Effects of Channeling on Damage Production in Iron*

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The displacement efficiency $K(E)$ for damage production by energetic iron atoms in α iron was computed by simulating complete elastic collision cascades in a bcc atomic array on a high-speed computer. Energies in the range $0.1 \leqslant E \leqslant 30$ keV were considered. Above 1 keV, $K(E)$ decreased monotonically as a consequence of progressively more frequent knock-on channeling. Relative to their values in the low-energy, nonchanneling range, the energy-dependent displacement efficiency given by this study and that given by Sigmund's theory are in agreement. Our extrapolated $K(E)$ value at 50 keV was 0.6 that at 1 keV. Damage production by primary knock-ons, *per se*, was attenuated by quasichanneling. Pure channeling was observed only for higher order knock-ons. In the case of reactor irradiation, the computed $K(E)$ leads to an over-all damage reduction of 35% relative to that predicted by simple cascade theory. This indicates that the ignoration of channeling effects (crystal structure) in simple cascade theory is not totally responsible for its overestimation of damage production by at least a factor of 2.

THE possibility that injected keV-energy atoms or ions follow open channels along the principal crystallographic directions in a target crystal was suggested by the results of machine calculations which treated the exact crystal structure of the target. In this regard, we observed channeling in our collision cascade calculations for the square planar lattice and wurzite structure (BeO),[1,2] and Robinson and Oen[3] observed it in their penetration and range calculations for cubic structures. This effect was subsequently verified by Piercy *et al.*[4] in ion bombardment experiments wherein the ion beam was oriented perpendicular to the principal crystallographic planes of single crystal targets.

Specific examples of knock-on atom channeling, during the evolution of a collision cascade, were first given by our cascade calculations.[2] This note summarizes similar computer experiment results for bcc iron in the form of a displacement function $g(E)$ for elastic atomic collisions. The displacement function is the average number of atoms displaced in a cascade initiated by an atom of energy E. The computational model used is described elsewhere in detail.[1,2] In short, it was assumed that a collision cascade could be described as a branching sequence of binary collision events determined by a repulsive interaction potential between a moving atom and a stationary lattice atom. A screened Coulomb potential was used to determine the distance of closest approach, r_0, and the scattering angle was taken to be the hard-sphere scattering angle associated with the collision diameter defined by r_0. In the final paragraph of this paper a comparison test is described which indicates that the damage production results given by this approximation are in close agreement with those of a more exact model.

Given an energy in the range 0.1–30 keV, iron atoms were emitted from a point midway between two lattice sites in the bcc iron lattice along sixteen randomly selected directions within the *nonchanneling* directional range associated with this point. The displacement function for this energy was taken to be the average number of atoms displaced in the sixteen collision cascades and written in the form

$$g(E)=1+K(E)E/E_d, \tag{1}$$

where E is the atom energy and E_d is the displacement energy. $K(E)$ will be referred to as the displacement efficiency. Of the several simple cascade theory models, i.e., those which assume that the lattice structure can be replaced by a randomized solid, the displacement criteria used in the Snyder-Neufeld model[5] are most similar to those used in the present study. The pertinent displacement energy for use in a comparison of our results with those of simple cascade theory is 16 eV, in that we used 4 eV as the sublimation energy for iron. The basis for these statements is fully described in an earlier publication.[2]

A plot of $K(E)$ is given in Fig. 1 along with the displacement efficiencies of four other models. It was clearly demonstrated that the monotonic decrease in $K(E)$ for $E>1$ keV was the result of knock-on atom channeling and quasichanneling[6] by plotting the cascade trajectories. Channeling influence is seen to be barely perceptible below 2 keV. This result is consistent with those of Erginsoy and Vineyard[7] who found no evidence for the channeling of iron knock-on atoms with energies of 1 keV or less in their machine calculations. They did

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[2] J. R. Beeler, Jr. and D. G. Besco, J. Appl. Phys. **34**, 2873 (1963).
[3] M. T. Robinson and O. S. Oen, Appl. Phys. Letters **2**, 30 (1963); Phys. Rev. **132**, 2385 (1963).
[4] G. R. Piercy, F. Brown, J. A. Davies, and M. McCargo, Phys. Rev. Letters **10**, 339 (1963).
[5] W. S. Snyder and J. Neufeld, Phys. Rev. **97**, 1636 (1955); F. Seitz and J. S. Koehler, Solid State Phys. **2**, 305 (1956), see pp. 380–385.
[6] Damage is produced in quasichanneling but not in pure channeling. Specifically, quasichanneling behavior includes unstable low-index channeling and movement in higher index channels.
[7] C. Erginsoy and G. H. Vineyard (private communication).

