CONF-750965--1

DECHANNELING MEASUREMENTS OF DEFECT DEPTH PROFILES
AND EFFECTIVE CROSS-CHANNEL DISTRIBUTION
OF MISALIGNED ATOMS IN ION IRRADIATED GOLD

By

P. P. Pronko

For Presentation at
International Conference on
Atomic Collisions in Solids
Amsterdam
September 22-26, 1975

NOTICE
This report was prepared as an account of work sponsored by the United States Government. Neither the United States nor the United States Energy Research and Development Administration, nor any of their employees, nor any of their contractors, subcontractors, or their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness or usefulness of any information, apparatus, product or process disclosed, or represents that its use would not infringe privately owned rights.

MASTER

U of C - AUA - USERDA

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

ARGONNE NATIONAL LABORATORY, ARGONNE, ILLINOIS

operated under contract W-31-109-Eng-38 for the
U. S. ENERGY RESEARCH AND DEVELOPMENT ADMINISTRATION

ABSTRACT

Defect depth profiles for self ion and He^+ irradiated gold are obtained from single and multiple scatter dechanneling analysis in single crystal gold films. Quantitative defect densities are obtained through use of atomic scattering cross sections. Integral damage profiles are extracted from the dechanneling spectra and subsequently differentiated to yield the volume concentration of defects as a function of depth. Results from the self ion irradiations suggest that incident ions produce defect distributions across depths much greater than predicted by random stopping theory. This is in agreement with TEM observations of others.(15) Comparison of the experimental profiles is made with theoretical vacancy distributions predicted by defect diffusion in a radiation environment. Similarities are observed for the low fluence irradiations suggesting that profile characteristics may be controlled by rapid migration and loss of interstitials to the film surfaces during irradiation. Information on the across-channel distribution of misaligned atoms in the damaged films is obtained with the steady increase of transverse energy model applied to the dechanneling spectra. A predominance of slight misalignment is observed with no contribution to dechanneling coming from atoms displaced significantly close to the center of the channels. This is in keeping with what is expected for crystal distortions caused by the strain fields associated with vacancy cluster defects.

1. INTRODUCTION

The charged particle channeling technique can be a useful tool for measuring defect profiles in ion irradiated crystals. Although much work of this type has been done on silicon and germanium, there has been very little published on the application of the method to measuring heavy ion induced damage depth distributions in metals. In metallic crystals the defects from irradiation, observable by dechanneling, usually consist of point defect clusters, dislocations, faults, etc. These defects introduce distortions in the alignment of the atoms in the crystal rows, through the long-range strain fields that are set up, and thereby introduce observable dechanneling of an aligned beam. In most cases, no direct backscattering from defects is detected in these systems, since the average atomic displacement involved are on the order of, or less than, a few tenths of an angstrom from the atomic row.

The various principles of dechanneling have been discussed previously and can be considered in terms of their applicability to interactions with atoms that are displaced by varying amounts from the perfect strings that constitute the channeling potential. These different approaches to the problem include diffusion in transverse energy space, (1) steady increase of transverse energy, (2) multiple scattering, (3) plural scattering, (4) and single scattering. (5) The various methods of analysis are individually applicable to those problems that fulfill the conditions of the model associated with the dechanneling mechanism. The precise character of the interaction mechanism for channeled particles with defects in metals is only partially understood. As a first approximation to dechanneling depth distributions in metals the present work examines the results that emerge from single and multiple scattering analysis of measured spectra taken from single crystal thin film specimens of self ion and He^+ irradiated gold. The damage levels were deliberately kept at or below the saturation level for black spot defect clusters as observed by TEM. In order to obtain information about the across-channel displacement distribution of misaligned atoms in the damaged crystal, an analysis of the dechanneling data is done on the basis of the steady increase of transverse energy model using parameters obtained from the multiple scattering analysis.

In addition to its simplicity, the following arguments can be proposed for single or multiple scatter dechanneling analysis.

a) Dechanneling theory predicts that diffusion in transverse energy becomes significant beyond about one micron in depth. (6,7,8) Less complex treatments should be possible, therefore, at shallower depths.

b) Results of our own experiments and those of Swanson et al. (10,11) indicate that for certain cases thermal and defect dechanneling are linearly separable and may be treated as independent phenomena.

