expression can be evaluated readily, and yields

$$\sigma_1=344\epsilon^2\gamma. \tag{11}$$

There are eight second-nearest neighbors at a distance $\sqrt{3}b$ from the interstitial. Because this distance is so large, the (almost exact) method applied above to nearest neighbors is too cumbersome. We shall evaluate the sum which occurs in the expression for A_2 by replacing it with an integral, corresponding to a uniform distribution of the eight atoms over a spherical surface of radius $\sqrt{3}b$.

$$\textstyle\sum_2 \mathbf{q}\cdot\mathbf{u}_L e^{-i\mathbf{q}\cdot\mathbf{L}} \longrightarrow (2ga^3/\pi L^3)\int qL\cos\theta e^{-qL\cos\theta}d\Omega.$$

One finds, then,

$$A_2=(64^2g^2/27)[\cos\sqrt{3}bq-(\sqrt{3}bq)^{-1}\sin\sqrt{3}bq]^2.$$

Using Eq. (10), the corresponding average cross section is

$$\sigma_2=753g^2\gamma. \tag{12}$$

There are 24 third-nearest neighbors, 30 fourth-nearest neighbors, etc. We shall assume that it is justified to treat the scattering from the remaining region of the lattice as though it were a continuum. The appropriate terms in the summation, Eq. (4), can be evaluated as follows:

$$\textstyle\sum_{3+} \mathbf{q}\cdot\mathbf{u}_L e^{-i\mathbf{q}\cdot\mathbf{L}} \longrightarrow 4g\int_{r_0}^\infty\int q\cos\theta e^{-iqL\cos\theta}d\Omega dL,$$

where the lower limit, r_0, of the radial integration is the radius of a sphere of volume equal to 14 atomic volumes.

$$(4\pi/3)r_0^3=14a^3/4.$$

The integrations yield

$$A_{3+}=256\pi^2g^2(qr_0)^{-2}\sin^2(qr_0).$$

The cross section associated with this term is

$$\sigma_{3+}=385g^2\gamma. \tag{13}$$

We must consider next the inteference or cross terms of (4) that arise from our decomposition of the sum-

mation into three parts. The first such term is

$$A_{1,2}=-\frac{256\epsilon g}{3\sqrt{3}}(\textstyle\sum_i q_i b\,\sin q_i b)\left(\cos\sqrt{3}bq-\frac{\sin\sqrt{3}bq}{\sqrt{3}bq}\right).$$

This expression must be averaged over all orientations of the crystal axes. The following integral occurs for each of the three terms in the summation.

$$\tfrac{1}{2}\int qb\cos\theta\,\sin(qb\cos\theta)\,\sin\theta d\theta=-\cos bq+(bq)^{-1}\sin bq.$$

Consequently, the average value of $A_{1,2}$ is

$$A_{1,2}'=\frac{256\epsilon g}{\sqrt{3}}\left(\cos\sqrt{3}bq-\frac{\sin\sqrt{3}bq}{\sqrt{3}bq}\right)\left(\cos bq-\frac{\sin bq}{bq}\right).$$

Using Eq. (10), as before, to determine the average cross section, we find

$$\sigma_{1,2}=-449\epsilon g\gamma. \tag{14}$$

The calculation of the inteference term associated with nearest neighbor scattering and third and further neighbor scattering proceeds similarly.

$$A_{1,3+}'=192\pi\epsilon g\left(\cos bq-\frac{\sin bq}{bq}\right)\frac{\sin qr_0}{qr_0}.$$

