A Theoretical Estimate of the Effect of Radiation on the Elastic Constants of Simple Metals*

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Interstitial atoms and vacancies play an important role in the theory of solids and of radiation damage. It is difficult to separate and measure unambiguously these lattice disturbances in metals. It is suggested that measurements of changes in elastic constants may be appropriate in such investigations.

An approximate theoretical treatment is given of the change in elastic constants of simple metals caused by the presence of a given small fraction of interstitial atoms and vacancies. The elastic coefficients are calculated from atomic interaction potentials (a simple exponential function for copper and a Morse function for sodium) with relaxation effects taken into account. The presence of a small fraction of interstitials and vacancies results in large increases in the elastic coefficients of copper. Lattice vacancies alone were found to decrease the elastic coefficients, the change being essentially a bulk effect. Consequently, increases in the elastic moduli measure primarily the fraction of interstitial atoms. In sodium, large relaxation occurs around an interstitial and this atomic readjustment reduces the effect of the interstitial to the magnitude of a bulk effect.

It is concluded that the theoretically predicted effects should be easily observable in copper or similar metals, provided thermal annealing is prevented. Changes in elastic constants, therefore, may serve as a useful tool for distinguishing between interstitial atoms and lattice vacancies.

I. INTRODUCTION

RADIATION damage may be described briefly as the result of atomic displacements caused by the passage of neutrons or fast charged particles through the material.[1] Many physical properties are drastically changed by the radiation. Our understanding of these effects is still rather rudimentary for two reasons: first, it is by no means clear just what sort of disturbances are left behind in the lattice and, second, the theories which relate atomic displacements to physical properties are themselves poorly developed.

For the purposes of the present study, radiation damage is pictured as the result of the presence of interstitial atoms and vacancies which have been produced by the high energy incident particles. On an atomic scale this must be the primary result of knocking the atoms about within the lattice. If the lattice disturbances cluster, however, either during irradiation or subsequently (by annealing, for example), it may be more profitable to think of radiation damage as akin to cold work or thermal spikes. It is quite likely that differences between radiation damage and cold work in metals, which have been observed experimentally,[2,3] are the result of the presence of interstitials. Such high energies are required for the formation of interstitials in such a substance as copper[4] that their production thermally or even by cold work is most unlikely. They are easily produced, however, by direct knock-ons.

It is clear that it is important to find out whether interstitials exist, in fact, in a close-packed crystalline lattice. The most convenient and best understood physical properties, such as electrical and thermal conductivity of metals, are not well suited to such an investigation since both interstitials and vacancies are scattering centers. It would be very difficult to separate and measure unambiguously the two types of disturbances.

A simple physical argument indicates that elastic constants may be quite sensitive to the presence of interstitial atoms. In general, a bulk property is not expected to be changed appreciably by the displacement of a relatively small percentage of atoms. In close packed metallic substances, however, the elastic constants are determined primarily by the repulsive interactions of the closed ion shells. This potential is of an exponential nature and varies extremely rapidly with interatomic distance. As the interaction distance is shortened, for example by creating an interstitial, the energy of the system increases sharply on the repulsive side of the potential curve. The creation of vacancies by removal of atoms results essentially in the destruction of some normal interactions. Thus, one expects the influence of the interstitials to outweigh heavily the effect of the vacancies.

The main purpose of this paper is to describe some theoretical calculations that have been carried out in an attempt to arrive at a quantitative estimate of the effect of radiation on the elastic coefficients of simple metals. In addition to yielding information concerning interstitials and vacancies, the elastic properties themselves are of interest as influenced by lattice disturbances. It is well known[1,2,5] that many mechanical properties of materials are appreciably changed by irradiation. Mechanical properties, however, are not understood well enough, except in the range of perfect elasticity, to permit a theoretical study of radiation effects. The elastic constants of metals, however, are

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[1] For recent declassified articles on radiation damage in solids see F. Seitz, Disc. Faraday Soc. No. 5, 271 (1949); J. C. Slater, J. Appl. Phys. 22, 237 (1951).

[2] Martin, Austerman, Eggleston, McGee, and Tarpinian, Phys. Rev. 81, 664 (1951).

[3] Eggleston, Bowen, and Kropschot, paper given at Chicago meeting of AIP, October 24, 1951.

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

[5] T. H. Blewitt and R. R. Coltman, Phys. Rev. 82, 769 (1951).

sufficiently well understood theoretically to make it profitable to carry out some calculations concerning the effect of radiation on elastic properties.

