

ON THE NUMBER OF ATOMS DISPLACED BY IMPLANTED IONS OR ENERGETIC RECOIL ATOMS

Cite as: Appl. Phys. Lett. **14**, 114 (1969); <https://doi.org/10.1063/1.1652730>

Submitted: 03 October 1968 . Published Online: 17 October 2003

P. Sigmund



View Online



Export Citation

ARTICLES YOU MAY BE INTERESTED IN

[Molecular dynamics simulation of radiation damage cascades in diamond](#)

Journal of Applied Physics **117**, 245901 (2015); <https://doi.org/10.1063/1.4922457>

[Recoil contribution to ion-implantation energy-deposition distributions](#)

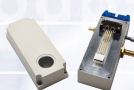
Journal of Applied Physics **46**, 3385 (1975); <https://doi.org/10.1063/1.322243>

[Ion and electron irradiation-induced effects in nanostructured materials](#)

Journal of Applied Physics **107**, 071301 (2010); <https://doi.org/10.1063/1.3318261>



**THE WORLD'S RESOURCE FOR
VARIABLE TEMPERATURE
SOLID STATE CHARACTERIZATION**



OPTICAL STUDIES SYSTEMS



SEEBECK STUDIES SYSTEMS



MICROPROBE STATIONS



HALL EFFECT STUDY SYSTEMS AND MAGNETS

WWW.MMR-TECH.COM

AIP
Publishing

rors M_3 and M_4 , and adjusting the uncompressed pulse delay by moving P_3 , it is possible to direct most of the beam of the uncompressed pulse and part of the compressed pulse beam below the beam splitter and have these pulses scan across each other inside the dye cell, thereby obtaining a measure of the squared envelope function $A^2(t)$. Actually, the fluorescence intensity is proportional to $\int A^2(t)B^2(t-t')dt$, which approximates $A^2(t')$ when the function $B^2(t-t')$ is sufficiently narrow. At the same time, that part of the compressed pulse that is intersected by the beam splitter produces a fluorescence intensity proportional to $\int B^2(t)B^2(t-t')dt$, which usually appears as a sharp line in the photograph, and one can estimate readily the degree of resolution in the envelope measurement from the sharpness of this line. [If this latter fluorescence intensity display produces a sharp line, we have some confidence that we are measuring an average $A^2(t)$ that is heavily weighted in favor of a small number of identical pulses.]

Although an accurate measure of $A^2(t)$ will require more sophisticated photographic techniques than we are using at present, two interesting results have been obtained. First, the width of the display for the scan of the uncompressed pulse with itself [$\int A^2(t)A^2(t-t')dt$] is considerably narrower than for the simultaneously measured scan of the compressed with the uncompressed pulse [$\int A^2(t)B^2(t-t')dt$], as would be expected. The ratio of the widths appears to be about 1.4. (It would approach $\sqrt{2}$ for Gaussian pulses with large compression ratio.) The second result is that the pulse envelope is unsymmetrical,¹¹ and in all cases observed so far the rise time of the pulse is larger than the fall time. Figure 4 shows a microdensitometer trace of a (squared) pulse envelope made in this way. The asymmetry is greater in this particular pulse than in any of the other pulses measured so far. The ratio of rise time to fall time is

about three on the microdensitometer trace, although the cut-off may be actually sharper, the trace being limited by the resolution of the microdensitometer. Pulse shape measurements made with single pulses will probably be more meaningful than those averaged over the pulse train.

It is a pleasure to acknowledge the technical assistance of R. Bodurtha and R. Michaud as well as the many fruitful discussions with W. H. Glenn and A. J. DeMaria.

Note added in proof. The width ratio referred to above would be expected to be the other way around. Our result is probably due to the low amplitude part of the pulse that is not readily visible in the ordinary display. The author is indebted to Robert A. Fisher for pointing out this error.

¹A. J. DeMaria, D. A. Stetser, and H. A. Heynau, *Appl. Phys. Letters* 8, 174 (1966).

²A. J. DeMaria, D. A. Stetser, and W. H. Glenn, Jr., *Science* 156, 1557 (1967).

³J. A. Armstrong, *Appl. Phys. Letters* 10, 16 (1967)

⁴W. H. Glenn, M. J. Brienza, *Appl. Phys. Letters* 10, 221 (1967).

⁵J. A. Giordmaine, P. M. Rentzepis, S. L. Shapiro, and K. W. Wecht, *Appl. Phys. Letters* 11, 216 (1967).

⁶A. J. DeMaria, W. H. Glenn, Jr., M. J. Brienza, and M. E. Mack, *Proc. IEEE* (January 1969).

⁷C. E. Cook, *Proc. IRE* 48, 310 (1960).

