

This procedure also yielded values which agree generally with the literature. We found that the temperature dependences of both  $m_d$  and  $m_c$  are quite similar in samples having the same type of carrier. Such a result would be anticipated from the known values of the anisotropy ratio  $K$ . The fact that they did indeed have similar thermal characteristics may be considered as evidence of their correctness since they were obtained from very different procedures. The actual temperature dependence of the effective masses has been found to increase with increasing temperature and it approaches  $T^{0.5}$  for  $n$ -type and  $T^{0.8}$  for  $p$ -type material at 300°K. Furthermore, the values for  $m_c$  and  $m_d$  indicate that a four-valley model is to be preferred in the conduction band. In the valence band we infer that there is a zone-centered maximum, which increases in prominence with

increasing temperature, in addition to the other (probably four) valence-band maxima.

#### ACKNOWLEDGMENTS

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## Point Defect Studies in Gold by Electron Irradiation at Low Temperatures. I. Threshold Displacement Energy and Displacement Cross Section\*

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The damage production on 99.999% pure 0.00025-in.-thick gold foils was measured as a function of incident electron energy in the range from 1.3 to 2.2 MeV. The effective threshold displacement energy was measured to be near 35 eV. It was found that reasonable agreement between the experimental and theoretical values of the displacement cross section could only be achieved with an unusually low value of the resistivity of a Frenkel pair ( $\rho_F = 0.89 \times 10^{-4}$   $\Omega$ -cm/unit fractional concentration). By comparison, in copper the agreement between the theoretical and experimental cross section ( $\rho_F = 1.2 \times 10^{-4}$   $\Omega$ -cm/unit fractional concentration) is somewhat better. This is interpreted to indicate that directional effects in the displacement process are considerably more important in gold than in copper, and that, for energies near the threshold energy, displacements in gold are possible only in a small solid angle centered about one crystallographic direction, most likely the  $\langle 100 \rangle$  direction.

### I. INTRODUCTION

IN the study of point defects in metals, the noble metals—copper, silver, and gold—have received the major attention. Among these three, copper has been studied most intensively but gold has received increasing attention recently. The shift from copper to gold may be traced to the fact that, despite a large effort, the point defect characteristics in copper remain inadequately understood, and that the annealing characteristics in gold, following irradiation, are significantly different from copper and silver or, as a matter of fact, almost any metals which have been examined.

The threshold displacement energy in gold has been variously reported to be  $>40$  eV,<sup>1</sup> near 40 eV,<sup>2</sup> and be-

tween 33 and 36 eV.<sup>3</sup> The experiments discussed in this paper were undertaken to measure the damage production as a function of the electron energy and thus to afford a comparison between the experimental and theoretical values of the displacement cross section.

In part II of this paper a description of the experimental equipment and techniques is given. Part III deals with the experimental results. The theoretical displacement cross section and a comparison of experimental and theoretical results is given in part IV. A discussion of the results is given in part V.

### II. EXPERIMENTAL METHODS

#### A. Specimen Preparation

In order to achieve minimum energy degradation of the bombarding electrons in the specimens 0.00025-in.-

\* This work was supported by the U. S. Atomic Energy Commission.

<sup>1</sup> P. G. Lucasson and R. M. Walker, *Phys. Rev.* **127**, 485 (1962).

<sup>2</sup> R. B. Minnix and P. E. Shearin, *Bull. Am. Phys. Soc.* **8**, 196 (1963).

<sup>3</sup> W. Bauer and A. Sosin, *J. Appl. Phys.* **35**, 703 (1964).

