Dynamics of Radiation Damage in a Body-Centered Cubic Lattice. II. Higher Energies*

C. ERGINSOY, G. H. VINEYARD, AND A. SHIMIZU†
Brookhaven National Laboratory, Upton, New York
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Computer studies in the dynamics of radiation damage in a body-centered cubic lattice representing α iron are extended to knock-on energies up to 1500 eV. The mean number N_d of defects created is calculated first for a knock-on of 100 eV in a large variety of directions. In one "representative" direction the knock-on energy is varied up to 1500 eV. It is seen that N_d increases approximately linearly with knock-on energy E. The usual formula $N_d=E/2E_d$ can be used with an effective threshold energy E_d of 50 to 55 eV. Dynamic features of a single collision and a cascade of collisions are investigated. The free-atom binary model is not adequate for a single collision for the purpose of estimating the transfer of kinetic energy. In a cascade, the initially localized kinetic energy of the knock-on is seen, in a relatively short time, to divide into equal amounts of potential energy in the lattice and total kinetic energy of moving atoms. The process of channeling of an iron atom projected into the lattice along a low-index direction is studied with the same model. The range of the channeled atom is found to be proportional to the $\frac{3}{2}$ power of its initial energy, in disagreement with the predictions of the impulse approximation and in agreement with recent experiments.

1. INTRODUCTION

IN the previous paper in this series,[1] radiation damage events in a body-centered cubic lattice representing α iron were investigated at near-threshold energies. In the present paper we continue this work and investigate events initiated by selected knock-ons of energies up to 1500 eV. The same model of iron and the same computational techniques are used that were described in I. References to earlier work on face-centered cubic lattices, in which the computational techniques were first developed and were applied to a model of copper, are also to be found in I. Since the publication of that paper, a detailed account of the computer programs has been issued in the form of an internal report.[2]

The general scheme is to consider a set of several hundred to a thousand atoms, interacting with fairly realistic forces, augmented by special forces on the boundary atoms simulating the influence of the surrounding material. Initially, the atoms are at rest on the sites of a perfect lattice, and the start of a radiation damage event is taken to be the sudden transfer of momentum to one of the atoms in the set (the primary knock-on) by an irradiating particle. The classical equations of motion of all the atoms in the set are then solved by a high-speed computer. This gives a detailed description of the dynamic stages of the damage process and also the final configuration of the crystal in its damaged state after the agitation has subsided.

In the present paper a systematic investigation of the damage produced by knock-ons of a large variety of directions at 100 eV is first presented. Also results of a series of dynamic events in which the knock-on had an energy up to 1500 eV in certain selected directions are given. The transfer of energy from the knock-on to the first struck atom is investigated in detail. A correlation is found between the direction of the primary knock-on and the direction of motion and kinetic energy of the first struck atom (the secondary knock-on). Conclusions are reached concerning the average number of lattice defects produced, as a function of the energy of the primary knock-on, up to 1500 eV. Finally, an investigation of the process of channeling of an energetic atom in a crystal lattice, encountered in ion-bombardment experiments, is made by means of the same computational methods for the case of an energetic iron atom introduced into an α-iron lattice. Channeling for the $\langle 100\rangle$ and $\langle 111\rangle$ directions is considered. The form of the energy dependence of the maximum range of channeled atoms is deduced.

2. EVENTS INITIATED BY A 100-eV KNOCK-ON

In I the displacement probability $P_d(E)$ (defined as the probability for creating at least one Frenkel pair by a knock-on of energy E and random direction) was calculated numerically for our model of α iron. It was shown that the $P_d(E)$ versus E curve has a "two-step" nature and rises rather slowly with energy from zero at $E\sim 18$ eV. It reaches 0.5 at $E\sim 40$ eV and 0.75 at $E\sim 60$ eV.

In order to investigate damage events in which at least one defect is always created, i.e., the realm where $P_d(E)=1$, we have chosen a knock-on energy of 100 eV and have carried out a large number of calculations (49 dynamic runs) at this energy with different knock-on directions. A knock-on of 100 eV in iron can be produced by bombardment with electrons of 2.5 MeV or above.

Single vacancies, divacancies, and double vacancies were produced in these events, together with the corresponding number of interstitials. By a divacancy we

* Work performed under the auspices of the U. S. Atomic Energy Commission.
† Permanent address: NAIG Nuclear Research Laboratory, Kawasaki, Japan.
[1] C. Erginsoy, G. H. Vineyard, and A. Englert, Phys. Rev. 133, A595 (1964), to be referred to as I throughout the present paper.
[2] A. Larsen, Brookhaven National Laboratory Report 7979 (unpublished), available on request from the Technical Information Division, Brookhaven National Laboratory, Upton, New York, 11973.

mean two vacancies in nearest sites. Results are given in Fig. 1, which shows a stereographic plot of the knock-on directions together with the number and type of defects made by the knock-on at that particular direction. The calculation in each event was run for a sufficiently long time to ascertain the number of defects and the stability of the damaged configuration. The boundaries shown between the regions must be considered as approximate since in some cases rearrangements were observed towards the end of the run whereby a divacancy dissociates into two vacancies through a mechanism of replacements.