The average cross section is

$$\sigma_{1,3+}=53\epsilon g\gamma. \tag{15}$$

Finally, the interference term associated with second-nearest neighbor scattering and all further neighbors yields

$$A_{2,3+}=\frac{2048\pi g^2}{3\sqrt{3}}\left(\cos\sqrt{3}bq-\frac{\sin\sqrt{3}bq}{\sqrt{3}bq}\right)\frac{\sin qr_0}{qr_0}, \tag{16}$$

and

$$\sigma_{2,3+}=249g^2\gamma.$$

The total effective cross section is the sum of the six terms, (11) to (16). Using Huntington's values for ϵ and g, quoted above, we find

$$\sigma=14.1\gamma.$$

If we assume that second-interest neighbors are not displaced, then we must sum only (11), (13), and (15). This sum yields

$$\sigma=16.2\gamma.$$

Since the second-nearest neighbor displacement probably has a value between these two extremes, we shall adopt the following intermediate value for the effective cross section:

$$\sigma=15\gamma. \tag{17}$$

It is of interest that the major contribution to this cross section arises from the nearest neighbor displacements alone. In fact σ_1, Eq. (11), has a value 15γ; the remaining five terms are individually much smaller and sum to zero.

III. RESISTIVITY OF INTERSTITIAL STRAINS

We shall evaluate next the residual resistivity associated with the elastic strains caused by one atomic percent of interstitial atoms. The resistivity is given by

$$\rho_0=\hbar k_0\sigma/100e^2, \tag{18}$$

where the effective cross section σ has been found to be

$$\sigma=15m^2C^2/4\pi^2N^2\hbar^4. \tag{19}$$

The resistivity arising from scattering by lattice vibrations in the temperature region above half the Debye temperature θ is[5]

$$\rho_l=\frac{3\pi m^2C^2T}{4\mu e^2\hbar\kappa\theta^2}, \tag{20}$$

where μ is the mass density of the metal. The theoretical formula (20) does not take into account the contribution of umklapp processes to the lattice resistivity. Consequently, we must equate ρ_l to only the fraction f of the experimental resistivity that can be attributed to normal scattering processes:

$$\rho_l=f\rho_{\text{exp}}. \tag{21}$$

Combining Eqs. (18) to (21), we find

$$\rho_0=15f\left(\frac{\mu k_0\kappa\theta^2}{300\pi^3\hbar^2N^2T}\right)\rho_{\text{exp}}. \tag{22}$$

It should be noted that the effective mass m and the electron-lattice interaction constant cancel out and do not appear in (22). The numerical factor in the brackets of this equation has a value 0.767, with $\theta=315°$K and $T=293°$K. The experimental resistivity of pure copper at 20°C is 1.673 μohm cm.

We have only to determine the factor f. Bardeen[7] has studied the relative contribution of normal and umklapp processes to the resistivity of monovalent metals. His results are contained in the integral, Eq. (51), of his paper. This integral evaluated over the interval $(0,2^{-2/3})$ is associated with normal scattering processes, whereas the value for the interval $(2^{-2/3},1)$ is associated with umklapp processes. The integrations yield the following value for copper:

$$f=0.50.$$

The residual resistivity is, therefore,

$$\rho_0=9.6\ \mu\text{ohm cm}.$$

IV. RESISTIVITY OF VACANCY STRAINS

We shall treat the scattering from the strain field about a vacancy in a manner similar to that used above

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

for interstitials. The displacement of the twelve nearest neighbors of a vacancy has been estimated by Huntington and Seitz[8] and is described by the relation

$$\mathbf{u}=\lambda\mathbf{L}.$$

The parameter λ depends to some extent on the ion core repulsive law that is used. For exponential repulsion, Huntington and Seitz found a value, $\lambda=-0.025$. The displacements of further neighbors were not estimated. We have seen for the interstitial case, however, that almost the entire scattering is associated with nearest neighbor displacements, and this feature will undoubtedly obtain for vacancies also. Therefore, we shall evaluate only this one contribution to the cross section. When one uses the method applied to second-nearest neighbors of interstitials, Eq. (4) becomes

$$A=144\lambda^2[\cos\sqrt{2}bq-(\sqrt{2}bq)^{-1}\sin\sqrt{2}bq]^2.$$

Using Eq. (10), the corresponding average cross section is

$$\sigma=1200\lambda^2\gamma=0.75\gamma.$$

The residual resistivity associated with the strains resulting from one atomic percent of vacancies is, therefore,

