Displacement Cross Sections for Fast Electrons Incident on Gold*

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The displacement cross section for electrons producing radiation damage in solids has been computed, using the Mott series for relativistic Coulomb scattering. The results are compared with the widely used formula of Seitz and Koehler, based on a low-Z approximation due to McKinley and Feshbach. For low-Z elements, the formula of Seitz and Koehler was found to be accurate. For gold the displacement cross section computed from the Mott series is, in the region of 2–4 MeV bombarding energy, about twice as large as the value obtained from the approximate formula. The behavior of the cross section near threshold and at very high energies has been considered. For high-Z values the displacement cross section shows predominantly a parabolic rise near threshold. At very high energies it falls slowly toward a finite value. The implications of these calculations for various experiments on radiation damage in gold are briefly discussed.

I. INTRODUCTION

When a solid is irradiated with electrons, the lattice is damaged by the displacement of atoms.[1,2] In the most primitive model of the production of radiation damage by electrons it is supposed that the effective collisions are two-body Coulomb collisions between electrons and nuclei, which are assumed to be free and initially stationary. The binding of the atom to its lattice site is, then, taken into account by assuming further that an atom is certain to be displaced, and a vacancy created, if the energy T transferred in the collision to the atom exceeds a minimum value E_d, and that no damage occurs if the energy transfer is less than this critical amount. The theory resembles Bohr's original discussion of the scattering and energy loss of a charged particle traversing matter.[3]

The largest amount of energy is transferred to a free atom at rest in a head-on collision and is equal to

$$T_m=\frac{2ME(E+2mc^2)}{(M+m)^2c^2+2ME}, \tag{1}$$

where M is the mass of the struck atom, while m is the mass of the electron and E its initial kinetic energy. The energy transfer corresponding to a scattering angle θ can be determined from the approximate relationship

$$T=T_m\sin^2(\theta/2), \tag{2}$$

valid when $M\gg m$. In the naive model of radiation damage production, damage will occur only if the incident electron has an energy greater than a threshold value E_t which corresponds to a maximum energy transfer $T_m=E_d$. At energies $E>E_t$, all those electrons are effective in removing an atom from its lattice site which are scattered by an angle greater than θ_m given by the formula

$$E_d=T_m\sin^2(\theta_m/2). \tag{3}$$

Figure 1 shows, for several metals used in radiation damage studies, how T_m depends on E. Since E_d is of the order of 20–100 eV, it is seen that electrons can damage a solid only when they have relativistic energies. The cross section which measures the efficacy of an electron in producing damage must, therefore, be calculated by the use of relativistic quantum mechanics. Since the forces responsible for the electron scattering are Coulomb forces, and since atomic screening as well as the finite size of the nucleus is neglected, Mott's relativistic cross section formula for scattering from a point charge must be used.[4]

The quantity of greatest interest in the interpretation of radiation damage experiments is the displacement cross section,

$$\sigma_d=2\pi\int_{\theta_m}^{\pi}\frac{d\sigma}{d\Omega}\sin\theta d\theta. \tag{4}$$

More sophisticated displacement cross sections can be defined, taking into account the likelihood that in a

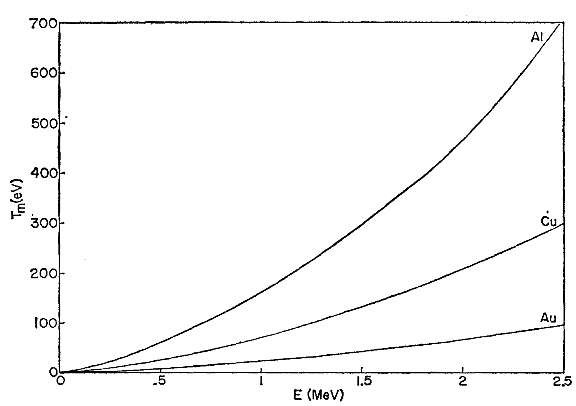

FIG. 1. Maximum energy transfer T_m in eV vs incident electron energy E in MeV for Al, Cu, and Au.