It was estimated, on the basis of these dynamic events, that approximately 63% of the knock-ons of 100 eV create one Frenkel pair and 37% create two Frenkel pairs. Thus the mean number of pairs is $\bar{N}_d(100)=0.63+2\times0.37=1.37$. About 57% of the cases where two pairs were created consisted of a divancy and two well-separated interstitials. The others went into configurations where the two vacancies are in second- or fourth-neighbor sites with respect to one another. No double vacancies in third-neighbor sites were observed in these events.

Single-vacancy regions surrounding the [111], [100], and [110] directions are associated with knock-ons that replace a nearest neighbor, second neighbor, and third neighbor, respectively. This also is the pattern observed at near-threshold energies, which was described in detail in I. The knock-on is found to initiate a sequence of replacements and to leave one vacancy behind. The interstitial is formed several lattice distances away.

There is, in addition, a large region of knock-on directions in the interior of the triangle where single vacancies are produced for a different reason. A knock-on in such directions collides with a relatively far neighbor, and the struck atom does not receive sufficient kinetic energy for displacement because the direction in which it moves is also an "internal" direction where the displacement threshold is high.[3] As a result only one Frenkel pair is created.

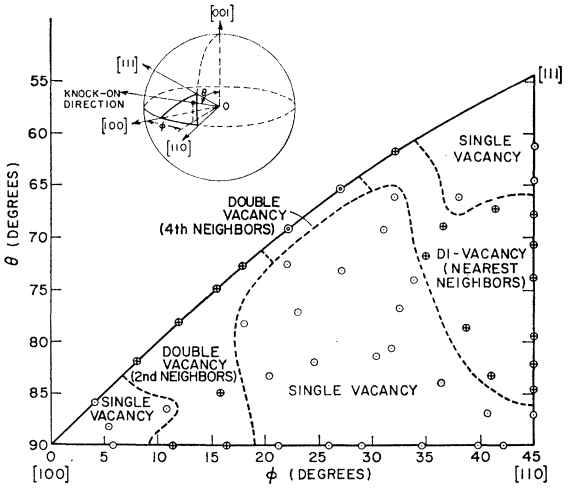

FIG. 1. Distribution of the single, di-, and double vacancies belonging to the Frenkel defects produced by a knock-on of 100 eV. The azimuthal and polar angles φ and θ define the initial knock-on direction. Only the fundamental triangle bounded by the [100], [110], and [111] directions is shown.

The correlation between the direction of the 100-eV knock-on and the direction and kinetic energy of the first-struck atom is illustrated in Figs. 2 and 3. In Fig. 2 the first-struck atom is a nearest neighbor and in Fig. 3 it is a second neighbor. The impact parameters (in units where the lattice constant equals 2) and kinetic energy transferred to the struck atom (in eV) are indicated on the diagrams. As the direction of the knock-on is changed away from a low-index plane [$(1\bar{1}0)$ in Fig. 2 and (001) in Fig. 3] in the sense of the arrows in the left-hand part of each figure, the direction of the struck atom changes in the sense of the arrows in the right-hand portion. This is an illustration for the point made earlier, i.e., that for a knock-on in an "internal" direction (away from low-index axes or planes) the first struck atom moves also in an "internal" direction.

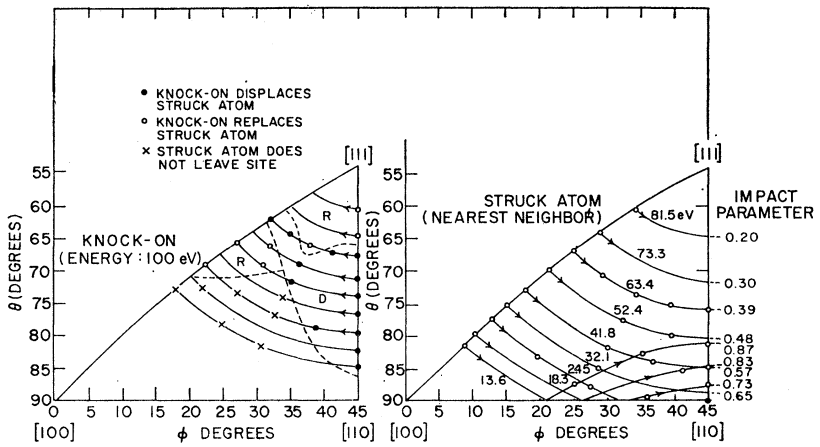

FIG. 2. Correlation between the direction of the 100-eV knock-on and the direction and energy of the struck atom. The trajectory nearest to the [111] pole in the left-hand diagram corresponds to that nearest to the [111] pole in the right-hand diagram, and so on. As the direction of the knock-on changes in the sense of the arrows in the left-hand triangle, the direction of the struck atom changes in the sense of the arrows in the right-hand triangle. The struck atom is a nearest neighbor. Collision impact parameters and the transferred kinetic energy are shown.

[3] See Fig. 15 in I.

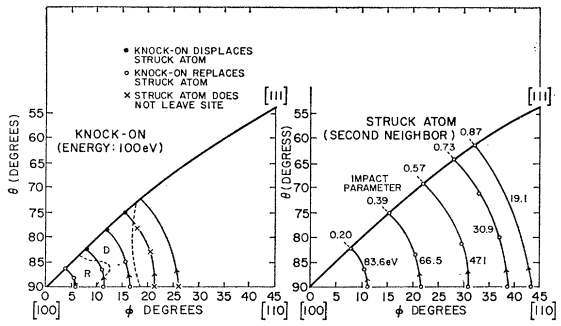

FIG. 3. Same as in Fig. 2 except that struck atom is a second neighbor.