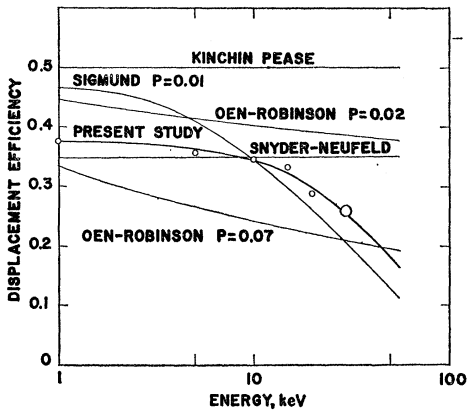

FIG. 1. Displacement efficiency reduction due to channeling.

not consider energies above 1 keV. Our results indicate that the damage reduction caused by channeling is not significant unless the energy of the primary exceeds 5 keV.

Figure 2 illustrates, simultaneously, the two important knock-on channeling effects observed. Trajectory T1 is that of a quasichanneled, 3458-eV primary knock-on, displaced by a 15-keV primary, and trajectory T2 is a pure channel trajectory of a 1325-eV secondary displaced by the primary knock-on. The primary knock-on was displaced into a ⟨142⟩ channel, the secondary into a ⟨110⟩ channel in which it traveled 704 Å. These two events alone caused a 10% damage reduction in the 15-keV primary cascade relative to the damage predicted by simple cascade theory. All observed instances of pure channeling along low-index directions were initiated by quasichanneled atoms as illustrated in Fig. 2.

On the interval $0.5<E<1$ keV, $K(E)$ maintained a constant value 0.375, thereafter dropping smoothly to 0.30 at 0.1 keV. It exceeds the Snyder-Neufeld value (0.35) on $0.5<E<$keV become twice the sublimation energy was subtracted from the energy transfer to a knock-on rather than the displacement energy. Below 0.5 keV, $K(E)<0.35$ because unstable Frenkel pair formation is there prevalent and the program automatically removed this configuration. Simple cascade theory does not fully account for this circumstance.

Also appearing in Fig. 1 are plots of the displacement efficiencies given by the analytical models of Sigmund,[8] and of Oen and Robinson.[9] These theories assume; (1) an energy-independent channeling probability, P, per displacement event, (2) no subsequent damage by channeled atoms, and (3) that an atom, once channeled, remains in this state. Both reduce to the Kinchin-Pease model[10] for $P=0$. Sigmund's theory differs from the

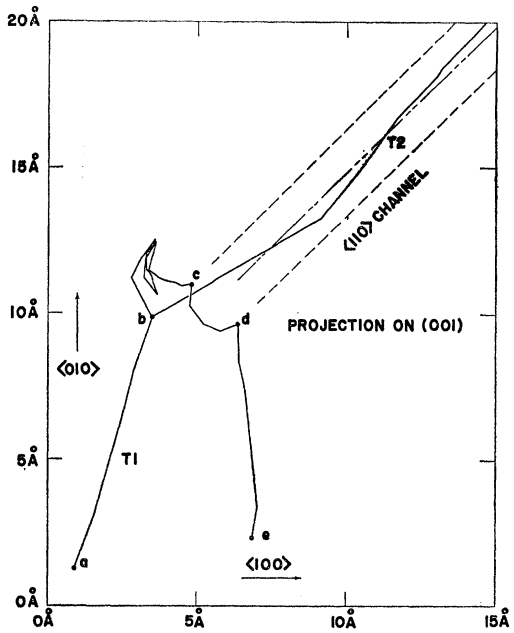

FIG. 2. Quasichanneling illustration. Trajectory T1 is that of a quasichanneled 3458-eV primary knock-on: part (a-b) along ⟨142⟩, part (b-c) along ⟨001⟩, part (c-d) along ⟨1$\bar{1}$0⟩, and part (d-e) along ⟨0$\bar{1}$0⟩. Trajectory T2 represents pure ⟨110⟩ channeling of a 1325-eV secondary knock-on displaced by the primary knock-on at (b).

Oen-Robinson model principally through the introduction of a forwardly peaked scattering distribution.

In their paper, Oen and Robinson suggest that $P=0.07$ is appropriate for copper. Sigmund thought this value to be too large and adopted $P=0.01$ in his calculations. An Oen-Robinson model curve also appears for $P=0.02$. Indications from the machine calculations of Erginsoy and Vineyard, and the present study are that damage reduction due to channeling is negligible for primary energies below 5 keV. Keeping in mind that the displacement efficiency for no channeling is 0.5 for the two analytical models and 0.375 for the present study, it follows that Sigmund's model more closely agrees with the machine calculations than does that of Oen and Robinson. Above 15 keV, Sigmund's $K(E)$ values are about 25% less than the cascade simulation machine values. If quasichanneling of primary knock-ons is in fact as prevalent as the cascade calculations suggest, the greater damage reduction predicted by the two analytical models is primarily a consequence of their assumptions (2) and (3).

An attempt to bracket the degree of damage reduction due to channeling in a neutron irradiation experiment was made by computing the damage increment produced by primary knock-on atoms in a given energy range, assuming an inelastic-scattering threshold of 56 keV. A Monte Carlo calculation was used to compute the primary knock-on atom energy spectrum and the number of primary knock-ons produced per neutron.