$$\rho_0=0.5\ \mu\text{ohm cm}.$$

V. INTERFERENCE BETWEEN DEFECT AND STRAIN SCATTERING

In order to obtain a value for the resistivity associated with an imperfection, we must add the scattering effects arising from the interstitial atom itself (or vacancy) and from the strained region of the lattice. The question of importance here is the magnitude of the interference term. The treatments of Jongenburger[2] and Blatt[4] employ a partial wave method. Only the S, P, and D waves contribute significantly to the scattering. Consequently, the angular dependence of the scattered wave can be written

$$h(\theta)=e^{i\delta_0}\sin\delta_0+3e^{i\delta_1}\sin\delta_1\cos\theta+5e^{i\delta_2}\sin\delta_2(3\cos^2\theta-1)/2,$$

where δ_0, δ_1, and δ_2 are the S, P, and D phase shifts. Similarly, the angular dependence of the wave scattered from the nearest neighbors of an interstitial can be written

$$h'(\theta)=K[\cos bq-(bq)^{-1}\sin bq],$$

where K is a real, positive constant (if C is negative). The contribution of the interference term to the effective scattering cross section will be proportional to

$$I=\int_0^\pi h'(h+h^*)(1-\cos\theta)\sin\theta d\theta. \qquad (23)$$

This integral can be evaluated readily and yields

$$I=K(-0.717\sin2\delta_0-0.521\sin2\delta_1+1.778\sin2\delta_2).$$

Using Blatt's[4] phase shifts for interstitial scattering, we find $I=0.058K$.

This interference term must be compared with the corresponding squared terms for scattering by the defect,

$$J=2\sum_{l=0}^{2}[(2l+1)\sin^2\delta_l-2l\sin\delta_l\sin\delta_{l-1}\cos(\delta_l-\delta_{l-1})], \qquad (24)$$

and nearest-neighbor displacement scattering,

$$J'=0.70K^2.$$

Using Blatt's phase shifts, we find $J=0.78$. Since J'/J must be about $9.6/0.7=14$, it follows that $K\sim4$. Therefore, $I/J'\sim0.02$, a value which indicates that the interference term contributes a resistivity of only $+0.2$ μohm cm. One should not be surprised that the interference term is so small since the phases of both scattered waves oscillate in sign as a function of scattering angle. Two alternative sets of phase shifts derived by Blatt using different scattering potentials yield -0.2 and $+0.6$ μohm cm for the interference term, indicating that the relative smallness of this term is a feature of the interstitial scattering phenomenon and does not depend on detailed assumptions.

We shall calculate now the interference term associated with vacancy scattering by the same method. We have, now,

$$h'(\theta)=-K[\cos\sqrt{2}bq-(\sqrt{2}bq)^{-1}\sin\sqrt{2}bq],$$

where K is an appropriate real, positive constant. The sign of $h'(\theta)$ is opposite to that for the interstitial case since the nearest neighbor displacements are inward for vacancies. The evaluation of the integral (23) yields

$$I=-K(1.120\sin2\delta_0-2.564\sin2\delta_1+0.546\sin2\delta_2).$$

Using Jongenburger's[2] phase shifts for vacancy scattering, we find $I=0.114$. The corresponding squared term for scattering from the defect is given by Eq. (24), using Jongenburger's phase shifts, and yields $J=0.92$. The squared term for scattering from nearest neighbors yields $J'=1.33K^2$. Since J'/J must be about $0.5/0.9=0.56$, it follows that $K\sim0.6$. The contribution of the interference term to the resistivity is therefore $+0.1$ μohm cm. An alternative set of phase shifts given by Jongenburger yields an interference term of 0.0 μohm cm. One observes that the relative smallness of the interference term obtains also for vacancy scattering.

VI. RESISTIVITY OF INTERSTITIALS AND VACANCIES

The contributions to the residual resistivity of interstitial atoms and vacancies are summarized in Table I.