c) According to plural scattering theory, (4) keV He^+ ions passing in a random direction through a thousand angstroms of gold will be near the single scattering limit. From the observed dechanneled fraction at saturation damage in the gold specimens being examined, it is estimated that about 10% of the atoms will be affected by the strain fields from the vacancy clusters introduced by self ion bombardment. Thus, the channeled beam will see many fewer lattice atoms to scatter from compared to an amorphous material and should therefore be well into the single scattering regime. In addition, Jack (12) has shown that thermal dechanneling of keV protons in copper fits a single scattering theory suggesting that other forms of small lattice atom displacements should produce similar patterns.

d) For shallow depths (<0.5 micron) it is the high transverse energy component of the beam that has the greatest probability of interacting with slightly displaced atoms. As is pointed out by Eisen, (13) single scattering events should then be sufficient to cause dechanneling. Preliminary work on the observed damage spectra, for approximately uniform distributions of damage, compared to calculated spectra using the steady increase of transverse energy model, shows that the high transverse energy component of the beam carries greatest probability for dechanneling from defect clusters in gold (see Section 5).

The choice of single or multiple scattering as a dominant mechanism is both target and projectile dependent. Estimates of the relative dominance of each mechanism can be obtained by a comparison of their associated dechanneling probabilities. This is done in the next section.

2. DEFECT DEPTH PROFILES

General observations of heavy ion damage in metals show a sigmoidal build up of dechanneled fraction across the damaged region of bulk specimens with an approximately linear region of dechanneled fraction behind it. The transition

from the damaged to the undamaged region is therefore definable. The dechanneled fraction behind the damage zone can be ideally treated as having a constant additive component introduced by the defects.

The attenuation model of dechanneling considers the channeled beam as an exponentially attenuated function of depth. Single and multiple scatter dechanneling both produce such an exponential attenuation. In single scattering the root mean square scattering angle per defect is greater than the critical angle for channeling. In this case the basic equation for dechanneling has been given as (14)

$$\chi'(z) = 1 - \{1 - \chi(z)\} \exp [-\gamma(z)] \quad (1)$$

where

$$\gamma(z) = \sigma_{ss} \int_0^z N(z') dz' = -\ln[(1 - \chi'(z))/(1 - \chi(z))]. \quad (2)$$

The volume concentration of defects as a function of depth z is given by $N(z)$ with σ_{ss} being the single scatter dechanneling cross section per defect. The measured quantities $\chi(z)$ and $\chi'(z)$ are the dechanneled fractions before and after damage, respectively. Equation 2 is the integral damage concentration and results directly from the measurement. The actual volume concentration is obtained by solving for $\gamma(z)$ in terms of the dechanneled fractions and differentiating with respect to depth. The damage profile is then given by inversion of Equation 1 as:

$$N(z) = - (1/\sigma_{ss}) d\{\ln [(1 - \chi'(z))/(1 - \chi(z))]\}/dz. \quad (3)$$

In performing the data analysis, $\gamma(z)$ is calculated point by point from the observed spectra. The depth scale is determined from the usual conversion of multi-channel energy to depth through known stopping power values. In the case of films of known thickness the depth scale can be obtained by equating the low energy cut-off with the film thickness. A smooth multiple order polynomial curve in z is fit to these points through a least squares computer program. This polynomial is used as the integral damage profile and is differentiated to yield the final volume distribution. By using this procedure, statistical counting fluctuations and experimental noise are eliminated as problems in the extraction

of the damage profile. Since the dechanneled fraction behind the damage zone is usually a constant fraction above the undamaged spectra, the differentiation in Equation 3 produces an effective zero of damage in that region. If this condition is not achieved it is an indication that some perturbation to the transverse energy distribution has occurred.

The single scatter dechanneling cross section σ_{ss} can be taken as the cluster cross section or the atomic cross section for atoms within the defect cluster. In the present work the atomic single scattering cross section was used, where $\sigma_{ss} = \pi Z_1 Z_2 e^2 d / 2E$ is the total dechanneling cross section per displaced atom obtained by integrating the Rutherford cross section from ψ_1 (the critical angle) to π . The major contribution to this function comes from the region close to ψ_1 since the Rutherford cross section is peaked at small angles. In Equation 4 the nuclear charge of incident and target particle is Z_1 and Z_2 , respectively; e is the electronic charge, d is the atomic spacing along the string atoms and E is the energy of the incident ion.