⁸J. R. Klauder, A. C. Price, S. Darlington, and W. J. Albersheim, *Bell System Tech. J.* 39, 745 (1960).

⁹E. B. Treacy, *Phys. Letters* 28A, 34 (1968).

¹⁰This measurement was suggested by W. H. Glenn.

¹¹Simultaneous measurements of the scan of the pulse with itself always give the expected symmetry.

ON THE NUMBER OF ATOMS DISPLACED BY IMPLANTED IONS OR ENERGETIC RECOIL ATOMS*

P. Sigmund †

Metallurgy Division, Argonne National Laboratory
Argonne, Illinois 60439

(Received 3 October 1968)

The validity of the Kinchin-Pease formula is re-examined on the basis of recent progress in the theory of collision cascades and irradiation experiments on semiconductors and metals.

The average number of Frenkel pairs produced in a solid by an energetic heavy ion or recoil atom is

usually estimated by the formula¹

$$N(E) = E/2E_d, \quad (1)$$

where E is the ion energy and E_d an effective displacement threshold energy. Despite frequent use of this formula, its validity has never been confirmed experimentally. Contrary, it has been an

*This work was performed under the auspices of the U.S. Atomic Energy Commission.

†Visiting Scientist on leave from Kernforschungsanlage, Jülich, Germany.

intriguing problem for many years that Eq. (1) appeared to overestimate $N(E)$ in irradiated metals and semiconductors by a factor of two to ten,² and the only attempt to measure the energy dependence of $N(E)$ over a large energy range (50–200-keV recoil atoms in gold) gave a quadratic rather than linear relationship.³ Several attempts to modify Eq. (1) by improving the underlying assumptions^{4–7} were more or less successful in pushing $N(E)$ down to smaller values as compared to Eq. (1), but the great number of uncertain parameters made reliable predictions virtually impossible.

A new feature came into this discussion when Davies *et al.*⁸ reported as many as 3000 displaced atoms per ion in silicon crystals bombarded with 40-keV Sb⁺ ions. With their technique—backscattering of a channeled 1-MeV He⁺ beam—they detect every atom displaced more than ~ 0.2 Å from a lattice site and not located in a regular interstitial hole. This result is insensitive to implantation temperature between about 100° and 300°K.⁹ Since E_d is about 14 eV in Si,¹⁰ $N(E)$ would be 1400 according to Eq. (1). The question arises whether we deal with 3000 dynamical displacement processes, such that we would have the first example where Eq. (1) *underestimates* the damage rate; in other words, can we push the theoretical “prediction” up by a factor of two?

Let us recall the assumptions underlying Eq. (1). (1) Random slowing-down. (2) Elastic collisions. (3) Hard-sphere scattering. (4) An atom recoiling with energy T is displaced when $T > E_d$. (5) No energy is lost if $T > E_d$ while all energy is lost if $T < E_d$. (6) An atom of energy E makes a replacement collision if $E - T < E_d$.

Assumption (1) *overestimates*⁶ $N(E)$, so we may neglect lattice effects throughout this paper. If assumptions (2) and (3) are dropped Eq. (1) is modified to

$$N(E) = \xi \nu(E)/(2E_d), \quad (1a)$$

where $\nu(E)$ is the amount of energy *not* lost to electronic excitation,⁵ and ξ a factor < 1 dependent on the atomic interaction.^{5,7} Recent calculations¹¹ indicate that $\xi \approx 0.8$. If we want to be flexible with respect to assumptions (4)–(6) it is convenient to consider the *recoil density* $F(E, E_0)dE_0$, defined as the average number of atoms recoiling with an energy (E_0, dE_0) as a consequence of a primary ion slowing down from E to zero energy. $F(E, E_0)$ satisfies the following integral equation:

$$0 = \int_0^E K(E, T) dT [F(E, E_0) - F(E-T, E_0) - F(T-U, E_0) - \delta(T-E_0)], \quad (2)$$

where $K(E, T)$ is the differential cross section and U a binding energy lost by an atom when leaving a lattice site. Equation (2) holds strictly only for elastic collisions, but electronic energy loss could easily be superimposed. It is also assumed that the primary ion is of the same type as the target atoms, but generalization to unequal masses is

straightforward. Equation (2) is similar to the equation defining the collision density,¹² the main difference being that the collision density counts *both* collision partners after every collision, which would add another source term $\delta(E-T-E_0)$ in Eq. (2).

If we solve Eq. (2) for the power approximation of the Thomas-Fermi cross section,¹³ $K(E, T) \propto E^{-m} T^{-1-m}$, where $0 \leq m \leq 1$ we obtain the asymptotic solution

$$F(E, E_0) = \frac{m}{\psi(1) - \psi(1-m)} \frac{E}{(E_0 + U)^{1-m} E_0^{1+m}}, \quad (3)$$

for $E \gg E_0 \gg U$,

where $\psi(x) = d[\ln \Gamma(x)]/dx$. This result is asymptotically exact and has been derived by use of Laplace transform⁷ in connection with a series expansion in powers of U . Equation (3) holds also for unequal masses of ion and target.