II. THE PHYSICAL MODEL

As stated above, changes in physical properties caused by irradiation are pictured as the result of random displacement of atoms. A perfect lattice is assumed in which radiation creates lattice vacancies and interstitial atoms. These disturbances will be preserved in their metastable positions provided the specimen is kept at a sufficiently low temperature to prevent annealing. The number of interstitials and vacancies will be assumed to be small enough so that interaction between the distrubances may be neglected. The problem is then to calculate the elastic coefficients of a crystal lattice containing a given small fraction of interstitials and vacancies.

Two characteristic systems will be investigated. One is the close-packed face-centered cubic lattice in which primarily the closed-shell repulsive interactions determine the elastic constants.[6] This description is suitable for the noble metals and the calculations will be carried out for copper. It will be assumed that the interstitial lodges in the geometrically favorable position, namely, in the body-centered position of the face centered unit cube. The second system is that typified by the alkali metals, namely the body-centered cubic. The calculations will be carried out for sodium. In this system both attractive and repulsive interactions must be taken into account.[6] Again, it will be assumed that the interstitial lodges at the geometrically favorable position, namely, in the center of the face of the body-centered unit cube. The calculations will be carried out for the undistorted lattice first. Relaxation around the lattice disturbances is calculated and discussed in Sec. VI.

The elastic coefficients of a homogeneous material are calculable if the atomic interactions are known as a function of the distance of separation of the atoms. A radiation damaged material is, however, locally inhomogeneous. It is very difficult to take proper account of this inhomogeneity. In the present approximation, therefore, the real material was replaced by an approximately equivalent homogeneous material in which the interactions ascribable to the lattice disturbances are smeared over the whole crystal. Thus, the geometry of the original lattice is retained but the potential energy of the system is modified according to the number of contacts formed and broken by the creation of interstitials and vacancies.

It is evident that quite drastic approximations have been made in order to carry out the calculations with a reasonable amount of labor. It will be seen from later sections that the results are quite clear-cut and the present approximation is considered adequate in indicating the direction and the order of magnitude of the changes in elastic coefficients to be expected from "frozen in" radiation damage.

III. MATHEMATICAL FORMALISM

The elastic coefficients of a crystal are given by the second derivatives of the elastic potential energy per unit volume with respect to the strains. Fuchs[6] discusses the derivation of these equations and further details may be found in unclassified reports by the writer.[7] Only the final working equations will be given here. It has been found that summation over nearest neighbors is sufficient for the face-centered cubic lattice, while nearest and next nearest neighbors must be taken into account in the body-centered cubic system.[6,7]

The final working equations are:

Face centered cubic, nearest neighbors,

$$\begin{aligned} A &= r_e^2(d^2U/dr^2)_{r_e} + 7r_e(dU/dr)_{r_e} \\ 2B &= r_e^2(d^2U/dr^2)_{r_e} + 3r_e(dU/dr)_{r_e} \\ K &= 2C/\Omega_0 = (24/9\sqrt{2}r_e)(d^2U/dr^2)_{r_e}, \end{aligned} \tag{1}$$

where Ω_0 = volume per atom $= \delta^3/4$, and r_e = interatomic distance $= \delta/\sqrt{2}$.

Body-centered cubic,

$$\begin{array}{lll} & \text{Nearest neighbors} & \text{Next nearest neighbors} \\ A = & \dfrac{16}{3} r_e \left(\dfrac{dU}{dr}\right)_{r_e} & + \dfrac{4}{\sqrt{3}} r_e \left(\dfrac{dU}{dr}\right)_{2r_e/\sqrt{3}} + \dfrac{8}{3} r_e^2 \left(\dfrac{d^2U}{dr^2}\right)_{2r_e/\sqrt{3}} \\ 2B = & \dfrac{16}{9} r_e \left(\dfrac{dU}{dr}\right)_{r_e} + \dfrac{8}{9} r_e^2 \left(\dfrac{d^2U}{dr^2}\right)_{r_e} & + \dfrac{4}{\sqrt{3}} r_e \left(\dfrac{dU}{dr}\right)_{2r_e/\sqrt{3}} \\ K = & \dfrac{2C}{\Omega_0} = \dfrac{\sqrt{3}}{r_e^2}\left(\dfrac{dU}{dr}\right)_{r_e} + \dfrac{2}{\sqrt{3}}\dfrac{1}{r_e}\left(\dfrac{d^2U}{dr^2}\right)_{r_e} & + \dfrac{3}{2}\dfrac{1}{r_e^2}\left(\dfrac{dU}{dr}\right)_{2r_e/\sqrt{3}} + \dfrac{2}{\sqrt{3}}\dfrac{1}{r_e}\left(\dfrac{d^2U}{dr^2}\right)_{2r_e/\sqrt{3}} \end{array} \tag{2}$$

where Ω_0 = volume per atom $= \delta^3/2$, r_e = interatomic distance $= \sqrt{3}\delta/2$, $U(r)$ = potential energy per atom, $A = (c_{11} - c_{12})\Omega_0$, $2B = c_{44}\Omega_0$, $2C = K = \frac{1}{3}(c_{11} + 2c_{12})\Omega_0$, c_{ij} = elastic coefficients in dynes/cm^2, and K = bulk modulus.