For multiple scattering one proceeds in the same fashion as above except that the dechanneled fraction is given by (3)

$$\chi'(z) = \chi(z) + (1 - \chi(z)) \exp \left\{ -[\psi_1^2 / \Omega(z)] \right\}$$

where

$$\Omega(z) = \sigma_{ms} \int_0^z N(z') dz'. \quad (4)$$

In this case the volume concentration of damage is given as:

$$N(z) = - (\psi_1^2 / \sigma_{ms}) d \left\{ \ln[(\chi'(z) - \chi(z)) / (1 - \chi(z))] \right\}^{-1} / dz. \quad (5)$$

The atomic multiple scattering dechanneling cross section is:

$$\sigma_{ms} = (\pi/2) \psi_1^4 d^2 \ln(1.29\epsilon) \quad (6)$$

where ψ_1 is the critical angle for scattering and ϵ the Lindhard dimensionless energy parameter.

Comparison of the dechanneling probability for single and multiple scattering under given channeling conditions is a useful procedure for determining the relative contribution from each mechanism. For single scattering $P(z) =$

$\exp(-\gamma(z))$ from Equation 1 and for multiple scattering $P(z) = \exp(-\psi_1^2/\Omega(z))$ from Equation 4. These quantities are plotted in Fig. 1 for 0.27 and 2 MeV He^+ in gold as a function of the areal density of defects. It is seen that the effect of increasing the probe energy is to decrease the interaction probability as well as to cause a greater difference between the single and multiple scattering probabilities at the higher energy. The horizontal line drawn at $P = 1 \times 10^{-2}$ is the sensitivity limit in single alignment. As damage is introduced it must cause dechanneling to greater than 1% before it will be observable. It is seen in the graph that for the 0.27 MeV probe the single scattering process will dominate as one comes out of the sensitivity limit which will correspond to $\sim 2 \times 10^{15}$ scattering points per cm^2 . This single scattering dominance will exist for dechanneling of less than 10%. In examining the 2 MeV curve it is evident that as soon as the sensitivity limit for observable dechanneling is reached one is into the multiple scattering regime and continues to be so throughout the entire range thereafter. It is thus on the basis of these results that single scattering is used to analyze the 0.27 MeV data and multiple scattering applied to the 2 MeV measurements.

3. RESULTS

We will deal first with the results from the 5000 Å single crystal gold foil specimen that was irradiated in a random direction with 2 MeV He^+ ions. Since the damaging beam, at 2 MeV, passes completely thru the film before coming to rest, it can be assumed that the energy deposition is approximately uniform across the film. Likewise it is known that in addition to the defect clusters which are formed by the energetic collisions of the He^+ with gold atoms, a large number of Frenkel pairs will also be generated. Since this bombardment was done at room temperature, it can be concluded that, in addition to spontaneous collapse of collision cascades, a certain amount of kinetic redistribution of interstitials (and possibly vacancies) from the Frenkel pairs will occur thru activated migration processes.

Fig. 2 shows the measured differential damage distribution as observed with 2 MeV He^+ dechanneling in the 5000 Å films that were irradiated in a random direction (as determined by backscattering) with 2 MeV helium ions. It is seen

that for intermediate fluences the defect distribution is nearly uniform across the specimen as expected; however, at low dose a double peaking of the defect concentration occurs near the front and back surfaces. At higher fluences, near saturation, the distribution shows a tendency toward having preferential build up of defects on the back (or deep) side of the film. These characteristics of the distributions will be given further discussion below.

The results from the 270 keV He^+ probe of the heavy ion damage in 1200 Å single crystal films on rock salt are presented in Figs. 3, 4, and 5. These correspond to 540, 270 and 80 keV self ion damage in a random orientation as determined from He^+ backscattering. The irradiation fluences used for damaging ranged from 3.8×10^{10} to $2 \times 10^{13} \text{ cm}^{-2}$. It is immediately evident that the defect profiles extend across the entire 1200 Å and bear little resemblance to the results of random stopping theory which, for example, predict, for 540 keV self ion damage in gold, a gaussian like distribution with mean depth of 380 Å and rms width of 200 Å. The present results are in qualitative agreement with those of Merkel et al. (15,16) where stereo transmission electron microscopy measurements were made of black spot defect cluster distributions in 800 Å single crystal gold films. There it was found that at energies between about 100 and 500 keV the defect profiles were generally much broader and deeper than expected and were distributed generally throughout the film. It was felt that unavoidable heavy ion channeling is probably responsible for this, with the defects being produced as the gold ions dechannel and undergo random collisions. As in the 2 MeV He^+ data the heavy ion damage shows an approximately uniform distribution of defects across the film for intermediate fluence. In this region there are a total of approximately 1.5×10^{21} misaligned atoms per cm^3 associated with the overall cluster strain fields. For the lowest fluences a double peaking is again observed and as saturation is approached a tendency toward an increasing concentration of defects on the back or deep side of the film is evident. This pattern is observed for both the 540 and 270 keV bombardments. The 80-keV irradiations exhibit the near surface peaking for all fluences with the number of misaligned dechanneling centers never exceeding 0.7×10^{21} which is not yet at the level where the other distributions show a transition away from the double peak behavior.