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[1] F. Seitz and J. S. Koehler, in *Solid State Physics*, edited by F. Seitz and D. Turnbull (Academic Press Inc., New York, 1956), Vol. 2, p. 305. Our notation follows the usage of this reference wherever possible.

[2] A. N. Goland, Ann. Rev. Nucl. Sci. **12**, 243 (1962).

[3] N. Bohr, Kgl. Danske Videnskab. Selskab, Mat. Fys. Medd. **18**, No. 8 (1948).

[4] M. E. Rose, *Relativistic Electron Theory* (John Wiley & Sons, Inc., New York, 1961), where references to the original work are found.

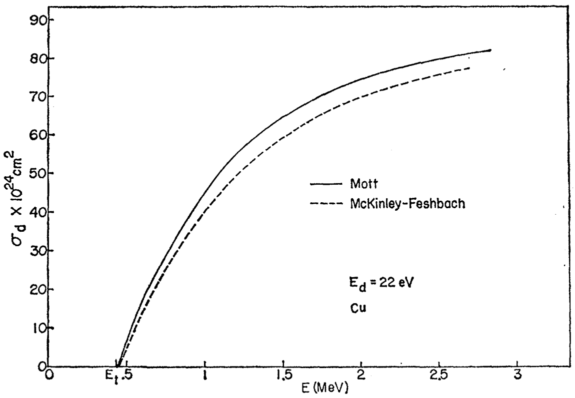

FIG. 2. Displacement cross section in barns vs incident energy E in MeV for copper. $E_d=22$ eV. The solid curve is exact; the dashed curve represents the McKinley-Feshbach approximation.

crystalline solid it might be easier to displace the atom in certain directions than in others, but for most purposes the crude definition given by Eq. (4) appears adequate.

In the past, workers in solid-state physics have usually been content to evaluate the differential Coulomb cross section for use in Eq. (4) on the basis of an approximate formula given by McKinley and Feshbach[5] who expanded the Mott series in powers of α and α/β. Here, $\alpha=Ze^2/\hbar c$ and $\beta=v/c$, v being the velocity of the electrons incident on a nucleus of charge Ze. Retaining only the first approximation of McKinley and Feshbach, Seitz and Koehler[1] derived a formula for the displacement cross section,

$$\sigma_d=\frac{\pi}{4}(b')^2\left\{\frac{T_m}{E_d}-1-\beta^2\ln\frac{T_m}{E_d}+\pi\alpha\beta\left[2\left(\frac{T_m}{E_d}\right)^{1/2}-\ln\frac{T_m}{E_d}-2\right]\right\},\quad(5)$$

where

$$b'=\frac{2Ze^2}{mv^2}(1-\beta^2)^{1/2}.\quad(6)$$

It was the purpose of this work to evaluate the displacement cross section for various values of v and Z, notably for gold, by accurate numerical computation, using the original Mott series. A comparison of the results with those obtained from the approximation (5), to be referred in the following as the *McKinley-Feshbach approximation*, is made.[6]

II. CALCULATION

A program was written in GAT language for the UNIVAC 1105, similar to the program outlined by Sherman.[7] Our program was tested by comparison with Sherman's and Feshbach's[8] results. The calculations covered the energy region below 4 MeV thoroughly, but a few sample points at higher energies were also obtained. For aluminum ($Z=13$) the McKinley-Feshbach approximation was verified to be in excellent agreement with the exact results. For copper ($Z=29$), Fig. 2 shows the Mott displacement cross section to exceed the McKinley-Feshbach approximation by a few percent—far too little to affect significantly the interpretation of radiation damage work on copper. The value of E_d chosen, 22 eV, is that inferred from radiation damage experiments.[9]

