

was found earlier by Weiner⁹ in the computer simulation of the modified Frenkel-Kontorova model with φ [Fig. 1(a)] = $0.3b$. Although it is no longer possible to speak of dislocation velocity past v_B , it is still possible to compute the front velocity v_F , the velocity at which potential-well boundaries are crossed by the lead atom of the disturbed region.

(3) As the stress level continues to increase, and $v_F \rightarrow 1$, atom collisions begin to occur.

(4) Two types of waves are caused to propagate through the lattice by these phenomena: (a) a backward-moving breakdown wave, and (b) a forward-moving collision wave.

Several cross checks have been made of the computer-simulation results. (i) The atomic displacements corresponding to the Atkinson-Cabrera solution have been determined analytically, and it is found that they do, in fact, lead to multiple-well crossings, contrary to the *a priori* assumption, at a steady-state velocity $v_B(P)$. (ii) As the rate of stress rise is decreased in the computer-simulation studies, the velocity at which breakdown is first observed decreases and approaches the theoretical value of $v_B(P)$ computed under (i) above. (iii) Computer-simulation runs have been made in which the stress is increased to a value slightly larger than that required for breakdown and is then held constant. Breakdown and the subsequent growth of the extended fault region occurs in much the same manner as in the increasing stress program for Fig. 2. Details of these cross checks will be published

elsewhere.⁸

In summary, then, we conclude that the Atkinson-Cabrera solution does *not* provide support for the hypothesis that dislocations may be accelerated to supersonic speeds since it ceases to be valid at velocities greater than $v_B < 1$.

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Identification of Irradiation-Induced Al-Mn Dumbbells in Al Crystals by Backscattering

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By measuring the energy spectra of backscattered 1-MeV He⁺ ions from Al-0.09 at.% Mn crystals, it was found that Mn atoms were displaced from lattice sites by irradiation with 0.3–1.0-MeV He⁺ ions at 35°K. Annealing results and an analysis of $\langle 110 \rangle$ and $\langle 111 \rangle$ axial channeling and $\{100\}$ planar channeling indicated that the Mn atoms were displaced by trapping irradiation-induced interstitial Al atoms, forming Al-Mn atom pairs in the $\langle 100 \rangle$ dumbbell configuration.

An analysis of the spectra of backscattered high-energy ions from single crystals can be used to determine the position of foreign atoms in the host lattice.¹⁻⁴ This technique, based on the channeling phenomenon, has been widely applied to the location of ion-implanted impurities in

semiconductors³⁻⁶ and in metals.⁷⁻⁹ Under suitable conditions, the positions of impurity atoms can be determined to within 0.1–0.2 Å, for concentrations as low as 10⁻⁴ atomic fraction.⁴ The method has great potential for studying impurity-point-defect interactions. The application of this

method to crystals doped with impurities from the melt has yet to be fully exploited.¹⁰

We have chosen an alloy Al-0.09 at.% Mn for our initial investigation of the interaction of irradiation-induced point defects with impurities because (a) Mn atoms are sufficiently heavier than Al atoms for accurate backscattering studies, (b) Mn has strong interactions with point defects in Al,¹¹⁻¹³ (c) an impurity concentration of ~0.1 at.% is approximately equivalent to the saturation point-defect concentration created by irradiation at low temperatures,¹⁴ and (d) in dilute substitutional alloys, as contrasted with ion-implanted samples, all the impurity atoms are in lattice sites.

From electrical-resistivity data, it has been concluded that self-interstitial Al atoms are trapped by impurity atoms in electron- or neutron-irradiated Al.^{12, 13, 15} Such trapped interstitial atoms are presumed to be released during stage-II recovery (60–150°K) or during stage-III recovery (150–270°K) in Al.^{12, 13, 15, 16} Our results give the first direct evidence for the displacement of impurity (Mn) atoms by the trapping of self-interstitial atoms, and demonstrate that the resultant interstitial Al-Mn pair has the <100> dumbbell configuration. This is the calculated stable form of a self-interstitial atom¹⁷ in a fcc crystal.