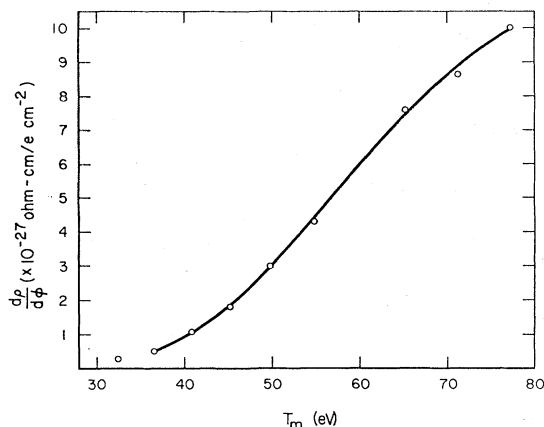


FIG. 1. The experimental values of resistivity increase per unit integrated flux as a function of the maximum energy imparted a lattice atom.

thick gold foils were used. The foil was prepared by rolling 99.999% pure 0.002-in.-diam wire, purchased from Sigmund Cohn Corporation, between tantalum foils after a thorough cleaning.<sup>4</sup> Then gold potential leads were spotwelded approximately 2 in. apart on a 3-in. length of gold foil. The foil was then cleaned and annealed at 670°C for 2 h by passing an electric current through it in air. The actual specimen was then prepared from the length of foil between the potential leads. After mounting the specimen on the holder and mounting the holder on the cryostat the specimen was reannealed at 670°C for 2 h by passing a current through it in air.

The residual resistivity of the various foils used in these experiments ranged from  $4.5 \times 10^{-9}$  to  $5.7 \times 10^{-9}$  Ω-cm. We believe that a considerable part of the residual resistivity is due to the size effect and a high susceptibility to unavoidable cold work.

The resistivity increase  $\Delta\rho$  was computed from the measured increase in electrical resistance  $\Delta R$  measured at 4.2°K, using the measured value of resistance at room temperature  $R_{300}$ , and the tabulated value of the room temperature resistivity  $\rho_{300}$  ( $2.44 \times 10^{-6}$  Ω-cm). The relationship used is

$$\Delta\rho = (\rho_{300}/R_{300})\Delta R. \quad (1)$$

Note that this relationship holds only since the potential leads were spotwelded to the specimen in such a manner that the irradiated length of the specimen extends beyond the portion of the specimen over which the resistance is measured.

### B. Irradiations Near 13°K

The liquid-helium cryostat and electrical instrumentation used in these experiments have been fully described elsewhere.<sup>5</sup> With a measuring current of 0.4 A, the experimental accuracy of the resistivity readings was  $\pm 2 \times 10^{-12}$  Ω-cm.

<sup>4</sup> K. Herschbach, Phys. Rev. **130**, 554 (1963).

<sup>5</sup> A. Sosin and H. H. Neely, Rev. Sci. Instr. **32**, 922 (1961).

In some of the runs a 0.00025-in.-thick aluminum foil was placed approximately 7 in. from the sample. This results in a more uniform beam over the 1-cm<sup>2</sup> irradiation area. The energy correction due to the aluminum foil is negligible. The energy of the Van de Graaff accelerator was calibrated at one point using the Be( $\gamma, n$ ) nuclear reaction at 1.655 MeV. The energy uncertainty was  $\pm 15$  keV. The estimated error in the measurement of the total integrated flux is about 5%. The temperature of the gold specimens never rose above 13°K with 2-MeV electron current densities of  $5 \mu\text{A}/\text{cm}^2$ .

### III. EXPERIMENTAL RESULTS

Figure 1 shows the plot of  $d\rho/d\phi$ , the resistivity increase per unit integrated electron flux, versus  $T_m$ , the maximum energy that can be imparted a lattice atom by the bombarding electron. The quantity  $d\rho/d\phi$  is the measured slope of the resistivity increase versus integrated flux of electrons curve at a fixed energy  $E$ . The relationship between  $T_m$  and  $E$  is<sup>6</sup>

$$T_m(\text{eV}) = \frac{560}{A} \frac{E}{mc^2} \left[ \frac{E}{mc^2} + 2 \right], \quad (2)$$

where  $mc^2 = 0.511$  MeV and  $A = 197$  for gold.