The same dynamic events provide a means of comparing the kinetic energy transferred in a collision of given initial impact parameter inside the lattice with the free binary collision case. By initial impact parameter we mean the perpendicular distance from the site of the struck atom to the initial direction of the knock-on. The comparison is shown in Fig. 4. The solid line represents the case of a binary collision between free atoms. It is seen that the kinetic energy transferred (taken at its maximum value) in a collision in the lattice, is a function not only of the initial impact parameter but of the initial direction of the knock-on with respect to the lattice. In only a small region of impact parameters (approximately between 0.5 and 0.6) do the transferred energies show agreement. For smaller impact parameters the transferred energies are smaller than in the binary case because a significant part of the initial kinetic energy goes into potential energy along a row in the lattice.[4] The decrease of the transferred energy is largest when the struck atom is a third neighbor, because a large amount of energy is lost to neighbors before the actual impact. On the other hand, for impact parameters larger than about 0.5, the energies transferred are larger than in the binary collision between free atoms because the knock-on is deflected toward the struck atom by intermediate collisions. It would appear from these calculations, therefore, that some caution is necessary in applying the formulas for free collisions with a given initial kinetic energy, a given force law, and a given impact parameter to collisions taking place within a lattice.

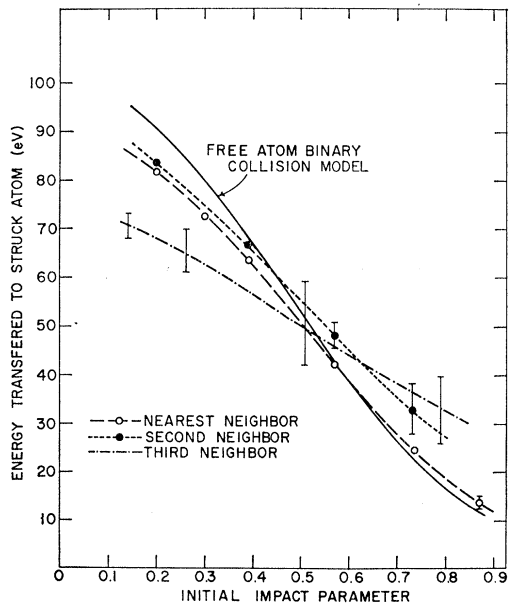

FIG. 4. Kinetic energy transferred by a 100-eV knock-on in a collision with a neighbor. Note that the free-atom binary collision model overestimates energy transfer for small impact parameters and underestimates it for large impact parameters. The spread shown by vertical bars is due to different knock-on directions for a constant impact parameter.

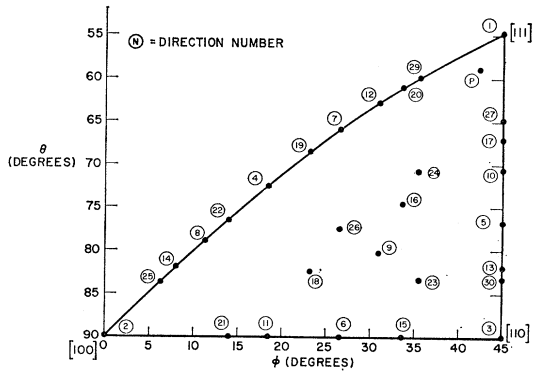

FIG. 5. Distribution of directions to neighboring sites. Direction 1 views nearest-neighbor site, direction 2 second-neighbor site, direction 3 third-neighbor site, etc. Distinct directions up to No. 30 are shown. Note that a large fraction of such directions lie in the symmetry planes. Direction No. 9 is chosen for knock-on in most dynamic runs above 100 eV. A few events were also run with direction marked *P*.

3. HIGHER ENERGY EVENTS

A. Collision Cascades

A series of events extending to higher energies has also been run, and will now be described. Because the time required for a computation mounts rapidly with increasing energy, relatively few computations were made, and a systematic coverage of knock-on directions and energies was not possible. It was decided to employ a variety of energies and one knock-on direction of low symmetry, in the expectation that this would be a representative direction and would give results most nearly resembling those to be obtained by an average over all directions. The direction chosen was the vector (5, 3, 1), or in polar coordinates $\theta=80°$, $\varphi=30°$, shown as point 9 in Fig. 5. Knock-on energies ranging from 100 to 1500 eV were employed. Toward the upper end of this range the cascade was not confined within the fundamental set, and a technique of restarting sub-

[4] This point was discussed in detail for near-threshold energies in C. Erginsoy, *The Interaction of Radiation with Solids*, edited by R. Strumane, J. Nihoul, R. Geners, and S. Amelinckx (North-Holland Publishing Company, Inc., Amsterdam, 1964), p. 51.

sections of the cascade in a fresh set was employed. Calculations were continued to the point where the total number of displacements could be found with reasonable certainty, even though the precise end configurations were not determined. In addition, runs at three energies in the direction $\theta=58°$, $\varphi=42°$ (shown as point P in Fig. 5) were tried. Short runs in three other directions at 1000 eV were made. Table I shows the number of Frenkel pairs created at different energies.