Single crystals of Al-0.09 at.% Mn were grown from the melt by the Bridgman technique at a speed of 1 cm/h. Slices were spark cut, polished on successively finer emery paper and diamond grit wheels, vibratory polished for 16 h with 0.05- μ m alumina powder, and electropolished 100 sec in a solution of 20% perchloric acid plus 80% ethyl alcohol.

The samples were examined in the low temperature arm of the Chalk River 2.5-MV Van de Graaff accelerator, using backscattering of 1-MeV He⁺ ions.^{18, 19} The analyzing He⁺ beam was 1 mm in diameter, with divergence <0.1°. The beam current was 2–20 nA. The energies of backscattered ions were measured using a surface barrier detector at a scattering angle of 150°, with single and multichannel analyzers. The energy resolution was 20 keV full width at half-maximum. Each sample, mounted on a goniometer,¹⁸ was cooled to ~35°K by means of a self-contained refrigeration unit.¹⁹ A shield at the same temperature surrounded the sample, thus avoiding surface contamination from hydrocarbons. A heater attached to the sample holder was used to vary the temperature from 35 to

300°K. The temperature was measured with a copper-Constantan thermocouple. The crystals were damaged at 35°K by irradiating them with a 0.3- or 1-MeV He⁺ beam which was swept uniformly over a 5-mm-diam area.

The minimum yields [$\chi_{\min} = (\text{aligned yield}) / (\text{random yield})$] from Al atoms, obtained from the backscattering spectra of annealed crystals, were $(\chi_{\min})_{\text{Al}} = 0.045\text{--}0.055$ at 300°K and $(\chi_{\min})_{\text{Al}} = 0.015\text{--}0.025$ at 35°K, both in a <110> direction, and $(\chi_{\min})_{\text{Al}} = 0.09$ at 35°K in a <111> direction. In both <110> and <111> directions, the yields from Mn atoms indicated that >96% of the Mn atoms had replaced Al atoms at normal substi-

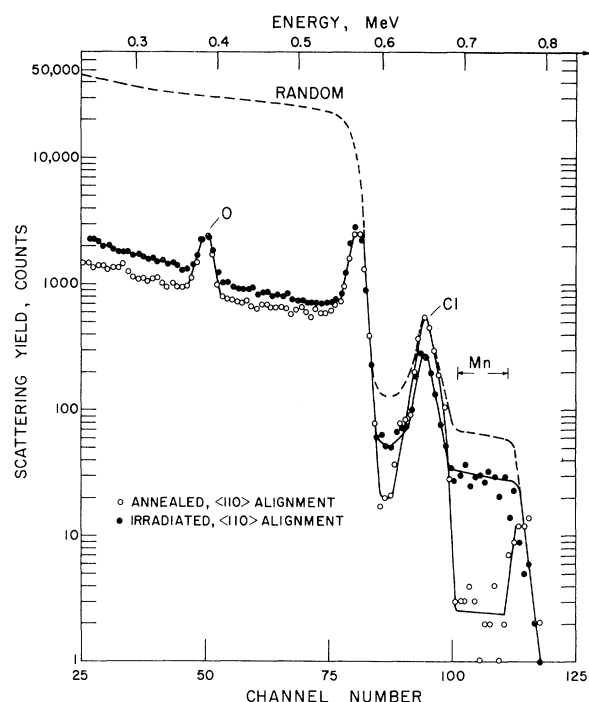


FIG. 1. Typical energy spectra of backscattered 1-MeV He⁺ ions from an Al-0.09 at.% Mn crystal at 35°K. The <110> aligned spectra are shown for an annealed crystal, and for the same crystal after irradiation in a random direction with $\sim 10^{16}$ 1-MeV He⁺ ions/cm² *in situ* at 35°K and annealing 10 min at 60°K. The irradiation increased $(\chi_{\min})_{\text{Al}}$ from 0.024 to 0.029, and $(\chi_{\min})_{\text{Mn}}$ from 0.039 to 0.48. [The damage caused by the analyzing beam in the [110] direction (4×10^{15} ions/cm²) was negligible compared with the damage from the random beam.] After annealing 10 min at 245°K, the aligned spectrum was identical to the spectrum before irradiation. Surface peaks are seen for both Al and Mn in the surface oxide film; an oxygen peak corresponding to this film is also present. The Cl peak is caused by a residual surface layer from the electropolishing solution. The peak is reduced somewhat by irradiation, perhaps because of sputtering.