[8] P. Sigmund, Phys. Letters **6**, 251 (1963).
[9] O. S. Oen and M. T. Robinson, Appl. Phys. Letters **2**, 83 (1963).
[10] G. H. Kinchin and R. S. Pease, Rept. Progr. Phys. **18**, 1 (1955).

An iron specimen of the size used by Chow *et al.*[11] was assumed. Damage reduction was 35% for irradiation by fission neutrons (average energy $\bar{E}=2$ MeV). Reductions of 32 and 22%, respectively, were obtained using a test-hole spectrum of a water-moderated reactor, $\bar{E}=0.94$ MeV, and that of a graphite-moderated reactor, $\bar{E}=0.11$ MeV.

Let us refer to the scattering approximation used in this study as the screened Coulomb hard-sphere (SHS) model and a scattering treatment using the Born-Mayer potential 2 of Gibson *et al.*[12] and the exact scattering-angle solution for this potential as the BME model. The SHS model overestimates the scattering angle in a comparison with the exact scattering angle for the screened Coulomb potential. Because of this we inferred an overly pessimistic judgement of the SHS model in a recent article[2] which should be corrected in view of subsequent results which will now be outlined. The cascade program was rewritten to accept an arbitrary potential and scattering-angle energy-transfer matrix. Calculations were then made for copper using both models and identical sets of initial conditions. The numbers of displaced atoms given by the two models agreed within 5% and the atom range given by the BME model for 1–5-keV atoms was about 20% larger than that given by the SHS model. We feel this comparison indicates that the realism of the SHS model damage results is nearly comparable to that of the BME model.

[11] J. G. Y. Chow, S. B. McRickard, and D. H. Gurinsky, *Radiation Damage in Solids* (International Atomic Energy Agency, Vienna, 1962), Vol. I, p. 277.
[12] J. B. Gibson, A. N. Goland, M. Milgram, and G. H. Vineyard, Phys. Rev. **120**, 1229 (1960).

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Measurement of Equilibrium Vacancy Concentrations in Dilute Aluminum-Silver Alloys*

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Precision measurements were made of the differential length expansions $(\Delta L'/L'-\Delta L^0/L^0)$ and differential x-ray lattice parameter expansions $(\Delta a'/a'-\Delta a^0/a^0)$ between specimens of pure aluminum and two dilute aluminum base alloys containing 0.52 and 0.94 at.% silver during slow reversible heating and cooling between the solidus and the solubility limit temperature. Absolute differences between the equilibrium vacancy concentrations in each alloy and the pure metal were then obtained from the relation

$$\Delta C_v=C_v'-C_v^0=3(\Delta L'/L'-\Delta L^0/L^0)-3(\Delta a'/a'-\Delta a^0/a^0).$$

Here, C_v is the equilibrium vacancy concentration and $\Delta L/L$ and $\Delta a/a$ are length and lattice parameter expansions. The prime and zero superscripts refer to the alloy and pure aluminum, respectively. Since C_v^0 is known from previous measurements, these differential data serve to determine C_v'. The differential length and lattice parameter measurements were carried out using the same general technique previously employed in the determination of equilibrium vacancy concentrations in a series of pure face-centered cubic metals, and yielded a relatively high precision in the determination of the extremely small differences involved. The addition of silver caused only small increases in the vacancy concentration. Values of ΔC_v equal to $(13\pm5)\times10^{-5}$ and $(12\pm5)\times10^{-5}$ were found for the 0.52 and 0.94 at.% silver alloys, respectively, at their solidus temperatures. These increments correspond to $\lesssim23\%$ of the concentration in pure aluminum. The results for both alloys could be fitted, within the estimated uncertainty of the data, to a simple first-order vacancy-solute atom binding model, where

$$\Delta C_v=12C_sC_v^0[\exp(-S_{vs}^b/k)\exp(E_{vs}^b/kT)-1].$$

Here, C_s is the solute concentration, and the best value of the binding energy, E_{vs}^b, was found to be 0.08 eV for an assumed binding entropy $S_{vs}^b=0$. This value was of the order generally expected from previous experiments. The significance of the apparent agreement between the data and the model were discussed.

I. INTRODUCTION

ABSOLUTE measurements of the concentration of vacant atomic sites in thermal equilibrium in a number of pure face-centered cubic metals at elevated temperatures have been carried out by Simmons and Balluffi[1–4] and d'Heurle *et al.*[5] The basic method used in these measurements has been to observe the difference between the macroscopic expansion, $\Delta L/L(T_r)$,

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[3] R. O. Simmons and R. W. Balluffi, Phys. Rev. **125**, 862 (1962).
[4] R. O. Simmons and R. W. Balluffi, Phys. Rev. **129**, 1533 (1963).
[5] F. H. d'Heurle, R. Feder, and A. S. Nowick, J. Phys. Soc. Japan **18**, 184 (1963).