The damage always was found to consist of interstitials and vacancies. The number of Frenkel defects N_d (that is, N_d=number of vacancies=number of interstitials) for the direction 9 is plotted against knock-on energy in Fig. 6. The plot is approximately linear over the entire range, and the curve $N_d=E/100$ (E in electron volts) runs precisely through 7 out of the 12 points. Alternatively, a straight line determined by least squares and constrained to pass through the origin is found to be $N_d=E/110$. In every run many replacement events occur for each defect created. Detailed counts of replacements were not made, but typically the number was about four times as large as N_d.

TABLE I. Results of higher energy calculations.

Knock-on energy (eV)	Knock-on direction[a]	N_d=Number of Frenkel pairs made
100	(9)	1
150	(9)	2
250	(9)	3
300	(9)	3
400	(9)	4
500	(9)	5
600	(9)	6
700	(9)	7
800	(9)	8
900	(9)	8
1000	(9)	8
1500	(9)	13
300	(P)	3
600	(P)	5
900	(P)	9

[a] Symbols represent designation on Fig. 5. (9) has polar angles $\theta=80°$, $\varphi=31°$ and (P) has polar angles $\theta=58°$, $\varphi=42°$.

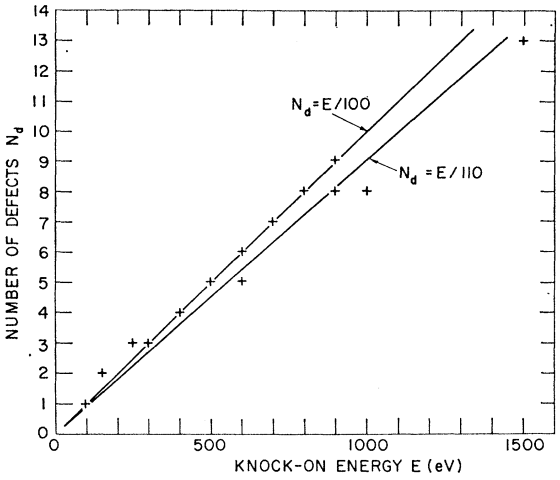

FIG. 6. Number of defects N_d as function of knock-on energy E. The line $N_d=E/100$ (E in eV) runs through 7 out of 12 points. A straight line determined by least squares and passing through the origin gives $N_d=E/110$.

Each cascade proceeds approximately as a sequence of two-body collisions: Although each atom is simultaneously interacting with all its neighbors, the interaction potential at normal neighbor distance is less than 0.2 eV, and the energetic interactions (collisions) which transfer most of the energy in a cascade take place between two atoms at a time. In each cascade the primary knock-on is found to end its trajectory by replacing a lattice atom rather than by going into an interstitial site. If sufficient kinetic energy is imparted to the replaced atom, this atom too is found to make a replacement. The path of such a sequence of replacements initiated by the primary may be termed the primary replacement sequence. Figure 7 shows a primary replacement sequence for the 300-eV knock-on. Projections of the trajectories on the x-z plane and x-y plane are shown. The kinetic energies acquired by the struck atoms are indicated by numbers. Sites where vacancies are ultimately created are shown by the letter V and replacement sites by the letter R. The trajectories of the side chains are not shown. Figures 8 and 9 give similar plots for the 700- and 1000-eV knock-on events. It is seen that the primary replacement sequence is longer for the larger energies.

Further light on the character of these events is afforded by examining the potential energy of the entire set of atoms during the course of the cascade. If the atoms were hard spheres, the potential energy would be zero except at the precise instants of contact of pairs. In the present calculations this is far from the case.

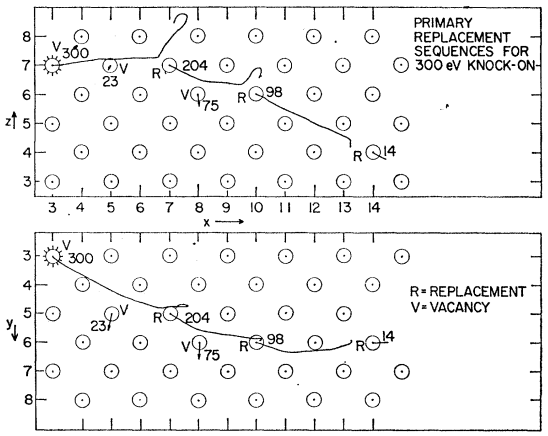

FIG. 7. Primary replacement sequences associated with 300-eV knock-on in direction No. 9 (Fig. 5). The kinetic energies transferred to displaced atoms (replacement sites shown by R) are indicated. Trajectories are projected on the x-z and x-y planes.