[6] K. Fuchs, Proc. Roy. Soc. (London) **A151**, 585 (1935); **A153**, 622 (1936).

[7] G. J. Dienes, North American Aviation Report No. SR-80 (1951); North American Aviation Report No. SR-125 (1951).

TABLE I. The elastic coefficients of Cu calculated by Eq. (3), in dynes cm^{-2} (low temperature). $D_0=2.8\times10^{-8}$ erg/atom, $r_e=2.55\times10^{-8}$ cm, and $\rho=0.200\times10^{-8}$ cm.

	Calculated	Experimental[a]
$c_{11}-c_{12}$	5.1×10^{11}	5.1×10^{11}
c_{44}	8.6×10^{11}	8.2×10^{11}
K	1.33×10^{12}	1.39×10^{12}

[a] Data from references 6 and 10.

IV. THE ELASTIC COEFFICIENTS OF COPPER AND SODIUM

Fuchs[6] has made a careful quantum-mechanical study of the cohesive forces and elastic coefficients in copper and the alkali metals. He has applied and extended the earlier work of Wigner and Seitz[8] and Seitz[9] on the cohesive forces in sodium and lithium. Two of his conclusions, important for the purpose of the present paper, may be stated as follows: 1. In copper the elastic coefficients are primarily determined by the closed shell repulsive interactions. This, apparently, holds even for the compressibility although one may expect purely volume forces to be of importance. 2. In the alkali metals both attractive and repulsive energies must be taken into account.

In neither case did Fuchs arrive at a simple function for U which could be conveniently used in the present calculations. Huntington and Seitz,[10] in their theoretical study of self-diffusion in copper, point out that a simple exponential function of the Born and Mayer type can be used satisfactorily to represent the repulsive interactions. This result, combined with the results of Fuchs' study, suggests that the elastic constants of copper may be adequately described by assuming U to be given, as a function of distance, r, by the relation

$$U=D_0e^{-r/\rho}, \tag{3}$$

where D_0 and ρ are adjustable constants. A single exponential function is an adequate approximation in this case because the second derivative of the attractive part of the potential energy is small compared to that of the repulsive part and can, therefore, be neglected.

This same approximation cannot be used for the alkali metals. To carry out the proposed calculation, it is important to find some simple function for U which can be used for calculating the elastic coefficients of alkali metals. Slater suggests[11] that a Morse function is a rather good approximation for the interatomic potential in metals. More recently Pauling[12] found that a Morse potential function can be used to calculate the compressibility of metals as a function of pressure. Consequently, it was thought that for sodium a function U may be used, given by

$$U=D_0[1-e^{-a(r-r_e)}]^2. \tag{4}$$

The use of the Morse potential function for describing the elastic coefficients of the alkali metals is discussed in detail in an unclassified report by the writer:[13] It is sufficient to state here that Eq. (3) has been found satisfactory for copper and Eq. (4) for sodium. The constants of Eqs. (3) and (4) have been calculated and the calculated elastic coefficients were found to be in good agreement with experimental values. The pertinent data are collected in Tables I and II. For sodium[14] it was necessary to sum over both nearest and next nearest neighbors.

It is concluded from these results that the elastic coefficients are quite well described by the atomic interaction potentials represented by Eqs. (3) and (4) for copper and sodium, respectively. It should be emphasized that, in both cases, only two adjustable constants (D_0 and ρ, and D_0 and a, respectively) are employed to fit three elastic constants. The equilibrium interatomic distance r_e is considered to be known and fixed.

V. INTERSTITIALS AND VACANCIES IN COPPER AND SODIUM

Sufficient background information is now at hand to carry out the theoretical estimate proposed in Sec. II. The calculations for copper will be described first since this metal represents the simpler case.