tutional sites.

Irradiations of $>10^{15}$ ions/cm² in a random direction with 0.3- or 1-MeV He⁺ ions at 35–65°K increased the $\langle 110 \rangle$ minimum yield $(\chi_{\min})_{\text{Mn}}$ for the Mn atoms drastically compared with the increase of $(\chi_{\min})_{\text{Al}}$ (see Fig. 1). After doses $\approx 10^{16}$ ions/cm² (depending on the energy), $(\chi_{\min})_{\text{Mn}}$ saturated at a value close to 0.60. (This is the extrapolated minimum yield; cf. Fig. 2.) Using a simple geometric model for the backscattering from Mn atoms in a channel, in which the ion flux is assumed uniform, this corresponds to a concentration of shadowed Mn atoms, $c = [1 - (\chi_{\min})_{\text{Mn}}] / [1 - (\chi_{\min})_{\text{Al}}] = 40\%$, which would equal the fraction of substitutional Mn atoms. The remaining 60% of Mn atoms would then be displaced sufficiently into the $\langle 110 \rangle$ channel to give the random yield.

Alternatively, 100% of the Mn atoms could be displaced by a smaller amount.⁴ In this case, an angular scan across a $\langle 110 \rangle$ direction would show an angular width of the Mn dip which was less than that of the Al dip. As shown in Fig. 2, this change in width was not observed. Furthermore, the presence of a narrow peak in the Mn yield at 0° from a $\langle 110 \rangle$ direction indicated that the Mn atoms were displaced far enough to reach the flux-peaking region. The peak-to-valley ratio of this peak was approximately 1.5, indicating that $\sim 60\%$ of the Mn atoms were displaced at least 1.3 Å, if the displacement was along a $\langle 100 \rangle$ direction. This conclusion is based

on the approximate flux distribution in the channel,⁵ $F_i = \ln(A_0/A_i)$, where A_0 is the channel area and F_i is the normalized flux at the edge of an area A_i defined by an equipotential contour. In this expression, multiple scattering is neglected.²⁰ It is also assumed that statistical equilibrium of ion positions in the channel has been achieved, which is not accurate, especially for depths of less than 1000 Å.^{20,21} However, since our Mn yields are averages from ~ 500 –1500 Å, any depth dependence of the yield will be averaged out.

In order to specify further the Mn atom displacements, an angular scan through a $\langle 111 \rangle$ direction was made. If the Mn atoms were displaced into body-centered positions, they would be entirely shadowed in this direction, but the observed shadowing of Mn atoms was only 63% for a dose of $\sim 10^{16}$ 0.3-MeV He⁺ ions/cm². This dose gave 43% shadowing in the $\langle 110 \rangle$ direction (for the extrapolated minimum yield, cf. Fig. 2), which indicated that no more than 20% of the Mn atoms could be in body-centered positions. However, the greater shadowing in the $\langle 111 \rangle$ direction can be more simply explained by a Mn atom displacement ≈ 1.3 Å in the $\langle 100 \rangle$ direction, which moves the Mn atoms from one $\langle 111 \rangle$ string close to a neighboring string (within 0.6 Å). The expected narrowing of the $\langle 111 \rangle$ channel for Mn atoms which are displaced in this way could not be verified from our results, because of large statistical errors in counting.