One notes from Fig. 1 that measurable damage production occurs at values of  $T_m \leq 35$  eV. We attribute these displacements to "soft spots" in the lattice associated with unavoidable impurities. This topic is incidental to this discussion and has been discussed in a separate publication.<sup>3</sup>

The experimental points shown in Fig. 1 include corrections for energy degradation and straggling of the electrons in the sample. The average energy of the electrons in the sample is, approximately,

$$\bar{E} = E_i - \frac{1}{2}\alpha t, \quad (3)$$

where  $E_i$  = incident electron energy,  $\alpha$  = energy loss per unit distance, approximately 0.1 MeV/0.001 in. (see Ref. 7),  $t = 0.00025$  in. (thickness of foil used in these measurements). Then

$$\bar{E} = E_i - 0.013 \text{ MeV}. \quad (4)$$

The calculation of the correction for electron straggling follows closely Refs. 8 and 9. The correction manifests itself in an additional resistivity increment

$$\Delta\rho' = a t \Delta\rho, \quad (5)$$

where

$$a = (w^2 \chi_0)^{-1};$$

$\chi_0$  = "radiation length," a characteristic of the material ( $34 \text{ gm}/\text{cm}^2$  in gold), and  $w$  is a function of the electron

<sup>6</sup> F. Seitz and J. S. Koehler, in *Solid State Physics*, edited by F. Seitz and D. Turnbull (Academic Press Inc., New York, 1956), Vol. II, p. 330.

<sup>7</sup> L. Katz and R. S. Penfold, Rev. Mod. Phys. **24**, 28 (1952).

<sup>8</sup> A. Sosin, Phys. Rev. **126**, 1698 (1962).

<sup>9</sup> C. N. Yang, Phys. Rev. **84**, 599 (1951).

energy with a value between 0.1 and 0.2. We then have

$$\Delta\rho' \approx 0.04\Delta\rho. \quad (6)$$

For electron energies used in these experiments, this correction is negligible.

#### IV. THEORETICAL DISPLACEMENT CROSS SECTION AND COMPARISON OF EXPERIMENTAL AND THEORETICAL RESULTS

Making the common assumption that the contribution to electrical resistivity due to interstitials and vacancies does not depend on the separation between an interstitial and a vacancy in a defect pair, the resistivity increase per unit integrated flux  $d\rho/d\varphi$  is proportional to the "displacement cross section"  $\sigma_d$ :

$$d\rho/d\varphi = \rho_F \sigma_d. \quad (7)$$

Here  $\rho_F$  is the resistivity of a unit concentration interstitial-vacancy (Frenkel) pairs (all specific resistivities throughout this paper will be given in units of  $\Omega$ -cm per unit fractional concentration of lattice defects).

The minimum energy required to displace an atom permanently from its lattice site is a function of the crystallographic direction in which the atom is driven as a result of the preliminary electron collision. In particular there are certain crystallographic directions in which the threshold displacement energy exhibits minimum values. The assumption which is frequently made of the existence of an "effective" displacement energy  $T_e$  is useful if the differential scattering cross section is nearly independent of the energy transferred to the atom, throughout the entire range over which the threshold displacement energy varies as a function of angle. When this is true, there exists an effective minimum scattering angle for the incident electron, measured in the center-of-mass coordinate system  $\theta_m$  given by Eq. (8),

$$T_e = T_m \sin^2(\frac{1}{2}\theta_m), \quad (8)$$

where  $T_e$  is the effective threshold displacement energy and  $T_m$  is the maximum energy transfer possible. The corresponding displacement cross section is given by

$$\sigma_d = 2\pi \int_{\theta_m}^{\pi} \frac{d\sigma}{d\Omega} \sin\theta d\theta. \quad (9)$$

The assumption implicit in Eqs. (8) and (9) can be written

$$T_d(\theta', \varphi') = T_e, \quad (10)$$

where  $\theta'$  and  $\varphi'$  denote the direction of the initial impulse given to the atom, measured with respect to a given crystallographic direction.