Let the fraction of interstitials produced by radiation be denoted by x. In the absence of any annealing the fraction of vacancies left behind is also x. In creating a vacancy 12 normal contacts are broken. Formation of an interstitial in the body-center position of the face-centered copper lattice requires 14 new contacts, 6 of them $(\sqrt{2}/2)r$ away and 8 of them $(\sqrt{3}\sqrt{2}/2)r$ away. Following the physical discussion of Sec. II, the total repulsive potential energy per atom may then be written,

$$U=(1-x)D_0\exp(-r/\rho)+x(6/12)D_0\exp[-(\sqrt{2}/2)r/\rho]+x(8/12)D_0\exp[-(\sqrt{3}\sqrt{2}/2)r/\rho]. \tag{5}$$

TABLE II. The elastic coefficients of Na calculated by Eq. (4), in dynes cm^{-2} (room temperature).[a] $D_0=5.19\times10^{-14}$ erg/atom, $r_e=3.68\times10^{-8}$ cm, and $a=1.06\times10^8$ cm.

	Calculated	Experimental[b]
$c_{11}-c_{12}$	1.159×10^{10}	1.159×10^{10}
c_{44}	4.26×10^{10}	4.26×10^{10}
K	4.15×10^{10}	4.20×10^{10}

[a] The elastic coefficients of Na at low temperature (see reference 14) (80°K) can also be satisfactorily fitted using $D_0=6.84\times10^{-14}$, $r_e=3.68\times10^{-8}$, and $a=1.087\times10^8$.
[b] Data from R. F. S. Hearmon, Revs. Modern Phys. 18, 409 (1946).

[8] E. P. Wigner and F. Seitz, Phys. Rev. 43, 804 (1933); 46, 509 (1934).
[9] F. Seitz, Phys. Rev. 47, 400 (1935).
[10] H. B. Huntington and F. Seitz, Phys. Rev. 61, 315 (1942).
[11] J. C. Slater, *Introduction to Chemical Physics* (McGraw-Hill Book Company, Inc., New York, 1939), pp. 450–456.
[12] L. Pauling, Science 111, 461 (1950).
[13] G. J. Dienes, North American Aviation Report No. SR-125 (1951).
[14] S. L. Quimby and S. Siegel, Phys. Rev. 54, 293 (1938).

If one neglects lattice relaxation and volume effects, the elastic coefficients of the damaged crystal are calculable from Eqs. (5) and (1) with all the derivatives evaluated at r_e. Physically this means that the change in repulsive energy has been spread out over the whole crystal and, in effect, the damaged lattice has been replaced by an equivalent homogeneous face-centered cubic lattice for which the repulsive interactions are given by Eq. (5) in place of Eq. (3).

In addition to the assumptions and approximations discussed so far, a further assumption is implicit in these calculations. Equation (5) assumes that the repulsive potential energy function, Eq. (3), fitted to the perfect lattice, remains valid over the considerably shorter interaction distances used in Eq. (5). From present knowledge of interaction forces it is impossible to estimate the degree of approximation involved.

The calculations indicated above have been carried out. The changes in the elastic coefficients are evidently proportional to x (fraction of interstitials or vacancies). It is of interest to give the results for two concentrations, $x=0.01$ (1 percent) and $x=0.05$ (5 percent), covering the range of concentration expected in irradiated materials. For consistency, the comparison is made relative to the calculated elastic constants of Table I. The results are summarized in Table III. In addition to the changes in the three fundamental elastic coefficients the corresponding values for the two Young's moduli are also given. Young's moduli, corresponding to the shear moduli c_{44} and $\frac{1}{2}(c_{11}-c_{12})$, are defined by

$$E_1=9Kc_{44}/(c_{44}+3K)$$
$$E_2=9K\cdot\tfrac{1}{2}(c_{11}-c_{12})/[\tfrac{1}{2}(c_{11}-c_{12})+3K].$$

The data in Table III indicate that large changes in the elastic moduli of copper are to be expected as a result of the creation of interstitials and vacancies. The higher elastic coefficients are entirely due to the presence of interstitials. Vacancies alone decrease the elastic coefficients. The effect of vacancies is easily calculable using the first term of Eq. (5) for U. Performing such a calculation it was found that 1 percent vacancies decrease the elastic coefficients very closely by 1 percent indicating that this change is primarily a bulk effect. These general results are physically to be expected as long as it is reasonable to derive the elastic properties from the closed shell interaction. If it is valid to consider irradiation to result in interstitials and vacancies then radiation damage is expected to increase the elastic coefficients in a metal such as copper and the increase in the elastic coefficients is primarily a measure of the number of interstitial atoms.