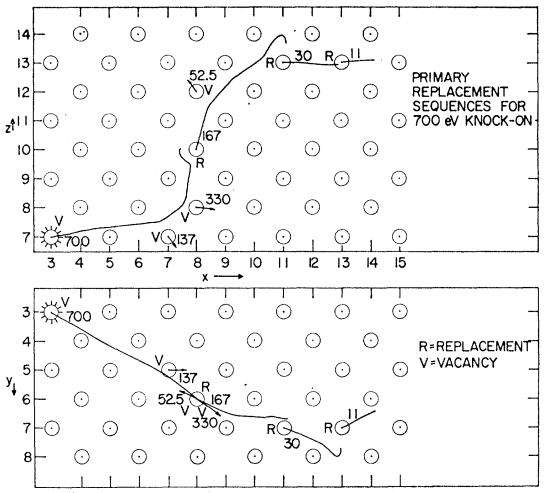

FIG. 8. Primary replacement sequences associated with 700-eV knock-on in direction No. 9 (Fig. 5).

Figure 10 shows the change in potential energy of the set as a function of time after the initiation of the cascade, for four different knock-on energies. The sharp peaks occur during the energetic collisions; beneath these peaks there is a rapidly growing "background," and after the early stages the sharpness of the peaks diminishes. In the time span represented, loss of energy at the boundaries of the set is negligible. If the calculations were continued to such long times that only small vibrations remained and if the set were big enough that boundary losses did not occur, the increase of potential energy would equal the mean potential energy of the lattice oscillators plus the small stored energy of the Frenkel pairs (of the order of 5 eV per pair). Since, by the virial theorem, the mean potential energy of the lattice oscillators equals the mean kinetic energy, the asymptotic values of curves such as those given in Fig. 10 should be nearly half the initial kinetic energy of the knock-on, actually being less than this by half the stored energy of the Frenkel pairs. It can be seen that in the relatively short time represented in Fig. 10 the curves are nearing their asymptotes, which means that the highly localized initial energy has now been rather well spread into lattice oscillations. The differences from any hard-sphere model are pronounced.

Figure 11 shows the change in potential energy of the set of atoms as a function of time for 1000-eV knock-ons in three different directions. Although the details of the curves differ, the rate of approach to the asymptotic limit is about the same and the qualitative behavior is very much like that of the lower energy events of Fig. 10.

B. The Number of Atoms Displaced

Treatments of radiation damage in simplified models that can be handled analytically are by now traditional. A number of models which differ in minor ways have been proposed.[5] In all of these, the damage process is viewed as a cascade of independent two-body collisions. Each collision is assumed to take place between a moving atom and a stationary atom of the lattice. The initial locations of the stationary atoms are taken to be random, and the effect of the lattice is introduced only through a certain threshold energy E_d such that a struck atom will be displaced if it receives more than the threshold energy. Several treatments, differing in minor ways over details of the displacement process, agree in predicting that the average number of displaced atoms N_d produced by the primary knock-on of energy E will, when ionization losses are not important, be given approximately by the formula

$$N_d = E/2E_d. \tag{1}$$

In the simplest theories, E_d is the same as the minimum threshold, but Sampson, Hurwitz, and Clancy,[6] and Snyder and Neufeld[7] have considered the effect of allowing for a displacement probability that rises linearly from zero to unity over a finite range of energy, and have shown that Eq. (1) remains a fair approximation if E_d is replaced by an effective threshold defined as that energy at which the displacement probability is $\frac{1}{2}$.

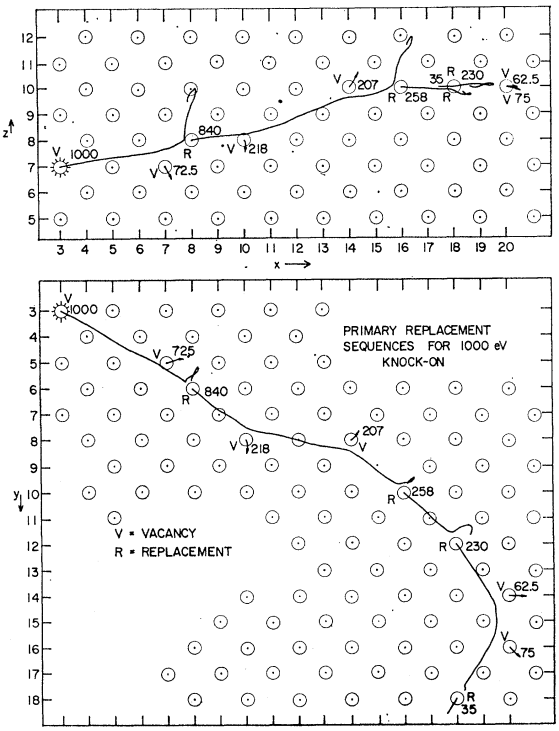

FIG. 9. Primary replacement sequences associated with 1000-eV knock-on in direction No. 9 (Fig. 5).

[5] For a review, see G. J. Dienes and C. H. Vineyard, *Radiation Effects in Solids* (Interscience Publishers, Inc., New York, 1957), Chap. 2.

[6] J. B. Sampson, H. Hurwitz, and E. F. Clancy, Phys. Rev. **99**, 1657 (1955).

[7] W. S. Snyder and J. Neufeld, Phys. Rev. **97**, 1636 (1955); **99**, 1326 (1955); **103**, 862 (1957).