In case  $T_m$  is less than the threshold displacement energy for certain crystallographic directions, the integration in Eq. (9) should not extend over all possible solid angles for which  $\theta$  exceeds  $\theta_m$ ; specifically that region of solid angle for which  $T_d(\theta', \varphi') > T_m$  should be

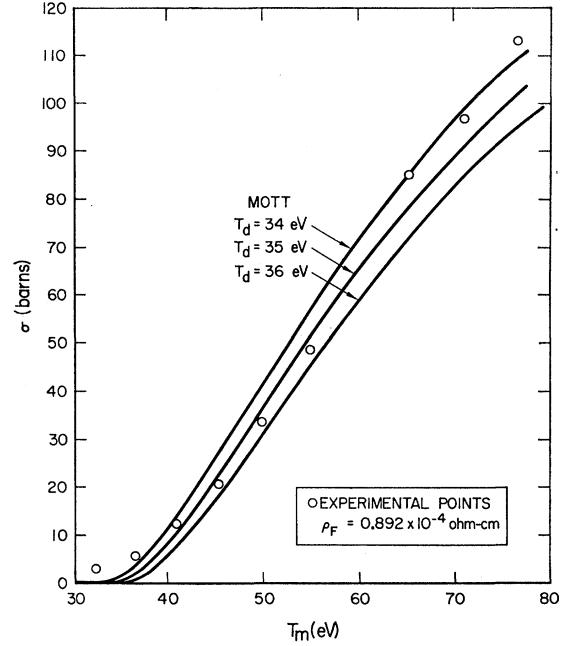


FIG. 2. The experimental and theoretical values of the displacement cross section as a function of the maximum energy imparted a lattice atom. The theoretical displacement cross section, solid curve, was calculated for values of  $T_d=34, 35,$  and  $36$  eV.

excluded. This will decrease the apparent value of  $\rho_F$  as defined in Eq. (7) if, in the reduction of the data, Eqs. (8)–(10) are assumed valid.

For  $d\sigma$ , the relativistic Coulomb scattering cross section due to Mott must be used. For elements with a value of  $Z < 30$  an approximation for  $d\sigma$  due to McKinley and Feshbach<sup>10</sup> and integrated by Seitz and Koehler<sup>6</sup> is available. This approximation is inadequate for elements with higher values of  $Z$  such as gold. Recently, a numerical calculation using the Mott series directly has been performed for gold by Khandelwal and Merzbacher.<sup>11</sup> The results of their calculations have kindly been made available to us for values of  $T_e$  of 34, 35, and 36 eV.<sup>12</sup> The results of their calculation for  $\sigma_d$  are shown in Fig. 2.

The experimental points for  $\sigma_d$  in Fig. 2 are calculated, using Eq. (7), the  $d\rho/d\varphi$  values of Fig. 1, and a value of  $\rho_F = 0.89 \times 10^{-4}$ . Although the choice of the value of  $\rho_F$  is arbitrary, we feel that the combination of  $\rho_F = 0.89 \times 10^{-4}$  and the theoretical value of  $\sigma_d$  calculated with  $T_e = 35$  eV give the best agreement for  $35 \text{ eV} \leq T_m \leq 77 \text{ eV}$ . Since the "excluded" portion of the solid angle over which integration should be performed is itself a function of energy, the energy interval over which even the apparent value of  $\rho_F$  is constant should

<sup>10</sup> W. A. McKinley, Jr., and H. Feshbach, Phys. Rev. **74**, 1759 (1948).

<sup>11</sup> G. S. Khandelwal and E. Merzbacher, Phys. Rev. **130**, 1822 (1963).

<sup>12</sup> These additional calculations were supported by the U. S. Atomic Energy Commission.

shrink to zero. The implications of this apparent value of  $\rho_F$  will be discussed further in the next section, in comparison with the corresponding value for copper.

An alternative method of comparison between experiment and theory not involving a choice of  $\rho_F$  is shown in Figs. 3 and 4. This method has been used extensively by Lucasson and Walker<sup>1</sup> and in part by Sosin.<sup>8</sup> In Fig. 3, the experimental damage rates and the theoretical displacement cross sections, following Khandelwal and Merzbacher,<sup>11</sup> have been divided by their respective values at an incident electron energy of 2.19 MeV ( $T_m=76.5$  eV); in Fig. 4, this "normalization" has been made at 1.80 MeV ( $T_m=54.8$  eV). The agreement in Fig. 3 is not particularly good. If it were necessary to deduce a value of  $T_e$  from this plot, it would appear that  $T_e > 36$  eV. Somewhat better agreement is evident in Fig. 4 in the range of energies  $T_m < 65$  eV. However, it is difficult to make any definite choice for the best value of  $T_e$  here. Obviously, the "normalization" technique is an entirely inadequate procedure in gold for gaining appreciable insight into the nature of the displacement theory. By comparison, some success for this procedure has been achieved in copper.<sup>1,8</sup>