4. DEFECT PROFILES FROM IRRADIATION AND DIFFUSION

One interpretation of the defect profiles obtained from the dechanneling analysis can be made through consideration of the theory of defect diffusion in a radiation environment. Rothman et al. (17) have considered the case of a uniform distribution of Frenkel pairs being generated by irradiation and simultaneously undergoing recombinational losses, migration to surfaces, and loss to internal sinks. This theory is particularly applicable to the case of the room temperature 2 MeV He^+ damage in the 5000 Å films since a large number of Frenkel pairs will be produced in addition to the heavy ion recoil cascades. The calculations predict vacancy profiles as shown in Fig. 6. The double peak near the foil surfaces is a consequence of the loss of interstitials to the surface resulting in a reduction of the vacancy-interstitial recombination in that region. On the surface side of these peaks the vacancy concentration is depleted due to loss of vacancies to the surface. The central minimum results from randomly moving interstitials annihilating vacancies through recombination before reaching the surface. As the irradiation proceeds, and steady-state conditions are approached, the central valley diminishes and a uniform distribution is achieved. Lam (18) has considered, in addition to the point defect case, the possibility of vacancies clustering into agglomerates as a consequence of migration. His cluster profiles are qualitatively similar to those obtained for the case of Frenkel pairs. This is significant since the dechanneling is really a consequence of the strain fields associated with defect clusters. There are, in the diffusion calculations, quantitative differences associated with the multiple vacancy profiles compared to the single vacancy profiles. For example, since di-vacancies and tri-vacancies are considered to be mobile, their profiles reflect the effects of a lower activation energy for migration (.58 eV for di-vacancies and .47 eV for tri-vacancies compared to .84 eV for single vacancies in silver) by being broader in the peaked region and of generally lower concentration than the single vacancy profiles.

The precise defect profile at any irradiation fluence will be controlled by the parameters associated with the kinetic processes under consideration. These parameters include specimen temperature, activation energy for interstitial and vacancy migration (including multiple vacancies), sink density, film thickness, etc. From these, it was found that film thickness and the ratio of the

relevant vacancy migration energy to specimen temperature were most dominant in controlling the shape of the profiles in the thin films and the time to steady state. Using the theory of Rothman et al. and the gold single vacancy migration energy of 0.85 eV, Lam's computer code (19) revealed that a temperature of 125°C was necessary to achieve profiles and time to steady state comparable with the results of the dechanneling analysis. These calculated profiles are shown in Fig. 7. The irradiations were done at room temperature and if beam heating were negligible one would be required to use an activation energy of 0.58 eV at 23°C to get the same profiles. This is more nearly the value expected for dominance by the di-vacancy migration energy.

It should be noted that, according to the theory, the formation rate of di-vacancies through migration and combination of single vacancies will be comparable, for short times to steady state, with the mutual recombination rate. (19) Thus, the production of di-vacancies in the ion irradiations is a significant process and their migration could be the dominating factor in subsequent production of larger clusters, thus requiring the use of a 0.58 eV activation energy. The precise nature of the clustering process is not clear. However, for purposes of comparison to the theory, one should only consider migration to nucleation sites and consequent clustering as the diffusional process by which the profiles evolve. Spontaneous formation of defect clusters during cascade collapse is not necessarily diffusion controlled and their distribution cannot be easily identified with the theory of defect diffusion in a radiation environment.

5. EFFECTIVE CROSS-CHANNEL DISTRIBUTION OF MISALIGNED ATOMS IN THE DEFECT CLUSTER STRAIN FIELD

The distribution of misaligned lattice atoms across a channel can in principle be understood by examining the way in which the defect clusters perturb the transverse energy of the probing beam. If the probability of a misaligned atom being anywhere in the channel is a constant then particles of any transverse energy would have equal probability of encountering it. However, if the majority of misaligned atoms were near to the atomic rows, then particles with trajectories of high transverse energy would have greater probability of encountering them compared to those nearer the channel centers having low transverse energy.