For gold ($Z=79$), the expansion parameters α and α/β are quite close to unity, and as remarked by Seitz and Koehler,[1] the first-order McKinley-Feshbach approximation is not expected to be useful. Indeed, Figs. 3 and 4 show a considerable departure of the Mott values from the approximate ones. The choice of E_d, 40 eV in Fig. 3 extending from threshold to 4 MeV, and 44 eV in the close-up of Fig. 4, was somewhat arbitrary but dictated by the experimental finding that E_d is greater than 40 eV.[9]

Similarly, it is known from residual resistivity measurements in gold[10] after irradiation with electrons of 2.54 MeV that E_d must surely be less than 100 eV. In order to utilize this experimental information for an approximate determination of E_d, it was thought worthwhile to compute the displacement cross section for gold at the fixed bombarding energy of $E=2.54$ MeV as a function of E_d. The results are shown in Fig. 5 and will be discussed in Sec. IV.

III. LOW- AND HIGH-ENERGY LIMITS

Since some determinations of E_d proceed by an attempt to locate experimentally the threshold energy

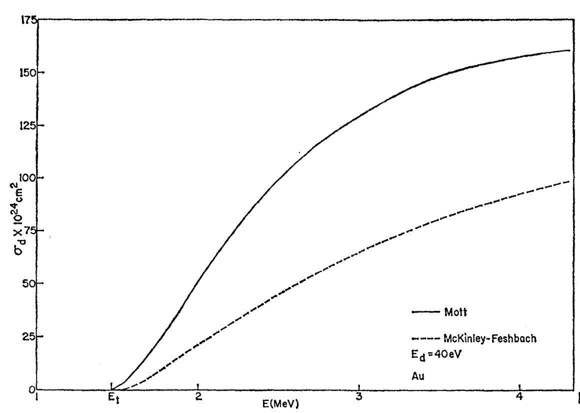

FIG. 3. Displacement cross section in barns vs incident electron energy E in MeV for gold. $E_d=40$ eV. The solid curve is exact; the dashed curve represents the McKinley-Feshbach approximation.

[5] W. A. McKinley, Jr., and H. Feshbach, Phys. Rev. **74**, 1759 (1948).
[6] E. Merzbacher and G. S. Khandelwal, Bull. Am. Phys. Soc. **7**, 543 (1962). See also O. S. Oen, ORNL Report 3464, 1962, p. 26 (unpublished).
[7] N. Sherman, Phys. Rev. **103**, 1601 (1956).
[8] H. Feshbach, Phys. Rev. **88**, 295 (1952).
[9] P. G. Lucasson and R. M. Walker, Phys. Rev. **127**, 485 (1962).
[10] J. B. Ward and J. W. Kauffman, Phys. Rev. **123**, 90 (1961).

TABLE I. Displacement cross section for electrons of energy E incident on Au ($Z=79$). $E_d=40$ eV was assumed.

	σ_d (b)	
E (MeV)	McKinley-Feshbach	Mott
2	20.1	50.7
4	93.2	158.9
6	118.9	165.9
8	128.3	159.2
10	131.7	151.8
20	130.7	131.2
∞	109.8	109.8

E_t, it is of interest to note that for high Z elements the rise of the displacement cross section very near the threshold can be adequately represented by the form $C(E-E_t)^2$. For gold, Fig. 4 shows this to be true for the McKinley-Feshbach as well as the Mott values of the cross section. For the former such a behavior near threshold can be deduced from an expansion in powers of $y=(T_m-E_d)/E_d$ of Eq. (5):

$$\sigma_d=\tfrac{1}{4}\pi(b')^2[(1-\beta^2)y+\tfrac{1}{2}\beta(\beta+\tfrac{1}{2}\pi\alpha)y^2+\cdots]. \quad (7)$$

A linear term is seen to be present but with a coefficient much smaller than that of the quadratic term. An expansion in powers of $(E-E_t)$ has a similar structure. Since E_d depends sensitively on the value of E_t, these results suggest caution in the determination of E_t and E_d by extrapolation of cross section data taken in the vicinity of the threshold.