The calculations for sodium, a body-centered cubic lattice, are carried out in an analogous manner with the modification that a Morse potential is to be used for U [Eq. (4)], and both nearest and next nearest neighbors are to be counted in calculating the elastic coefficients from U as shown by Eq. (2). In creating a vacancy 14 normal contacts are broken. Formation of an interstitial in the face-centered position of the body-centered sodium lattice requires the formation of 2 new contacts $(1/\sqrt{3})r$ away and 4 new contacts $(\sqrt{2}/\sqrt{3})r$ away. Analogous to Eq. (5), therefore, the total potential energy per atom may be written

$$U=(1-x)D_0\{1-\exp[-a(r-r_e)]\}^2 +x(2/14)D_0\{1-\exp[-a(r/\sqrt{3}-r_e)]\}^2 +x(4/14)D_0\{1-\exp[-a(2r/\sqrt{3}-r_e)]\}^2. \quad (6)$$

The elastic coefficients are then calculated directly from Eq. (2) using the expression for U given above.

The calculations indicated above have been carried out. The changes in the elastic coefficients are proportional to x and the results are again given for two concentrations ($x=0.01$ and $x=0.05$). For consistency, the comparison is made relative to the calculated elastic coefficients of Table II. The results are summarized in Table IV.

As Table IV shows, the predicted effects for sodium, calculated on the basis of a Morse function interaction, and in the absence of relaxation, are of the same order of magnitude as for copper calculated from the repulsive interactions. The effect of vacancies alone has also been determined in sodium. As in the case of copper, vacancies alone decrease the elastic coefficients and the change is again essentially a bulk effect, i.e., 1 percent vacancies decrease the elastic coefficients very closely by 1 percent. Thus, for sodium also, the increase in the elastic coefficients is primarily a measure of the number of interstitial atoms.

TABLE III. Effect of interstitials and vacancies on the elastic coefficients of copper (in dynes cm^{-2}).

	$x=0.00$	$x=0.01$	$x=0.05$
$c_{11}-c_{12}$(unirrad.)	5.1 $\times10^{11}$		
$c_{11}-c_{12}$(irrad.)		5.3 $\times10^{11}$	6.1 $\times10^{11}$
$\Delta(c_{11}-c_{12})$		0.2 $\times10^{11}$	1.0 $\times10^{11}$
$\Delta(c_{11}-c_{12})/(c_{11}-c_{12})$		3.9%	19.6%
c_{44}(unirrad.)	8.6 $\times10^{11}$		
c_{44}(irrad.)		9.4 $\times10^{11}$	12.6 $\times10^{11}$
Δc_{44}		0.8 $\times10^{11}$	4.0 $\times10^{11}$
$\Delta c_{44}/c_{44}$		9.3%	46.5%
K(unirrad.)	1.33 $\times10^{12}$		
K(irrad.)		1.45 $\times10^{12}$	1.93 $\times10^{12}$
ΔK		0.12 $\times10^{12}$	0.6 $\times10^{12}$
$\Delta K/K$		9.0%	45.0%
E_1(unirrad.)	2.125$\times10^{12}$		
E_1(irrad.)		2.32 $\times10^{12}$	3.11 $\times10^{12}$
ΔE_1		0.195$\times10^{12}$	0.985$\times10^{12}$
$\Delta E_1/E_1$		9.2%	46.3%
E_2(unirrad.)	1.355$\times10^{12}$		
E_2(irrad.)		1.417$\times10^{12}$	1.655$\times10^{12}$
ΔE_2		0.062$\times10^{12}$	0.3 $\times10^{12}$
$\Delta E_2/E_2$		4.56%	22.1%

VI. RELAXATION EFFECTS

Relaxation of the atoms around the lattice disturbances has so far not been taken into account. These atomic readjustments can be of considerable impor-

TABLE IV. Effect of interstitials and vacancies on the elastic coefficients of sodium (in dynes cm^{-2}).

	$x=0.00$	$x=0.01$	$x=0.05$
$c_{11}-c_{12}$(unirrad.)	1.159×10^{10}		
$c_{11}-c_{12}$(irrad.)		1.218×10^{10}	1.454×10^{10}
$\Delta[c_{11}-c_{12}]$		0.059×10^{10}	0.295×10^{10}
$\Delta[c_{11}-c_{12}]/(c_{11}-c_{12})$		5.1%	25.5%
c_{44}(unirrad.)	4.26×10^{10}		
c_{44}(irrad.)		4.37×10^{10}	4.81×10^{10}
Δc_{44}		0.11×10^{10}	0.55×10^{10}
$\Delta c_{44}/c_{44}$		2.6%	13.0%
K(unirrad.)	4.15×10^{10}		
K(irrad.)		4.42×10^{10}	5.5×10^{10}
ΔK		0.27×10^{10}	1.35×10^{10}
$\Delta K/K$		6.5%	32.5%
E_1(unirrad.)	9.58×10^{10}		
E_1(irrad.)		9.87×10^{10}	11.17×10^{10}
ΔE_1		0.29×10^{10}	1.59×10^{10}
$\Delta E_1/E_1$		3.0%	16.6%
E_2(unirrad.)	3.21×10^{10}		
E_2(irrad.)		3.35×10^{10}	4.01×10^{10}
ΔE_2		0.14×10^{10}	0.8×10^{10}
$\Delta E_2/E_2$		4.4%	24.9%

tance, particularly in the alkali metals.[15] The atoms around an interstitial will certainly move outwards to accommodate the interstitial atom. Similarly, the atoms around a vacancy tend to move toward the empty lattice site. If these atomic motions are relatively large, the increase in the elastic constants calculated in the previous section may be a serious overestimate.