A theory of dechanneling that can be applied to the problem of determining which trajectories are most likely to encounter misaligned atoms is the so-called steady increase of transverse energy model proposed by Lindhard (20) and applied to perfect crystals by Foti et al. (2) and to damaged crystals by Compisano et al. (21). Although the basic limitations of the assumption in this model are recognized (i.e., fixed transverse energy distribution with depth) it is felt that the approach represents a potentially tractable method for dealing with dechanneling from ion damage in metals. It is an obvious next step in sophistication beyond the simple approaches associated with the single and multiple scattering of section 2. The method in this section has certain features in common with those more elementary models (i.e., characteristic mean square scattering angle per collision); however, it recognizes and takes into account the fact that the transverse energy distribution of the probing beam in the axial channel is not a constant and that, therefore, a spatial distribution of probing trajectories can exist, with certain trajectories having greater probability of interacting with defects and thermally vibrating atoms than others. This approach begins to consider then such questions as the details of the relative displacement of dechanneling centers in terms of the atomic misalignment distances in a defect cluster.

In this model of dechanneling one follows the change in the average transverse energy as a function of depth. The changes in the transverse energy of a channeling particle will occur as a result of its encounters with vibrating nuclei, electrons and misaligned atoms.

Thus,

$$\frac{\delta \langle \epsilon_{\perp} \rangle}{\delta z} = \frac{\delta \langle \epsilon_{\perp} \rangle_n + \delta \langle \epsilon_{\perp} \rangle_e + \delta \langle \epsilon_{\perp} \rangle_d}{\delta z} = A_n f_n(\epsilon_{\perp}) + B_e f_e(\epsilon_{\perp}) + C_d f_d(\epsilon_{\perp}) \quad (7)$$

where n, e and d refer to nuclear, electronic, and defect contributions, respectively, and $\epsilon_{\perp}$ is the so-called reduced transverse energy given by $2E_{\perp}/E v_1^2$.

The various terms are broken up so that they consist of a constant representative of the system being examined, times a function, f, of the transverse energy only. This so-called f function describes the strength (or probability) of the interaction (with nuclei, electrons, or defects) in terms of the transverse energy being carried by the probing particle. For example, if the defects were such

that the misaligned atoms were uniformly distributed across the channels then $f_d(\epsilon_{\perp})$ would be a constant independent of $\epsilon_{\perp}$ since there would be equal probability of particles with any transverse energy encountering a misaligned atom. However, if there were a predominance of lattice atoms only slightly misaligned then $f_d(\epsilon_{\perp})$ would have a high value for large transverse energy particles that probe near the channel walls and a lower value for particles constrained to probe near the channel centers, there being a regular function defined for the full gradation of transverse energies between these extremes.

The procedure to be followed in this method is to determine the initial transverse energy distribution acquired by a perfectly collimated beam upon entering the crystal and then determining through the change in this cross-channel energy, as described above, the depth at which a particle of given $\epsilon_{\perp}$ will reach the critical angle and dechannel. This is done by numerically integrating Equation 7 to determine the depth at which a particular transverse energy will be reached and then using the integral transverse energy function below (Equation 9) to determine the fraction of the particles whose transverse energy has exceeded that value. One constructs from this the fraction of the total beam that dechannels at a given depth. This fraction is directly comparable to the experimental dechanneled fraction.

Assuming a perfect surface, the initial transverse energy is determined by the idealized cylindrical geometry of the axial channel and is given as:

$$P(\epsilon_{\perp 0}) = \frac{c_a^2}{r_0^2} \frac{Ae^{\epsilon_{\perp 0}}}{(Ae^{\epsilon_{\perp 0}} - 1)^2} \quad (8)$$

The total number of particles having transverse energy between 0 and $\epsilon_{\perp 0}$ is the so-called integral transverse energy distribution and is

$$P(\epsilon_{\perp 0}) = \int_0^{\epsilon_{\perp 0}} n(\epsilon'_{\perp 0}) d\epsilon'_{\perp 0} = \frac{A - 1}{Ae^{\epsilon_{\perp 0}} - 1} \quad (9)$$

It is the integral transverse energy function that is actually used, since all particles reaching a critical value of transverse energy will be assumed to dechannel.

The various terms used in calculating the change in transverse energy with depth have been described before and are here applied directly.