## V. DISCUSSION OF RESULTS

Before continuing, we discuss the apparent value of  $\rho_F = 0.89 \times 10^{-4}$ . It is generally assumed that  $\rho_F = \rho_i + \rho_v$ , where  $\rho_v$  is the resistivity of a unit concentration of vacancies, and  $\rho_i$  is the resistivity of a unit concentration of interstitials. The resistivity of an interstitial has not been measured and theoretical values vary greatly<sup>13</sup> but suggest that  $\rho_i > \rho_v$ .<sup>14</sup> A commonly accepted experimental value<sup>15</sup> of  $\rho_v$  is  $1.5 \times 10^{-4}$ . Thus, one would expect a value of  $\rho_F$  greater than  $1.5 \times 10^{-4}$  and probably greater than  $3 \times 10^{-4}$ . This is obviously in striking contrast to the value of  $0.89 \times 10^{-4}$  deduced from the comparison of theory and experiment. This discrepancy in gold has also been pointed out by Khandelwal and Merzbacher.<sup>11</sup>

A possible explanation is that  $\rho_F < \rho_i + \rho_v$ , for close Frenkel pairs, or even  $\rho_F < \rho_v$ , for very close Frenkel pairs. It is conceivable that interference effects could give rise to such a phenomenon. If this effect were important in gold but not in copper, one could understand the observation that about 85% of the resistivity increase due to electron bombardment in copper, but only 30% in gold, disappears after an anneal at 80°K. However, this comparison is complicated by the fact that the extent of close pair recovery in gold is not known and close pair recovery may actually extend to 180°K.<sup>16</sup>

<sup>13</sup> G. J. Dienes and G. H. Vineyard, *Radiation Effects in Solids* (Interscience Publishers, Inc., New York, 1957), p. 66.

<sup>14</sup> A. W. Overhauser and R. L. Gorman, *Phys. Rev.* **102**, 676 (1956).

<sup>15</sup> R. O. Simmons and R. W. Balluffi, *Phys. Rev.* **125**, 862 (1962).

<sup>16</sup> D. W. Keefe and A. Sosin, *Bull. Am. Phys. Soc.* **9**, 282 (1964).

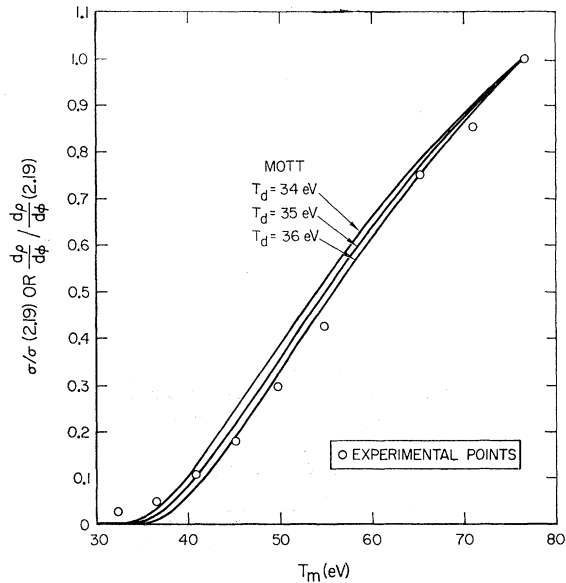


FIG. 3. Comparison of experimental results of  $d\rho/d\phi$  and the theoretical values of the displacement cross section normalized at 2.19 MeV, incident electron energy.