The outward motion of the atoms around an interstitial in copper is illustrated in Fig. 1. The repulsive interactions of the interstitial with its nearest neighbors push the atoms outward while the neighbors of the moving atom tend to restore it to its normal lattice position. Balance between these two forces will lead to an equilibrium displacement. The calculation is best carried out by finding the minimum in the potential energy of the whole system as a function of displacement, Δr. The displacement Δr is taken to be the same percentage of the atom to interstitial distance for each moving atom, that is, uniform distortion is assumed. This calculation is analogous to the one given by Dienes[16] for alkali halide crystals.

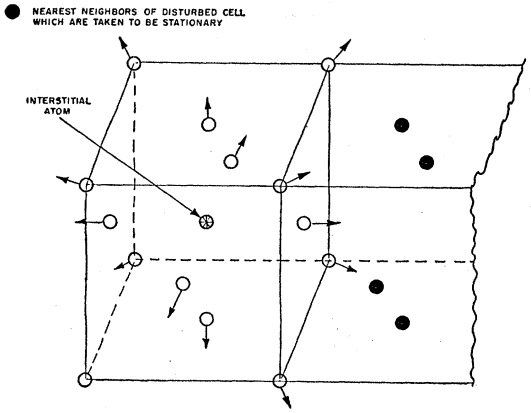

FIG. 1. Relaxation of atoms around an interstitial in copper.

In Fig. 1 part of the next cell in one direction is illustrated in order to show which atoms are assumed to remain at their lattice sites. The interstitial itself has fourteen neighbors which become displaced—six in the face-centered positions and eight at the corners of the cube. All atoms further away than these fourteen are assumed to suffer no displacement (Fig. 1). Each of these moving neighbors has twelve contacts which are changed by relaxation and must be evaluated. Of these twelve those which are not nearest neighbors of the interstitial are stationary. However, the nearest neighbors of the moving atom which are also nearest

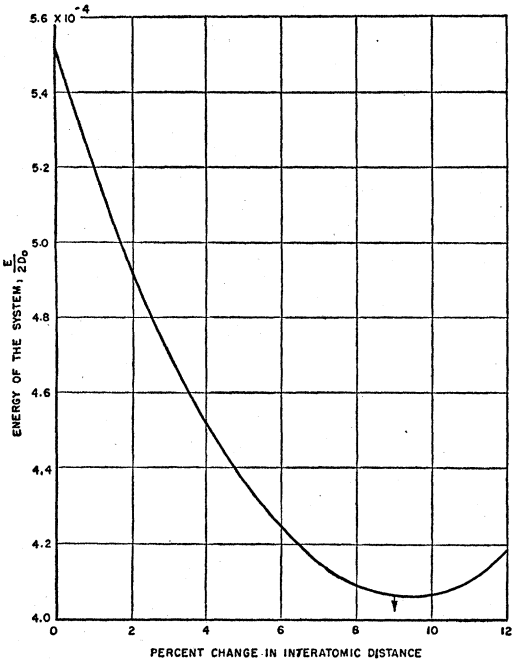

FIG. 2. Determination of equilibrium relaxation around an interstitial in copper.

neighbors of the interstitial have been displaced and their interactions were counted from the displaced position. These are the interactions which one must not count twice in the summation.

As an example of the procedure consider an atom normally in the face-centered position. After displacement the following interactions have changed and have been taken into account: (a) Interaction with interstitial. (b) Interaction with four nearest neighbors of the displaced face-centered atom which themselves have not moved (solid circles in Fig. 1). (c) Interaction with eight nearest neighbors of the displaced face-centered atom which themselves have been displaced. Similarly, for a corner atom the interactions are: (d) Interaction with interstitial. (e) Interaction with nine

[15] H. R. Paneth, Phys. Rev. **80**, 708 (1950).

[16] G. J. Dienes, J. Chem. Phys. **16**, 620 (1948).

nearest neighbors of the displaced corner atom which themselves have not moved. (f) Interaction with three nearest neighbors of the displaced corner atom which themselves have been displaced.