Thus,

$$\frac{\delta \langle \epsilon_{\perp} \rangle_n}{\delta z} = \frac{A_n f_n(\epsilon_{\perp})}{\delta z} = \left[\frac{\pi N d^2 \rho_{\perp}^2}{E C^2 a^2} \left(\frac{z_1 z_2 e^2}{d} \right)^2 \right] \times \left\{ \frac{(A e^{\epsilon_{\perp}} - 1)}{A(e^{\epsilon_{\perp}} - 1)} \left[(A e^{\epsilon_{\perp}} + 2/3) \left(1 - \frac{e^{-\epsilon_{\perp}}}{A} \right) \right]^3 \right\}, \quad (10)$$

which is the full vibrating nuclear contribution,

$$\text{and } \frac{\delta \langle \epsilon_{\perp} \rangle_e}{\delta z} = \frac{\pi z_1^2 e^2 N d}{E_o} \left(\frac{z_1 z_2 e^2}{d} \right) L_e \times \left\{ \frac{A e^{\epsilon_{\perp}} - 1}{A(e^{\epsilon_{\perp}} - 1)} \left[1 - \frac{e^{-\epsilon_{\perp}}}{A} \right] \right\}, \quad (11)$$

which is the non-thermal electronic contribution.

All terms in the above equations are as defined by Foti (2) with $\epsilon_{\perp}$ being the so-called reduced transverse energy. In order to account for the defects we have used a procedure where the defect contribution to the change in transverse energy is given as

$$\delta \langle \epsilon_{\perp} \rangle_d = G_d f_d(\epsilon_{\perp}) \delta z = \frac{2 \langle \theta^2 \rangle_t}{\psi_1^2} C(z) \delta z Q \exp \left\{ - \left[\frac{(\epsilon_{\perp}^* - \epsilon_{\perp})}{\epsilon_{\perp}} \right]^{1/2} \right\}. \quad (12)$$

In this equation $\langle \theta^2 \rangle_t^{1/2}$ is the mean square scattering angle per linear defect density, ψ_1 the critical angle, $C(z)$ the volume concentration of misaligned atoms in the crystal slice of δz . The quantity $\epsilon_{\perp}^*$ is the so-called critical value of the reduced transverse energy and is that value of $\epsilon_{\perp}$ at which a particle will dechannel. The quantity Q is a scaling factor for the exponential f function. This f function was obtained by trial and error fitting to the data and is discussed below.

Since the steady increase model assumes that a multiple scattering process is in effect, it is possible to estimate $\langle \theta^2 \rangle_t$ for the defects from the multiple scattering theory of Section 2. Likewise $C(z)$ can be taken from the same source when it is uniform with depth. This then allows a determination of Q to be made by fitting the theoretical and experimental dechanneling spectra, thus allowing the defect transverse energy function to be totally defined.

Calculations of the dechanneled fraction is obtained by using Equation 7 to determine the depth at which particles of initial transverse energy $\epsilon_{\perp 0}$ will reach the critical value $\epsilon_{\perp}^*$. This information is used with Equation 9, which gives the fraction of the particles starting out with energy equal to or greater than $\epsilon_{\perp 0}$, to find the total fraction of particles that dechannel at the depth of interest.

In addition to the $f_d(\epsilon_1)$ function used in Equation 12 the case of $f_d =$ constant was also examined. The latter being a case where the defect distribution would be uniform across the channel. A comparison of the experimental and theoretical dechanneling spectra for these two cases is presented in Figs. 8 and 9. It is obvious that the case of only slight displacement of lattice atoms is the correct picture inasmuch as the $f_d(\epsilon_1)$ function of Fig. 9 gives a far better fit to the experimental spectra compared to f_d being a constant.

Information about the cross channel distribution of the misaligned atoms can be obtained by examining this $f_d(\epsilon_1)$ function and comparing it to the similar functions used for electronic and thermal dechanneling. This is done in Fig. 10. Since the total transverse energy is a sum of kinetic and potential energy in the transverse plane, a determination can be made of the distance of closest approach of the probing particles to the channeling strings as a function of transverse energy. This is done by equating the total transverse energy to the string potential at the turning point in the transverse motion. Using the Lindhard (20) standard potential of

$$V(r) = - \frac{z_1 z_2 e^2}{d} \ln \left\{ \left(\frac{ca}{r} \right)^2 + 1 \right\}, \quad (13)$$

one can solve for r , the distance of closest approach of the probing particle to the string axis. Using the values of ϵ_1 in Fig. 10, a conversion is made from ϵ_1 to the minimum approach distance. The resulting scale is included in the upper abscissa of Fig. 10.

Examining the figure it is seen that the particles penetrating into the region between 0.45 and 0.2 Å of the channel walls are experiencing a change in their transverse energy, with those going closer to the walls being effected most significantly. For distances farther than ~0.45 Å particles are receiving negligible changes in their transverse energy. The distance from the strings to the channel center is $r_0 \approx 0.8$ Å, thus the misaligned atoms are a maximum of <1/2 the way to the channel center, with only a very few actually reaching that maximum distance. These results thus confirm the idea that the dechanneling points arise from the misalignments associated with the strain fields in the defect clusters and that the high transverse energy component of the beam is dominantly involved in the dechanneling from these defects.