In a separate experiment, measurement of the

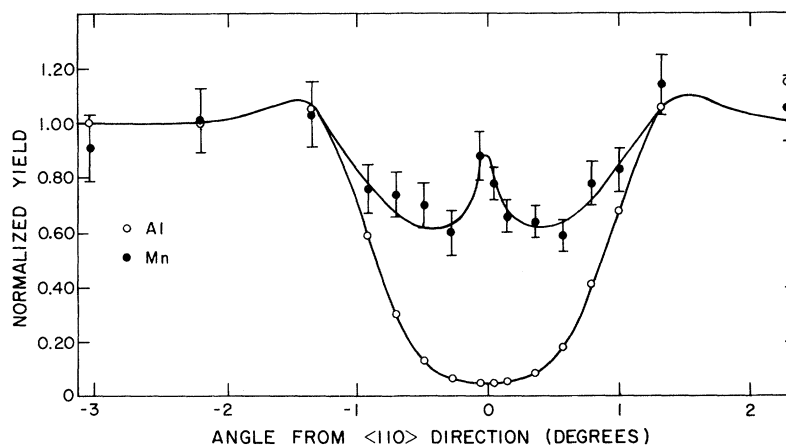


FIG. 2. Angular dependence of the normalized yield of backscattered He⁺ ions (incident energy 1 MeV) from Al and Mn atoms in an Al-0.09 at.% Mn crystal after irradiation at 65°K with $\sim 10^{16}$ 0.3-MeV He⁺ ions/cm². The yield is plotted as a function of the angle from the $[110]$ direction near the $(\bar{1}\bar{1}2)$ plane. The backscattering yield was measured from a depth of 1000 Å (for Mn this was an average from 500–1500 Å or twelve channels). Note that the angular dependence of the energy loss of the He⁺ ions is not nearly sufficient to cause an observable peak in Mn yield (Ref. 10).

channeling along a $\{100\}$ plane (at an angle of 5° from a $\langle 110 \rangle$ direction) showed a χ_{\min} for Mn of 0.31_6 , as compared with 0.25_7 for Al. These values corresponded to 92% of Mn atoms shadowed, whereas 69% were shadowed along the $\langle 110 \rangle$ direction (from the extrapolated minimum yield) for this irradiation. This result confirms a $\langle 100 \rangle$ displacement of Mn, since at most only $\frac{1}{3}$ of Mn atoms displaced in $\langle 100 \rangle$ directions will be in a given $\{100\}$ planar channel. The expected shadowing would thus be $69\% + \frac{2}{3} \times 31\% = 90\%$, in close agreement with the results.

It can be concluded that the Mn atoms were displaced approximately 1.3 \AA in $\langle 100 \rangle$ directions, which is close to the displacement expected if a Mn atom forms one half of an Al-Mn dumbbell interstitial configuration. Such a configuration would result from the trapping of a migrating Al self-interstitial atom (having either a metastable or stable configuration) by a Mn atom. It should be noted here that the displacement of Mn atoms cannot be a direct irradiation process, since at most about 0.1% of lattice atoms are directly displaced during the irradiation.

Annealing results support the Al-Mn dumbbell model. Following an irradiation at $\sim 35^\circ\text{K}$, a 10-min anneal at 60°K always caused the concentration of displaced Mn atoms to increase by $\sim 10\%$. This is expected, since long-range migration of self-interstitial Al atoms occurs from 40 to 50°K .²² The trapping of Al interstitial atoms by Mn atoms during the 35°K irradiation is assumed to occur mainly as a result of Al atom migration in recovery stage I_D , which is centered near 35°K .²² This stage is attributed to correlated (short range) interstitial-vacancy recombination.

During annealing from 180 to 245°K , more than 96% of the Mn atoms returned to their normal lattice sites, thus verifying that the displaced Mn atoms were in simple defect positions, rather than in defect clusters or Mn precipitates. As this annealing temperature range corresponds to recovery stage III in Al, these results indicate that at least some of stage-III recovery in irradiated Al is associated with release of self-interstitial atoms from impurity traps.

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