The summation required for evaluating the energy of the system evidently contains a large number of terms and is best accomplished by a point-by-point calculation for various values of Δr. The results are shown in Fig. 2 where the energy of the system, in units of $E/2D_0$, is plotted against the percentage change in interatomic distance, r. The minimum occurs at an outward equilibrium displacement of 9 percent.

Analogous calculations have been performed for relaxation inward around a vacant lattice site. The results are shown in Fig. 3 where the minimum is shown

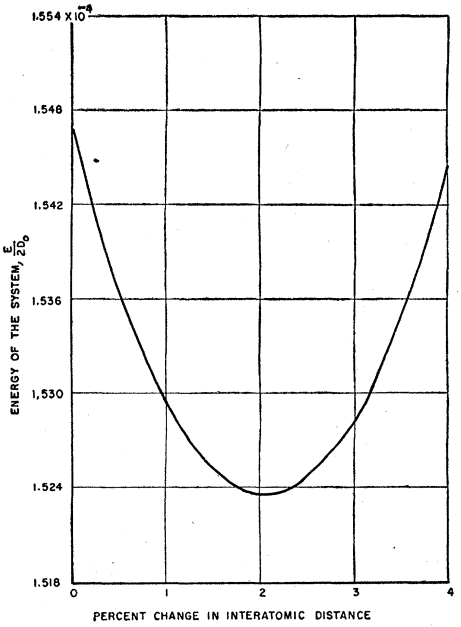

FIG. 3. Determination of equilibrium relaxation around a vacancy in copper.

to occur at an inward equilibrium displacement of 2 percent.

The equilibrium displacements having been determined, the total repulsive energy per atom, U, Eq. (5), can now be corrected for relaxation by taking into account all the altered interactions. Since the relaxation around a vacancy is small and the influence of the vacancies upon the elastic constants is also small, the relaxation corrections were applied only to the atoms surrounding the interstitial. From this point on the calculation is identical to that given in the previous section. The results show that the relaxation effects in copper decrease the influence of the interstitials, i.e., the increase in moduli resulting from the interstitials is not as large in the presence as in the absence of relaxation. The changes are, however, not large enough to modify any of the conclusions given in Sec. V, that is,

TABLE V. Effect of interstitials and vacancies on the elastic coefficients of copper (in dynes cm^{-2}).

Elastic coefficient	$x=0.00$[a]	$x=0.01$ Without relaxation	$x=0.01$ With relaxation
$c_{11}-c_{12}$	5.1×10^{11}	5.3×10^{11}	5.3×10^{11}
$\Delta(c_{11}-c_{12})$		0.2×10^{11}	0.2×10^{11}
$\Delta(c_{11}-c_{12})/(c_{11}-c_{12})$		3.9%	3.9%
c_{44}	8.6×10^{11}	9.4×10^{11}	9.2×10^{11}
Δc_{44}		0.8×10^{11}	0.6×10^{11}
$\Delta c_{44}/c_{44}$		9.3%	7.0%
K	1.33×10^{12}	1.45×10^{12}	1.42×10^{12}
ΔK		0.12×10^{12}	0.09×10^{12}
$\Delta K/K$		9.0%	6.8%

[a] x = fraction of interstials = fraction of vacancies.

the presence of interstitials in copper leads to a large increase in the elastic moduli even after relaxation. The results are summarized in Table V.

Relaxation effects in sodium are calculated in an analogous manner to that given for copper in the previous section except that the geometry is that of a body-centered cubic lattice and the interatomic interaction function is the Morse function [Eq. (4)]. The outward relaxation around an interstitial is illustrated in Fig. 4. The most important effect comes from the relaxation of the six nearest neighbors of the interstitial. Each of the moving atoms has fourteen contacts which must be taken into account, care being exercised in not counting twice the neighbors of the interstitial.

The total energy *vs* displacement curve is shown in Fig. 5. The minimum occurs at an outward equilibrium displacement of 30 percent. Evidently, relaxation around an interstitial in the more open body-centered cubic structure is far greater than in the close-packed copper lattice. Physically, this is a reasonable result.

Similar calculations for a vacent lattice site indicated that the lattice shows no relaxation around a vacancy within the accuracy of the nearest neighbor approximation. Since the influence of the vacancies is small to start with a more detailed calculation was not carried out.