The present calculations allow a check of the predictions of these models. Averaging over all directions of knock-on at 100 eV leads to $N_d=1.37$, which would be in accord with Eq. (1) for an effective threshold of $E_d=36$ eV. Although the mean number of displacements is far from a linear function of E in the near-threshold region (see I), the energy at which the mean number equals $\frac{1}{2}$ is approximately 39 eV, in surprisingly close agreement with this effective threshold of 36 eV. Finally, if the knock-on direction 9 gives a fair approximation to an average over-all knock-on direction, Fig. 6 can be compared with Eq. (1). The approximately linear dependence of N_d on E over a broad range above 100 eV is confirmed, and the effective threshold is found to be between 50 and 55 eV. It is to be noted that all these values of effective threshold energy are much higher than the minimum threshold which was found in I to be approximately 18 eV. There is some evidence of a slight falling off from linearity towards the upper end of the range, which has been discussed elsewhere.[4]

This rough validation of the now classic formula for N_d is gratifying, in view of the highly idealized models on which such theories are based. Furthermore, an effective threshold E_d considerably higher than the minimum threshold is plausible. Insofar as N_d is concerned, the chief influence of the lattice arrangement appears to be to introduce a complicated dependence of threshold energy on knock-on direction. This was discussed in detail in I. However, the spatial distribution of the damage is strikingly altered by the lattice. It has been pointed out in earlier work in this series and also in Sec. 2 of this paper that the collision chains tend to produce interstitials at some distance while the vacancies are left close together.

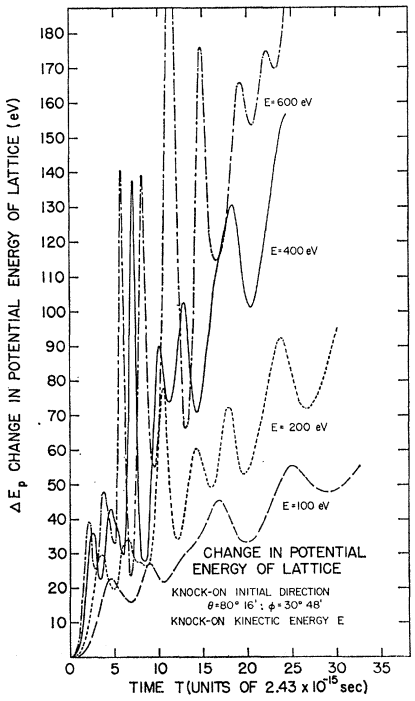

FIG. 10. Change in the potential energy of the lattice ΔE_p versus time T as cascade initiated by knock-on of energy 100, 200, 400, and 600 eV proceeds. Collisions give rise to peaks in the curves. Note that one-half of the knock-on energy goes into potential energy of the lattice in a relatively short time.

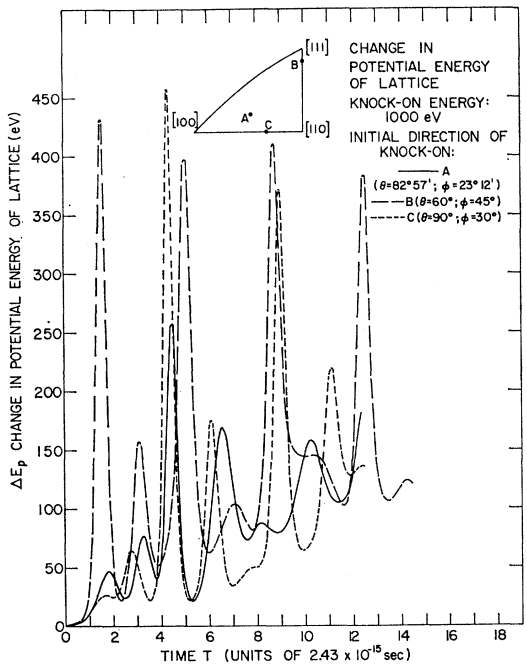

FIG. 11. Change in the potential energy of the lattice versus time for cascades initiated by a knock-on of energy 1000 eV and three different directions. Although details of individual collisions vary the "background" is approximately the same. The cascade has not proceeded long enough to show the leveling-off of the background at one-half of the initial knock-on energy.

4. CHANNELING

Considerable work has been done recently on the effects of the crystal lattice on the penetration and slowing down of heavy ions of energies in the keV range bombarding a surface along a low-index direction. The process of "channeling," first found in machine calculations,[8,9] has been verified experimentally.[10,11] Lehmann and Leibfried[12] approached the problem analytically and considered the energy-loss mechanism in the impulse approximation. The predicted maximum ranges of channeled ions are, of course, strongly dependent on the force law assumed, but an important result of the impulse approximation is that the rate of energy loss $-dE/dx$ is inversely proportional to energy E.

[8] M. T. Robinson and O. S. Oen, Bull. Am. Phys. Soc. **7**, 171 (1962); Appl. Phys. Letters **2**, 30 (1963); Phys. Rev. **132**, 2385 (1963).

[9] J. R. Beeler, Jr., and D. G. Besco, *Proceedings of the Symposium on Radiation Damage in Solids and Reactor Materials* (International Atomic Energy Agency, Vienna, 1962), Vol. 1, p. 43.

[10] G. R. Piercy, F. Brown, J. A. Davies, and M. McCargo, Phys. Rev. Letters **10**, 399 (1963); G. R. Piercy, M. McCargo, F. Brown, and J. A. Davies, Can. J. Phys. **42**, 115 (1964); D. A. Channing and J. L. Whitton, Phys. Letters **13**, 27 (1964).