Using what we feel is a minimum value of  $\rho_F = 1.5 \times 10^{-4}$  ( $\rho_F = \rho_v$ ) we find, using Eq. (7), that the experimental values of  $\sigma_d(T_m)$  are smaller than the theoretical values by a factor of 0.6. Physically, this implies that the probability of a permanent removal of a gold atom from a lattice site is 0.6 if the polycrystalline specimen is bombarded by electrons capable of transferring 35 eV to a gold atom in a head-on collision. If one chooses a more realistic value of  $\rho_F$ , such as  $2.7 \times 10^{-4}$  the upper limit to the displacement probability is reduced to 0.3. This low value can best be understood by considering the directional nature of the displacement process (i.e., the assumptions underlying Eq. (10) are not good in gold, at least for the case of electrons of energy  $\leq 2$  MeV). In copper, the calculations of Gibson *et al.*<sup>17</sup> indicate that the threshold displacement energy in the  $\langle 100 \rangle$  direction,  $T_{d\langle 100 \rangle}$ , is lowest (about 25 eV),  $T_{d\langle 100 \rangle}$  is almost as low, but  $T_{d\langle 111 \rangle}$  is near 85 eV. Their calculation may not be correct in detail since the interaction potential was chosen on the basis of a calculated minimum value of  $T_d$  as 25 eV, whereas experimental measurements show the minimum value of  $T_d$  to be 16–19 eV.<sup>3</sup> A comparison of the theoretical and experimental values of  $\sigma_d$  for copper, using the experimental results for  $d\rho/d\phi$  of Sosin<sup>8</sup> and Lucasson and Walker<sup>1</sup> with a value of  $\rho_F = 1.2 \times 10^{-4}$  in Eq. (7), and the theoretical value of  $\sigma_d$  with a unit probability of displacement at  $T_e = 19$  eV yields fair agreement between theory and experiment. Thus, the lower value of displacement probability that appears in gold is an indication that directional effects are more important in gold than in

<sup>17</sup> J. B. Gibson, A. N. Goland, M. Milgram, and G. H. Vineyard, *Phys. Rev.* **120**, 1229 (1960).

TABLE I. Tabulation of displacement energies.

Author		Potential, $V(r)$ ( $r_0$ =nearest neighbor distance)	$A$ (eV)	$B$	$E_F^{(110)}$ (eV)	$E_s^{(110)}$ (eV)	$E_F^{(100)}$ (eV)	$E_1^{(100)}$ (eV)	$\frac{2}{5}E_1^{(100)}$ (eV)
Copper	Seeger <sup>a</sup>	$A \exp\{-B(r/r_0-1)\}$	0.0765	13.6	61.6	34.2			
			0.079	13.0	48.2	25.9			
			0.041	16.6	141.0	85.4			
	Lehman and Leibfried <sup>b</sup> Gibson <i>et al.</i> <sup>c</sup> Nelson and Thompson <sup>d</sup> Present work using Brinkman <sup>e</sup> potential	$A \exp\{-Br/r_0\}$ $\exp\{-Br/r_0\}$ $AZ^2e^2$ $1-\exp(-Ar)$	0.051	13.0	35.0	17.0			
			0.051	13.0	30.0	30	40	10	4
			$2 \times 10^4$	13.0	60.0		65	38.5	15.4
Gold	Seeger <sup>a</sup>	$A \exp\{-B(r/r_0-1)\}$	0.04	16.2	113	67			
			0.088	16.6	302	185			
			0.022	20.1	426	168			
	Nelson and Thompson <sup>d</sup> Present work using Brinkman <sup>e</sup> potential	$A \exp\{-Br/r_0\}$ $\exp\{-Br/r_0\}$ $AZ^2e^2$ $1-\exp(-Ar)$	$8 \times 10^5$	15.0	800		700	90	36
			in $\text{cm}^{-1}$	15.5	563			54	22
			$7.45 \times 10^8$						

<sup>a</sup> See Ref. 20.  
<sup>b</sup> See Ref. 21.  
<sup>c</sup> See Ref. 17.  
<sup>d</sup> See Ref. 22.  
<sup>e</sup> J. A. Brinkman, *Radiation Damage in Solids* (Academic Press Inc., New York, 1962), p. 830.

copper. Stated differently, Eq. (10) is a better approximation for copper than for gold for  $T_m \leq 65$  eV.