[8] H. B. Huntington and F. Seitz, Phys. Rev. 61, 315 (1942).

TABLE I. Contributions to the residual resistivity of interstitial atoms and vacancies in Cu. The units are μohm cm per atomic percent of the imperfection.

	Interstitials	Vacancies
Defect scattering	0.7	0.9
Strain scattering	9.6	0.5
Interference term	0.2	0.1
Total resistivity	10.5	1.5

TABLE II. Stored energy and resistivity values of interstitials and vacancies in Cu. The ratios of stored energy to resistivity are given in cal/g per μohm cm.

	Energy of formation (ev)	Resistivity per percent (μohm cm)	$\left(\frac{\text{Stored energy}}{\text{resistivity}}\right)$
Interstitials	4	10.5	1.4
Vacancies	1.4	1.5	3.4
Int.-vac. pairs	5.4	12	1.6

It should be apparent that the accuracy of calculations of this type is necessarily limited, and it is difficult to estimate limits of error for the foregoing results. The displacements of atoms surrounding the imperfections are not known accurately. Fortunately, for the interstitial case, in which such effects play a very important role, the problem has received careful study.[6] The method we have used to evaluate the scattering arising from such displacements appears to be satisfactory. We have also estimated this scattering by treating all but the nearest neighbors in the continuum approximation. The result differed only slightly from that derived here, indicating again the major role played by nearest neighbor displacements and suggesting that little would be gained by treating third-nearest and further neighbors individually.

The rigid-ion model which we used to describe the electron-lattice interaction is not without objection, especially since Eq. (2) is only the first term in a power series in q, and therefore is not accurate for large scattering angles. However, as has been indicated previously, the same expression was used to calculate the high-temperature resistivity, with which the strain scattering was compared, so that any errors arising from the weakness of Eq. (2) tend to cancel.

VII. EXPERIMENTAL CONSIDERATIONS

Interstitials or vacancies can be produced in metals by irradiation with fast particles, plastic deformation, or quenching from high temperatures. In any particular case, it is very difficult to identify the type of defects that are produced or are involved in a subsequent annealing process. One of the authors[9] has emphasized the importance of measuring simultaneously two physical properties attributable to the imperfections, since the ratio of two specific property changes will probably differ according to the nature of the imperfection. Once such a property ratio has been measured or calculated with sufficient precision, it can be used as a tentative means of identification.

With regard to point imperfections in metals of the type we have been considering, the ratio of stored energy to resistivity is perhaps the most fundamental quantity of interest. Huntington[6] has estimated the energy of formation of an interstitial atom in Cu to be about 4 ev. The energy of formation of a vacancy is probably 1.4 ev, since the energy of self-diffusion is 2.1 ev and the energy of vacancy motion is presumed to be 0.7 ev according to the quenching experiments of Kauffman and Koehler.[10] The ratios of stored energy to resistivity that result from these values are presented in Table II.

Simultaneous measurements of stored energy and resistivity have been carried out for two annealing stages of irradiated copper in the temperature interval between -140°C and $+20$°C. The ratio of stored energy to resistivity was observed to be 1.7 cal/g per μohm cm for both annealing stages. Annealing kinetics[11] of the higher temperature stage (~ -30°C) has been observed to be bimolecular, so as to suggest interstitial-vacancy annihilation for the mechanism. Other reasonable interpretations,[12] however, have been proposed. The ratios of stored energy to resistivity that were computed in the present study provide strong evidence in favor of a hypothesis involving interstitial-vacancy annihilation. A mechanism involving only the disappearance of vacancies seems to be ruled out.

[9] A. W. Overhauser, Phys. Rev. **94**, 1551 (1954).

[10] J. W. Kauffman and J. S. Koehler, Phys. Rev. **97**, 555 (1955).

[11] A. W. Overhauser, Phys. Rev. **90**, 393 (1953).

[12] For a recent survey, see J. W. Glen, Advances in Phys. **4**, 381 (1955).