At extremely high energies the displacement cross section approaches a constant value because with increasing E the intrinsic decrease of the differential cross section is compensated by the increase of $1/\theta_m$ as θ_m approaches zero. Indeed, from Eqs. (1), (2), and (3) it is seen that as E increases, asymptotically,

$$\theta_m\sim\frac{1}{E}(2E_dMc^2)^{1/2}. \quad (8)$$

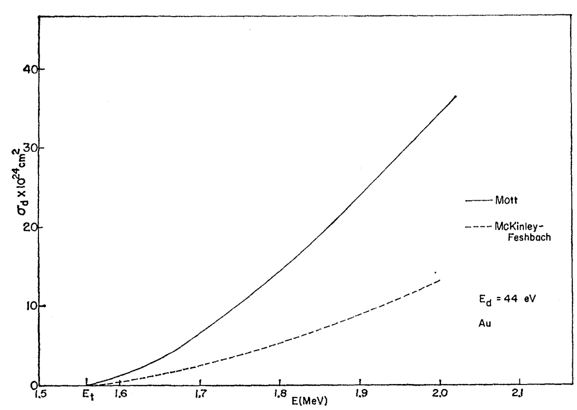

FIG. 4. Near-threshold behavior of displacement cross section in gold. $E_d=44$ eV. The solid curve is exact; the dashed curve represents the McKinley-Feshbach approximation.

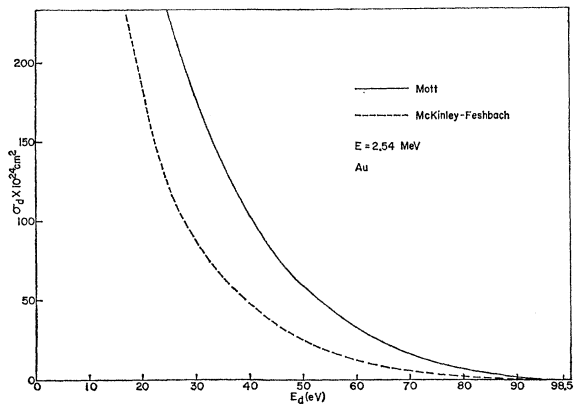

FIG. 5. Displacement cross section in barns vs E_d in eV for gold at a fixed energy (2.54 MeV) of incident electrons, see reference 10. The solid curve is exact; the dashed curve represents the McKinley-Feshbach approximation.

In the extreme high-energy limit, small angle scattering makes a dominant contribution to the displacement cross section. Near $\theta=0$, the differential cross section approaches the relativistic Rutherford value[11]

$$\frac{d\sigma}{d\Omega}=\frac{(b')^2}{16}\frac{1}{\sin^4(\theta/2)},$$

and with this value the displacement cross section will obviously approach

$$\sigma_d\sim\frac{\pi(b')^2}{8}\int_{\theta m}\frac{\theta d\theta}{(\theta/2)^4}=\frac{\pi(b')^2E^2}{2E_dMc^2}=\frac{2\pi Z^2e^4}{E_dMc^2}=140\frac{Z^2}{E_dA}\text{ b}, \quad (9)$$

where the numerical factor applies if E_d is given in eV.

The asymptotic value of σ_d is approached at an energy of about 10 MeV for low-Z elements. However, for Au and $E_d=40$ eV, the limiting value of the displacement cross section, 110 b, is approached much more slowly as can be seen from Table I. This table also shows that the displacement cross section has a maximum, which in the example at hand (Au, $E_d=40$ eV) is near $E=6$ MeV. At even higher energies the cross section *decreases* toward its asymptotic value, but it must be remembered that at such high energies the assumption of scattering from a point nucleus is no longer valid.