6. DISCUSSION

It is noteworthy in considering the outcome of the depth profiling analysis that similar results are obtained for the 0.27 and 2 MeV probes of thin film damage where the defects were introduced by different irradiations in 1200 and 5000 Å films, respectively. The two sets of results are similar both qualitatively and quantitatively; however, the first was done with single scattering analysis and the second with multiple scattering theory. It should be pointed out that the type of cluster formed by the 2 MeV He^+ irradiation and the 80-540 keV Au^+ irradiation will be similar since both incident ions, at the energies involved, will produce comparable recoil energies in the high-energy transfer regime. Comparison of the defect clusters, observable by TEM, shows that both irradiations produce very similar cluster size distributions. (16,22) The unusual aspect of the gold irradiations is that the defect distributions appear spread across the entire film. This result has a direct analog in the TEM data as well. (15,16)

The low dose profile shapes exhibit similarities to that predicted by the theory of diffusion in a radiation environment. However, the parameters required to get theory and experiment to agree indicate that either the effective specimen temperature was elevated to 125°C during the introduction of defects by the irradiation or the dominant vacancy migration energy was not 0.85 eV as known to be the case for single vacancies. If the specimen did remain at room temperature during the irradiation, then the dominant vacancy migration energy would have to be 0.58 eV in order to get the theoretical and experimental profiles to agree. This lower migration energy is much more in keeping with the expected value for di-vacancy motion. It should be noted that the dechanneling method does not see single vacancies but rather the misaligned atoms in the strain field of clusters of vacancies. If the rate controlling process for the production of clusters is the formation and migration of di-vacancies then the profiles as obtained with the lower migration energy are more easily explained.

Application of the transverse energy model for analysis of the dechanneling data appears to produce encouraging results. Information can be obtained from this model on the spatial distribution of the misaligned atoms across the channel being probed. This gives direct information about the internal defect cluster

strain field which to date is unavailable by other methods. The full potentiality of this kind of analysis is yet to be explored. The significant result in the present work is that the transverse spatial distribution is shown to consist dominantly of near channel wall atoms, dropping to an insignificant level at a distance of less than 25% across the channel. Thus, there are no observable contributions to dechanneling or scattering from atoms displaced toward the middle of the channel. This confirms the approach used in the depth profiling analysis where only dechanneling was considered important with direct back scattering from defect atoms being discounted.

ACKNOWLEDGMENTS

The author wishes to acknowledge helpful discussions with K. L. Merkle, H. Wiedersich, and S. J. Rothman. Computer calculation of the defect diffusion profiles was done by N. Q. Lam. Assistance with computer programming of the dechanneling data was contributed by D. G. Brunder.

FIGURE CAPTIONS

- Fig. 1. Dechanneling probability for He^+ in gold versus areal density of defects for single scattering (ss) and multiple scattering (ms) at 0.27 and 2 MeV.
- Fig. 2. Defect distributions obtained with Eq. 5 for 2 MeV He^+ dechanneling in 5000 Å single crystal gold film that was irradiated in a random direction with 2 MeV helium ions to the fluences indicated.
- Fig. 3. Defect distributions obtained with Eq. 3 for 0.27 MeV He^+ dechanneling in 1200 Å single crystal gold film after 540 keV self ion irradiation to the fluences indicated.
- Fig. 4. Same conditions as Fig. 3 except self ion irradiation of 270 keV.
- Fig. 5. Same conditions as Fig. 3 except self ion irradiation of 80 keV.
- Fig. 6. Vacancy profiles determined by Lam (19) using the theory from Ref. (17) for defect diffusion under uniform Frenkel pair production at room temperature. The parameters are $D_{1v} = 8.5 \times 10^{-13} \text{ cm}^2/\text{sec}$, $D_i = 3.6 \times 10^{-2} \text{ cm}^2/\text{sec}$, $E_{1v}^m = 0.85 \text{ eV}$, $E_i^m = 0.13 \text{ eV}$, $T = 23^\circ\text{C}$, sink density of $3.5 \times 10^{-6} \text{ atom fraction}$, displacement rate of $8 \times 10^{18} \text{ cm}^{-3} \text{ sec}^{-1}$, film thickness of 1200 Å.
- Fig. 7. Same as Fig. 6 except $T = 125^\circ\text{C}$. The times up to steady state and the near surface peak positions are here comparable to that associated with the self ion irradiations.
- Fig. 8. Theoretical and experimental dechanneled fraction versus depth for 2 MeV He^+ dechanneling from 2 MeV random damage in 5000 Å gold film with $f_d = \text{constant}$ in the theory of Section 5.
- Fig. 9. Same as Fig. 8 except $f_d = Q \exp \left\{ - \left[\frac{E_{\perp}^* - E_{\perp}}{E_{\perp}} \right]^{1/2} \right\}$.
- Fig. 10. Relative rate of change of transverse energy versus total transverse energy for thermal, electronic, and defect dechanneling of 2 MeV He^+ in gold. Also presented as rate of change of transverse energy versus closest approach distance to channeling walls as described in Section 5.