[11] H. Lutz and R. Sizmann, Phys. Letters **5**, 113 (1963); Z. Naturforsch. **19a**, 1097 (1964).

[12] C. Lehmann and G. Leibfried, J. Appl. Phys. **34**, 2821 (1963).

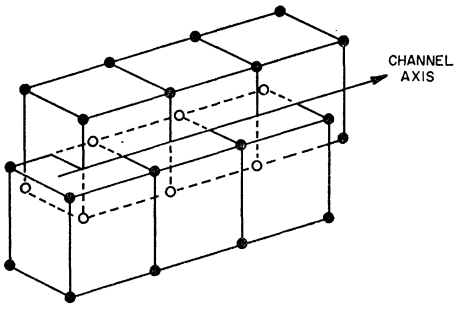

FIG. 12. Diagram showing the axis of a ⟨100⟩ channel in the bcc lattice.

The relation

$$-dE/dx \propto E^{-1} \tag{2}$$

leads to a maximum range $R_{\max}$ which behaves as

$$R_{\max} \propto E_0^2, \tag{3}$$

where E_0 is the initial energy.

Since our calculations on the collision processes in the lattice showed that the impulse approximation was not adequate to estimate energy transfers in the lattice, we carried out computations with our dynamic model on the energy loss of a 1000-eV Fe atom bombarding an Fe lattice along the ⟨100⟩ and the ⟨111⟩ directions. The same force law was employed that was used in other calculations reported earlier in the present paper.

Figure 12 shows a ⟨100⟩ channel in the bcc lattice. The bombarding atom was introduced into the lattice in several test positions shown in Fig. 13, with an initial direction parallel to the ⟨100⟩ axis. The kinetic energy of the bombarding atom is shown in Fig. 14 as a function of time. The leapfrog[13] technique was used in following the trajectory of the atom beyond the fundamental set. The energy curve shows characteristic "rippling" as the channeled atom passes successive lattice atoms. In addition there are large changes arising from occasional

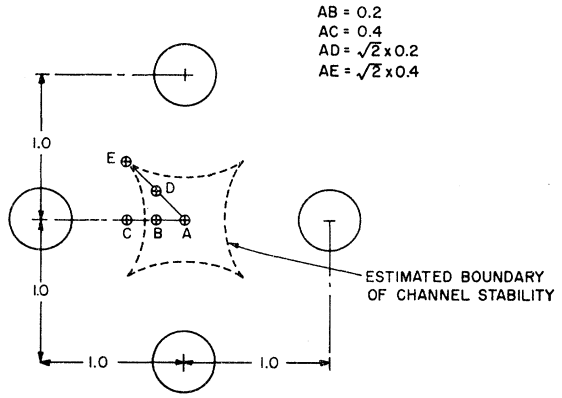

FIG. 13. Starting points in (100) plane for calculated channeled orbits are shown by letters A, B, C, D, and E. The initial kinetic energy of the channeled atom is 1000 eV and initial direction is [100]. The boundary of channel stability shown is approximate. Atoms starting in test positions outside the stability area are rapidly slowed down and proceed less than 10 lattice distances.

[13] See I, Sec. 2 and also Ref. 2.

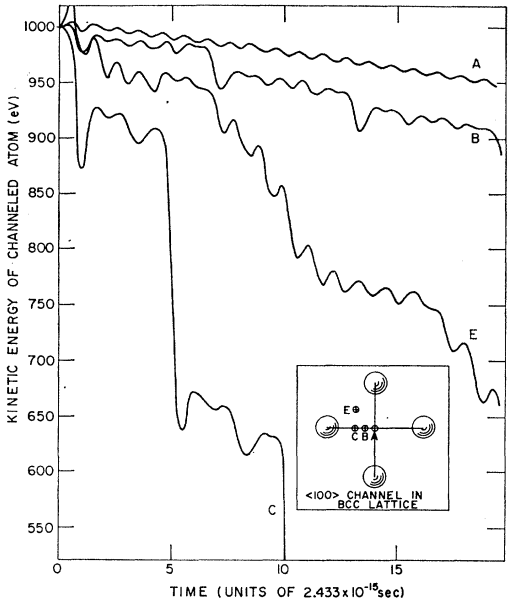

FIG. 14. Kinetic energy of channeled atom versus time for different test positions in ⟨100⟩ channel. Large changes in the kinetic energy are caused by relatively close collisions.

close encounters. It is found that the atom starting at the center of the channel (position A), where the potential is smallest, suffers the lowest rate of energy loss. When the bombarding atom starts far off the channel axis (e.g., position C) it undergoes wide excursions and suffers a rapid slowing down. It is, of course, impossible to define a clear boundary distinguishing those test positions that lead to channeling (long trajectories) and those that lead to a rapid slowing down as a result of a few large-angle collisions. However, a rough boundary for a "stable" channeled trajectory (longer than 10 lattice constants) is indicated in Fig. 13. The x-y plots of some trajectories are shown in Fig. 15.