Since a recoiling atom is displaced when $E_0 > E_d$ we get

$$N(E) = \int_{E_d}^E dE_0 F(E, E_0) = \frac{(1+U/E_d)^m - 1}{\psi(1) - \psi(1-m)} \frac{E}{U}, \quad (4)$$

for $E \gg E_d \gg U$.

It can be shown¹¹ that m has to be chosen in such a way that $K(E, T)$ describes collisions at *low* energies, i.e., $2E_d \approx E \approx 100 E_d$. This means¹³ $m \lesssim 1/4$. For $m = 0$ Eq. (4) reads

$$N(E) = \frac{6}{\pi^2} \frac{E}{U} \ln(1+U/E_d). \quad (4a)$$

This is an *upper limit* for the number of displaced atoms since loss of defects by replacement collisions has been neglected.

Since current models for displacement processes in metals and semiconductors are substantially different from each other, we divide the following discussion into two parts.

I. Semiconductors. We adopt the displacement model of Bäuerlein,¹⁴ i.e., E_d is determined by the number of bonds to be disrupted, $E_d = 4E_b$ for Si and Ge, where E_b is the bond energy. This implies that a dislodged atom does not have to travel far away from its site to form a stable defect, otherwise E_d would be higher. It also implies that replacement collisions, though possible, do not lead to a loss of defects, so Eq. (4a) should be adequate. With $U = E_d = 4E_b$ we obtain from Eq. (4a) $N(E) = 0.42 (E/E_d)$, which is essentially the same result as Eq. (1a), despite rather different underlying assumptions. Note that the present assumptions are those of Snyder and Neufeld,¹⁵ except for the cross section.

In a cascade where many defects are created, some atoms need not break all four bonds to get displaced. In fact, if *all* atoms within a certain region were displaced, only two bonds would have to be disrupted per atom, in the average. This would result in an increase of $N(E)$ by about a fac-

tor of 2. However, using recent estimates of the volume covered by high-energy cascades,^{16,17} we obtain $V(E) \approx 220 (E/\text{keV})^2$ atomic volumes for $E \lesssim 100$ keV in Sb⁺-bombarded Si, so a 40 keV cascade extends over a volume of about 360 000 atoms. If this figure is compared to the 3000 observed displaced atoms,⁸ it is realized that the assumption of all bonds being broken within a certain volume is hardly justified. Hence we conclude that collision cascade theory cannot account for 3000 displaced atoms under these experimental conditions. Note especially that we have left out of consideration the fact that the figure of Davies *et al.*⁸ does not include atoms knocked off into regular interstitial holes, and that the damage rate may be higher at some very low temperature. Both effects enhance the discrepancy.

It is supposed that an appreciable part of the observed effect is due to atoms surrounding vacancies and/or interstitials that are detected by the channeling technique because of lattice distortions (and, perhaps, enhanced vibrational amplitudes) greater than ~ 0.2 Å around the defects. At least in copper relaxations of this order of magnitude have been shown feasible by computer calculations.¹⁸ In view of the rather large concentration of defects (about 1%) it may even be that all atoms within the region of greatest defect density relax by a measurable amount. If this were the case, the measured $N(E)$ should not be linear in E , probably increase less steeply in the energy range under consideration.

II. Metals. A characteristic feature of displacements in metals is the large recombination volume of an isolated point defect, of the order of 100 atomic volumes or more.¹⁹ Thus, E_d is determined by the energy lost to the environment by an atom trying to escape the recombination volume. This has the consequence that in cascades many defects are lost by replacement collisions.²⁰ The bonding energy U is only a few eV²⁰ and thus negligible as compared to E_d . Equation (4a) predicts $N(E) = (6/\pi^2) E/E_d = 0.61 E/E_d$, which is about 50% more than the previous result Eq. (1a) that took into account replacement collisions. Actually, because of lattice structure there may be even more replacement collisions, resulting in a still lower damage rate²⁰ than Eq. (1a).