IV. CONCLUSIONS

Ward and Kauffman[10] have measured the increase in resistivity in a gold specimen after irradiation with 2.54-MeV electrons. Assuming that one electron is incident per cm^2, they found the change in resistivity to be $\Delta\rho_e=1.5\times10^{-26}$ Ω cm per (electron/cm^2). For a sample sufficiently thin to insure the absence of multiple

[11] J. H. Bartlett and R. E. Watson, Proc. Am. Acad. Arts Sci. **74**, 53 (1940).

large-angle scattering events, $\Delta\rho_e$ is related to the increase in resistivity $\Delta\rho_f$ due to the presence of one Frenkel pair (vacancy and interstitial) by the equation

$$\Delta\rho_e = \sigma_d \Delta\rho_f.$$

The resistivity increase due to a vacancy[12,13] is about $\Delta\rho_v = 1.7\times10^{-4}$ Ωcm. The resistivity increase $\Delta\rho_i$ due to an interstitial has not been measured; theoretical estimates of it vary greatly[14] but suggest that $\Delta\rho_i$ is greater than $\Delta\rho_v$. If the resistivity increase due to a Frenkel pair is the sum of the resistivities contributed by a vacancy and an interstitial, we can assume that

$$\Delta\rho_f > 1.7\times10^{-4}\ \Omega\ \text{cm}.$$

This estimate gives an upper bound for the value of the displacement cross section,

$$\sigma_d < 90\ \text{b}.$$

Using Fig. 5, we conclude that E_d for Au is presumably greater than 40 eV in agreement with the findings of Lucasson and Walker.[9] Recent experiments[15] suggest that E_d may be less than 40 eV. If this is so, it would appear either that the interstitials make an almost negligible contribution to the Frenkel resistivity, or that near threshold $\Delta\rho_f$ is not simply the sum of $\Delta\rho_v$ and $\Delta\rho_i$, or that the simple theory of the displacement cross section upon which this analysis is based is in need of revision.

ACKNOWLEDGMENTS

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[13] R. P. Huebener and C. G. Homan, Bull. Am. Phys. Soc. **7**, 543 (1962).
[14] G. J. Dienes and G. H. Vineyard, *Radiation Effects in Solids* (Interscience Publishers, Inc., New York, 1957), p. 66.
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Temperature Dependence of Lattice Parameters for Gd, Dy, and Ho

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The lattice parameters of single-crystal Gd, Dy, and Ho have been measured over their temperature ranges of magnetic ordering. The c axis and volume of all three hexagonal close-packed structures were found to increase with decreasing temperature below their respective Néel or Curie points. The temperature dependence of the c axes is in reasonable agreement with the exchange magnetostriction theory of Kittel. Discontinuities in the c axes were found for Dy and Ho, and a structure change to orthorhombic was found in Dy, at the antiferromagnetic-ferromagnetic transitions. This structure change is believed to account for the extraordinarily large values of magnetostriction reported for Dy.

INTRODUCTION

The series of heavy rare earths provide a system exhibiting complex magnetic spin structures with strong dependence on temperature.[1] Spiral configurations of several varieties, and first-order transitions between antiferromagnetic and ferromagnetic states, arise from energy balance among long-range exchange interactions, anisotropy resulting from crystal field–spin orbit effects, and direct exchange. Since indirect exchange in particular may depend strongly on crystal dimensions, and since Kittel has shown[2] that the interplay between exchange and elastic forces can give rise to first-order magnetic transitions when critical lattice dimensions are achieved through normal temperature variations, it is of interest to study the crystal cell dimensions as a function of temperature. This paper reports such studies for Gd, Dy, and Ho and discusses the measurements in terms of the magnetic properties and theories of the heavy rare earth metals.

EXPERIMENTAL DETAILS

The rare earths studied were in the form of single-crystal platelets approximately 0.1 mm thick and 1 mm² in area. The plate face was the (001) plane in all crystals examined. The crystals were found by spectrographic analysis to contain a total of 0.1% impurities, consisting mostly of the other rare earths. Lattice parameters were determined from 2θ values measured on a General Electric XRD-5 diffractometer. Scintillation counter output was displayed on a recorder chart together with angle markers, and peak positions were read from the chart to the nearest 0.01 deg. High-order reflections were used, e.g., (00 14) for c, and (700) and (440) for a.

* Contribution No. 848.
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