The slowing down of a bombarding atom introduced into the lattice along a ⟨111⟩ direction is shown in Fig. 16. In this case the atom was followed over a longer trajectory. Distances (in angstroms) covered in the lattice are also indicated. An interesting feature of these results is that the rate of energy loss is approximately constant. The relation

$$-dE/dt = \text{constant} \tag{5}$$

means that

$$-dE/dx \propto E^{-1/2}, \tag{5}$$

and the energy dependence of the maximum range is

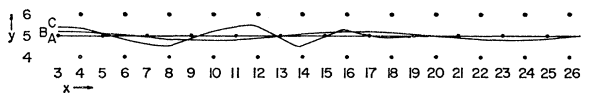

FIG. 15. Projections of ⟨100⟩ channeled trajectories in the x-y plane. Coordinates correspond to distances in units where lattice constant equals 2. Starting points of trajectories shown in Fig. 13.

found by integration to be

$$R_{\max} \propto E_0^{3/2}. \tag{6}$$

This relation is quite different from that predicted by the impulse approximation, $R_{\max} \propto E_0^2$. Recent experimental work[14] shows this $\frac{3}{2}$ power dependence for channeled heavy atoms at energies below 5 keV, where the slowing down is presumably due mainly to elastic collisions. At higher energies, on the other hand, when the impulse approximation would be expected to be valid, slowing down by inelastic processes (ionization and excitation) appears to affect the range sufficiently strongly that the energy dependence of the maximum range now changes towards another law given by

$$R_{\max} \propto E_0^{1/2}. \tag{7}$$

This corresponds to an energy loss of the form

$$-dE/dx \propto E^{1/2}, \tag{8}$$

which has been predicted[15] for the slowing down of a heavy particle moving in a degenerate electron gas with a velocity lower than the Fermi velocity. The same dependence was obtained by Lindhard[16] on the basis of the Thomas-Fermi approximation.

Regarding the possible implications of channeling for radiation damage, where all knock-on atoms start from lattice sites instead of being introduced into the lattice by bombardment, all our calculations performed to date (with knock-on energies up to 1500 eV) have failed to show any case where the trajectory of a knock-on was sufficiently long to be classified as "channeled." This causes us to doubt strongly that channeling processes play any significant role in radiation damage at low and intermediate energies. Different conclusions can be reached if different force laws are assumed. Beeler,[17] for instance, in a calculational model which takes a screened Coulomb potential and uses a hard-sphere approximation to find the scattering angle, has found channeling to occur in a bcc lattice. The possible effect of channeling on the displacement efficiency in radiation damage has been discussed theoretically by Oen and Robinson[18] and by Sigmund.[19] No experimental evidence exists as yet for these effects in radiation damage.

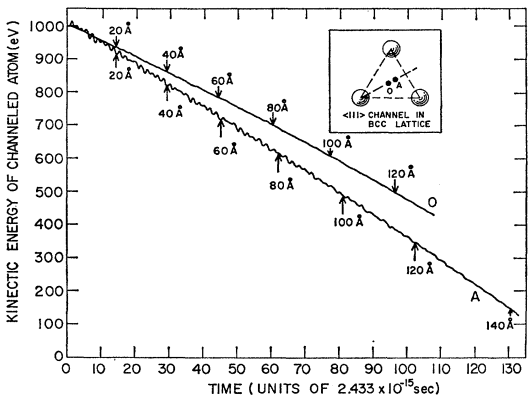

FIG. 16. Kinetic energy of ⟨111⟩ channeled atoms versus time. Distances covered by channeled atom in the crystal are shown at different times. Test position 0 corresponds to channel axis. Note the approximately linear dependence of kinetic energy on time.

5. CONCLUSIONS

(1) A primary knock-on with a kinetic energy of 100 eV and random direction creates an average of 1.37 Frenkel pairs in our model of α-iron. At higher knock-on energies E up to 1500 eV, the number of Frenkel pairs is estimated to rise approximately linearly with E according to the formula $N_d \cong E/2E_d$ where $E_d \cong 50$–55 eV. The calculations in the higher energy range were not sufficiently numerous, however, to give a very accurate value of N_d.

(2) The kinetic energy and initial direction imparted by a 100-eV primary knock-on to one of its neighbors in a collision are poorly approximated by a free-atom binary collision model which ignores the influence of other atoms in the lattice. Thus, at this energy, calculations on the outcome of a single collision must allow for the many-body aspects of the process to be even a fair approximation.

(3) At all energies up to 1500 eV, radiation damage in our model of α iron consists of vacancies and interstitials. No evidence for "amorphous zones" or defects more complicated than small clusters of vacancies has been found. As has been reported in earlier work the operation of focusing chains tends to produce the interstitials at some distance from the site of the primary knock-on, the vacancies closer in.

(4) Channeling effects along ⟨100⟩ and ⟨111⟩ directions have been found for an iron atom of 1000-eV kinetic energy introduced into the lattice from the outside. The rate of energy loss increases rapidly as the orbit is displaced from the channel axis. In the 1000-eV region, the impulse approximation does not give a good account of the rate of energy loss of a channeled atom. Instead, the time rate of change of energy is found to be approximately constant, leading to a range of a channeled atom proportional to $E_0^{3/2}$. This relationship agrees with recent experimental results.

(5) The present calculations give no reason to suppose that channeling has any importance in radiation damage at low and intermediate energies in the model assumed for α iron. This is because all moving atoms in a radiation damage cascade originate from lattices sites, and thus have a very low probability of entering channeled orbits.

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