Evaluation of the elastic constants in the relaxed lattice gave the results in Table VI. Comparison with

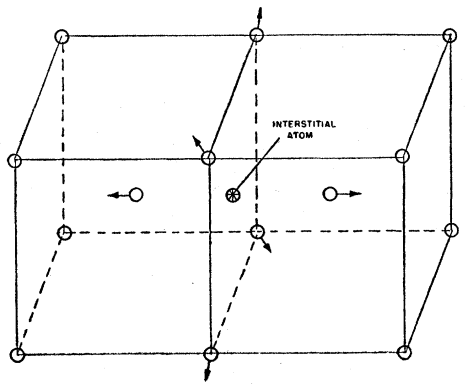

FIG. 4. Relaxation of atoms around an interstitial in sodium.

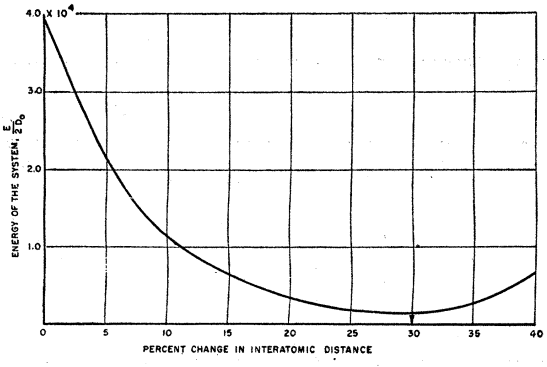

FIG. 5. Determination of equilibrium relaxation around an interstitial in sodium.

the unrelaxed lattice shows that atomic readjustments in the body-centered cubic lattice of sodium reduces the effect of the interstitial essentially to a bulk effect.

VII. SUMMARY

1. An approximate theoretical treatment is given of the change in elastic constants of simple metals caused by the presence of a given small fraction of interstitial atoms and vacancies. The elastic constants are calculated from interatomic potentials employing a simple exponential function for copper and a Morse function for sodium. Relaxation effects are taken into account.

2. A crystal containing interstitial atoms and vacancies is locally inhomogeneous. The major approximation of the theory is the replacement of the inhomogeneous lattice by an approximately equivalent homogeneous material in which the interactions ascribable to the lattice disturbances are smeared over the whole crystal. Thus, the geometry of the original lattice is retained in the present calculations, but the potential energy of the system is modified according to the number of contacts formed and broken by the creation of interstitials and vacancies.

3. The theoretically calculated changes in elastic coefficients are large in copper even in the presence of relaxation. In sodium, however, which has the more open body-centered structure, the relaxation around the interstitial is quite large. This atomic readjustment reduces the effect of the lattice disturbances to the magnitude of a bulk effect.

4. The presence of interstitial atoms and vacant lattice sites in a close-packed cubic crystal, such as copper, results in an appreciable increase in the elastic moduli. Vacancies alone decrease the elastic moduli by a magnitude corresponding essentially to a bulk effect. The increase in elastic coefficients, therefore, is due to the presence of interstitial atoms, with the increase being several orders of magnitude larger than would be predicted from a simple bulk effect.

TABLE VI. Effect of interstitials and vacancies on the elastic coefficients of sodium (in dynes cm^{-2}).

Elastic coefficient	$x=0.00$[a]	$x=0.01$ Without relaxation	$x=0.01$ With relaxation
$c_{11}-c_{12}$	1.159×10^{10}	1.218×10^{10}	1.166×10^{10}
$\Delta(c_{11}-c_{12})$		0.059×10^{10}	0.007×10^{10}
$\Delta(c_{11}-c_{12})/(c_{11}-c_{12})$		5.1%	0.6%
c_{44}	4.26×10^{10}	4.37×10^{10}	4.29×10^{10}
Δc_{44}		0.11×10^{10}	0.03×10^{10}
$\Delta c_{44}/c_{44}$		2.6%	0.7%
K	4.15×10^{10}	4.42×10^{10}	4.23×10^{10}
ΔK		0.27×10^{10}	0.08×10^{10}
$\Delta K/K$		6.5%	1.9%

[a] x = fraction of interstitials = fraction of vacancies.

5. The theoretically predicted effects should be easily observable experimentally provided interstitial atoms are, in fact, produced by irradiation, or by any other means, such as perhaps cold work at very low temperatures. To prevent annealing which may occur rapidly at room temperature the lattice disturbances must be produced and preserved at low temperatures.

6. The theoretical results strongly suggest that changes in elastic constants may serve as a useful and powerful tool for distinguishing between interstitial atoms and vacant lattice sites. Furthermore, since the mechanical properties of solids are known to be changed by irradiation, the study of elastic constants as a function of irradiation is of direct interest in yielding information about one of the fundamental mechanical properties.

Note added in proof:—Preliminary experiments by Bowman and Tarpinian (private communication, February, 1952) indicate that Young's modulus of copper increases by as much as 10 percent upon heavy cyclotron irradiation.

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