In gold, we suggest therefore, that displacements are possible only in a small solid angle centered about one crystallographic direction, most likely the  $\langle 100 \rangle$  direction, when  $T \gtrsim 35$  eV. The incorporation of this hypothesis into Eq. (9) is not possible at this time because the dependence of  $T_d$  on  $\theta'$  and  $\varphi'$  is not known. Attempts have been made by Sosin<sup>8</sup> and by Jan and Seeger<sup>18</sup> for copper and Erginsoy *et al.*<sup>19</sup> for  $\alpha$  iron to incorporate the directionality of the displacement process into the cross-section calculation.

We now turn to the lattice theory of displacements to

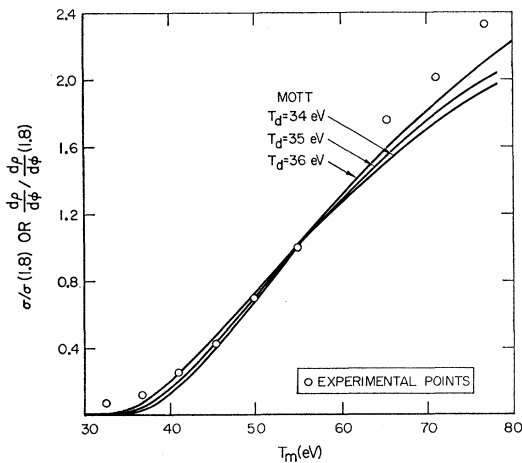


FIG. 4. Comparison of experimental results of  $d\rho/d\varphi$  and the theoretical values of the displacement cross section normalized at 1.8 MeV, incident electron energy.

<sup>18</sup> R. V. Jan and A. Seeger, *Stat. Phys. Sol.* **3**, 465 (1963).  
<sup>19</sup> C. Erginsoy, G. H. Vineyard, and A. Englert, *Phys. Rev.* **133**, A595 (1964).

investigate whether threshold displacement energies calculated from the interaction potentials of gold and copper can account for the experimental differences. We restrict our discussion to ejections in the closest packed direction,  $\langle 110 \rangle$  and  $\langle 100 \rangle$ . A copious amount of theoretical work has been done to determine the effect of close-packed directions on the propagation of energy and matter in fcc lattices. It is not the intent of this paper to review the literature in this field. A summary of the relevant results is given in Table I.  $E_F^{(110)}$  and  $E_F^{(100)}$  are defined as the upper energy limits of the propagation of energy (focussons), and, in addition, in the case of  $E_F^{(110)}$ , the upper energy limit of the propagation of matter (dynamic crowdion);  $E_s^{(110)}$  is defined as the lower energy limit of dynamic crowdion propagation, i.e., the threshold energy for displacements in a small solid angle about the  $\langle 110 \rangle$  direction.<sup>20,21</sup>  $E_1^{(100)}$  is the energy required to penetrate the plane defined by the four barrier atoms equidistant from the  $\langle 100 \rangle$  direction and halfway between the two atoms interacting in the  $\langle 100 \rangle$  direction.  $E_1^{(100)}$  was computed without taking the relaxation of the atoms into account and, therefore, its value is an upper limit. It is felt by Nelson and Thompson<sup>22</sup> that all collisions in the  $\langle 100 \rangle$  direction are of the replacement kind with a lower limit of  $\frac{2}{5}E_1^{(100)}$ .

Since we are interested in the creation of defects,  $\langle 110 \rangle$  focussons (not crowdions) are useful only to the extent that they create a defect at an imperfect region of the lattice, such as a stacking fault region or dislocation cores. This topic has been discussed by the authors<sup>3</sup> and it is felt that the magnitude of the effect is at most

<sup>20</sup> A. Seeger, *Radiation Damage in Solids* (International Atomic Energy Commission, Venice, 1962), Vol. I, p. 104.  
<sup>21</sup> C. Lehman and G. Leibfried, *Z. Physik* **162**, 203 (1961).  
<sup>22</sup> R. S. Nelson and M. W. Thompson, *Proc. Roy. Soc. (London)* **259**, 458 (1961).

a few percent of the total damage for the annealed samples used in the experiments.

We define a ratio

$$G = T_{d\langle 110 \rangle} / T_{d\langle 100 \rangle},$$

where  $T_{d\langle 110 \rangle} = E_z^{\langle 110 \rangle}$ , and  $\frac{2}{3}E_1^{\langle 100 \rangle} \leq T_{d\langle 100 \rangle} \leq E_1^{\langle 100 \rangle}$ .