However, especially in heavy metals, defect densities in keV cascades calculated from Eq. (1a) may become much higher than the stability limit determined by the recombination volume. In gold, for example, the primary concentration of Frenkel pairs has been estimated¹⁷ $c_F(E) \approx \text{keV}/2.1 E$ for $E \lesssim 1$ MeV, which means oversaturation at energies below about 100 keV. In an oversaturated cascade the number of stable defects is essentially determined by the volume of the primary damage and has little or no connection with the Kinchin-Pease formula. In gold we get¹⁷ $V(E) \approx 7 (E/\text{keV})^2$ atomic volumes. Assuming a recombination volume of 135 atomic volumes¹⁹ this yields

$$N(E) \approx 0.05 (E/\text{keV})^2 \text{ for } E \lesssim 100 \text{ keV} \quad (5)$$

in Au,

for a homogeneous distribution of vacancies and interstitials within $V(E)$. This will generally *underestimate* the damage, since considerable clustering of vacancies takes place,²¹ and thus higher defect concentrations can be achieved. Nevertheless, it is seen that $N(E)$ can be more than an order of magnitude smaller than Eq. (1a) would predict. Also, $N(E)$ may be proportional to E^2 , consistent with a preliminary experimental result.³ It is important to note that Eq. (5) is not valid at low energies where cascade dimensions may be modified by replacement sequences.²⁰ Thus, for small cascades in aluminum at a few hundred eV, the linearity of $N(E)$ with energy has been established recently.²² In gold, because of the small "random" dimensions, this linearity region may extend up to a few keV.

In very light metals the primary defect density is usually small enough to prevent spontaneous recombination from being dominant. In fact, measured damage rates in aluminum correspond closely to the expected value.² In heavier metals, however, in the energy range encountered in irradiations with neutrons, protons, etc., the deviations from the Kinchin-Pease formula may be so drastic because of rearrangement processes that Eq. (1) may not even be an order-of-magnitude estimate.

The author thanks J. A. Davies, L. Eriksson, and J. W. Mayer for extensive discussions. Interesting comments by H. H. Andersen, T. H. Blewitt, R. M. J. Cotterill, K. L. Merkle, and J. Wurm are gratefully acknowledged.

¹G. H. Kinchin and R. S. Pease, Rept. Progr. Phys. 18, 1 (1955).

²For a recent analysis of experiments on metals see W. Köhler and W. Schilling, Nukleonik 7, 389 (1965).

³W. Schilling and J. Völkl, Kernforschungsanlage Jülich Report, Jül-464 RW (1967).

⁴C. Lehmann, Nukleonik 3, 1 (1961).

⁵J. Lindhard and P. V. Thomsen in Radiation Damage in Solids (IAEA, Vienna, 1962), Vol. 1, p. 65.

⁶O. S. Oen and M. T. Robinson, Appl. Phys. Letters 2, 83 (1963); P. Sigmund, Phys. Letters 6, 251 (1963).

⁷M. T. Robinson, Phil. Mag. 12, 741 (1965); 17, 639 (1968).

⁸J. A. Davies, J. Denhartog, L. Eriksson, and J. W. Mayer, Can. J. Phys. 45, 4073 (1967).

⁹J. W. Mayer (private communication).

¹⁰R. L. Novak, Bull. Am. Phys. Soc. 8, 235 (1963).

¹¹P. Sigmund, Radiation Eff. (to be published).

¹²J. B. Sanders, Physica 32, 2197 (1966); M. T. Robinson, Phil. Mag. 12, 145 (1965).

¹³J. Lindhard, V. Nielsen, and M. Scharff, Kgl. Danske Videnskab. Selskab, Mat. Fys. Medd. 36, No. 10 (1968).

¹⁴R. Bäuerlein in *Radiation Damage in Solids*, D. S. Billington, Ed. (Academic Press Inc., New York, 1962), p. 358.

¹⁵W. S. Snyder and J. S. Neufeld, Phys. Rev. 97, 1636 (1955).

¹⁶P. Sigmund and J. B. Sanders, Proceedings of the International Conference on Applications of Ion Beams to Semiconductor Technology, P. Glotin, Ed. (Editions Ophrys, Paris, 1967), p. 215.

¹⁷P. Sigmund, G. P. Scheidler and G. Roth, Proceedings of the International Conference on Solid State Physics Research with Accelerators, A. N. Goland, Ed., Brookhaven Report BNL 50083 (C-52),

p. 374 (1968).

¹⁸M. Doyama and R. M. J. Cotterill in *Lattice Defects and Their Interactions*, R. R. Hasiguti, Ed. (Gordon & Breach, Science Publishers, Inc., New York, 1967), p. 79.

¹⁹F. Dworschak, C. Lehmann, H. Schuster, H. Wollenberger, and J. Wurm, Proceedings of the International Conference on Solid State Physics Research with Accelerators, A. N. Goland, Ed., BNL 50083 (C-52), p. 327 (1968).

²⁰C. Erginsoy, G. H. Vineyard, and A. Englert, Phys. Rev. 133A, 595 (1964).

²¹P. Sigmund, Bull. Am. Phys. Soc. 13, 464 (1968).

²²J. Wurm, F. Dworschak, H. Schuster, and H. Wollenberger, Verhandl. DPG (VI) 3, 86 (1968).