The value of  $G$  should give an indication of the shape of the threshold displacement energy surface around the  $\langle 100 \rangle$  direction. Referring to Table I, we see that for copper,

$$G_{\text{Cu}} < 30/17 = 1.8,$$

with a more realistic value of

$$G_{\text{Cu}} \approx 22/17 = 1.2.$$

Here we have used the results of Gibson *et al.*<sup>17</sup> that the value of  $T_{d\langle 110 \rangle}$  and  $T_{d\langle 100 \rangle}$  are quite close with  $T_{d\langle 100 \rangle} \leq T_{d\langle 110 \rangle}$ , and a "low" experimental value of  $T_d = 17$  eV for copper.<sup>3</sup>

Recently, Thompson<sup>23</sup> measured  $E_F^{\langle 110 \rangle}$  for gold to be  $E_F^{\langle 110 \rangle} = 280 \text{ eV} \pm 50 \text{ eV}$  by a sputtering experiment. This is in good agreement with the value of  $E_F^{\langle 110 \rangle} = 302$  eV in Table I. This allows us to use the corresponding value of  $E_z^{\langle 110 \rangle} = 185$  eV calculated with the same potential with some confidence. This rather large value of  $T_{d\langle 110 \rangle}$  implies directly that the experimental value of  $T_d = 35$  eV is associated with displacements in the  $\langle 100 \rangle$  direction. This is in excellent agreement with the value  $T_{d\langle 100 \rangle} = 35$  eV measured by Thompson<sup>24</sup> in recent sputtering experiments on gold. Then we have for the value of  $G$  for gold

$$G_{\text{Au}} \approx 185/35 = 5.3.$$

We can best summarize the experimental results presented here for gold and derived from previous experiments in copper, and the calculations discussed in the last few paragraphs by referring to a threshold dis-

placement energy surface. This is a surface, in the reference frame of the crystal lattice, generated by a vector whose length is proportional to the magnitude of the minimum energy which an atom must receive to be permanently displaced if initially directed along the direction of the vector. In copper and gold (or any fcc metals, presumably), this surface has "valleys" along the major symmetry directions— $\langle 100 \rangle$ ,  $\langle 110 \rangle$ , and  $\langle 111 \rangle$ —representing local minima.

We suggest that the displacement threshold energy surface in gold has the shape of a deep and narrow valley around the  $\langle 100 \rangle$  direction, but in copper the  $\langle 100 \rangle$  valley is considerably more gentle and shallow. Furthermore, the minimum of the  $\langle 110 \rangle$  valley in gold occurs at an appreciably higher value than the minimum of the  $\langle 100 \rangle$  valley; whereas in copper the two valleys are almost equally deep. Thus, in agreement with Seeger,<sup>20</sup> we feel that for  $T_d(\text{min}) \leq T_m \leq T_d(\text{min}) + 30$  eV, the production of direct displacements in gold is primarily confined to the  $\langle 100 \rangle$  direction, producing most likely the split interstitial configuration. In copper, for the same energy range, displacements occur in both the  $\langle 100 \rangle$  and  $\langle 110 \rangle$  directions. This lends support to the two interstitial models originally proposed by Meechan *et al.*<sup>25</sup> and Seeger<sup>20</sup> for copper. Since in this model the crowdion is mobile with an activation energy near 0.1 eV ( $35^\circ\text{K} \rightarrow 55^\circ\text{K}$ ), we expect no significant recovery associated with free migration in this temperature range ( $35^\circ\text{K} \rightarrow 55^\circ\text{K}$ ) in gold since the crowdion is not produced. The resistivity recovery in gold will be discussed in subsequent papers.

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<sup>23</sup> M. W. Thompson, United Kingdom Atomic Energy Authority Memorandum AERE M1262 (unpublished).

<sup>24</sup> M. W. Thompson (private communication).

<sup>25</sup> C. J. Meechan, A. Sosin, and J. A. Brinkman, *Phys. Rev.* **120**, 441 (1960).