REFERENCES

1. N. Matsunami and N. Itoh, Atomic Collisions in Solids, S. Datz, B. R. Appleton, and C. D. Moak, eds., Vol. 1, Plenum Press, New York (1975) p. 175.
2. G. Foti, F. Grasso, R. Quattrocchi, and E. Rimini, Phys. Rev. B 3, 2169 (1971).
3. L. C. Feldman and J. W. Rogers, J. Appl. Phys. 41, 3776 (1970).
4. J. E. Westmorland, J. W. Mayer, F. H. Eisen, B. Welch, Rad. Effects 6, 161 (1970).
5. R. R. Hart, Rad. Effects, 6, 51 (1970).
6. E. Bonderup, H. Esbensen, J. U. Andersen, and H. E. Schiott, Rad. Effects 12, 261 (1972).
7. N. Matsunami and N. Itoh, Phys. Lett. 43A, 435 (1973).
8. N. Matsunami, J. Phys. Soc. Japan 38, 848 (1975).
9. K. Morita and R. Sizmann, Rad. Effects 24, 281 (1975).
10. P. P. Pronko, to be published in Proceedings of the Intl. Conf. on Fundamental Aspects of Radiation Damage in Metals, Gatlinburg (1975).
11. M. L. Swanson, L. M. Howe, and A. F. Quenneville, Rad. Effects 25, 61 (1975).
12. H. E. Jack, Rad. Effects 13, 101 (1972).
13. F. H. Eisen, Channeling, D. V. Morgan, ed., J. Wiley, New York (1973) p. 415.
14. E. Bogh, Can. J. Phys. 46, 653 (1967).
15. K. L. Merkle, D. J. Dever, and J. R. Wrobel, Bull. Am. Phys. Soc. 18, 479 (1973).
16. P. P. Pronko and K. L. Merkle, Ion Beams in Metals, S. T. Picraux, E. P. EerNisse, and F. L. Vook, eds., Plenum Press, New York (1974) p. 481.
17. S. J. Rothman, N. Q. Lam, R. Sizmann, and H. Bisswanger, Rad. Effects 20, 223 (1973).
18. N. Q. Lam, J. Nucl. Materials 56, 125 (1975).
19. N. Q. Lam, private communication.
20. J. Lindhard, Dansk, Vid. Selsk. Mat. Fys. Medd. 34, No. 14 (1965).
21. S. U. Campisano, G. Foti and F. Grasso, Atomic Collisions in Solids, S. Datz, B. R. Appleton, and C. D. Moak, eds., Plenum Press, New York (1975) p. 905.
22. K. L. Merkle, P. P. Pronko, D. S. Gemmell, R. C. Mikkelsen, and J. R. Wrobel, Phys. Rev. B 8, 1002 (1973).

Fig. 1. Dechanneling probability for He⁺ in gold versus areal density of defects for single scattering (ss) and multiple scattering (ms) at 0.27 and 2 MeV.

Fig. 2. Defect distributions obtained with Eq. 5 for 2 MeV He⁺ dechanneling in 5000 Å single crystal gold film that was irradiated in a random direction with 2 MeV helium ions to the fluences indicated. DASHED CURVE IS RESULT FROM IRRADIATION ALONG THE <100> CHANNELING DIRECTION PRIOR TO RANDOM IRRADIATIONS

Fig. 3. Defect distributions obtained with Eq. 3 for 0.27 MeV He^+ dechanneling in 1200 Å single crystal gold film after 540 keV self ion irradiation to the fluences indicated.

Fig. 4. Same conditions as Fig. 3 except self ion irradiation of 270 keV.

Fig. 5. Same conditions as Fig. 3 except self ion irradiation of 80 keV.

in Gold, as

Fig. 6. Vacancy profiles_A determined by Lam (19), using the theory from Ref. (17) for defect diffusion under uniform Frenkel pair production at room temperature. The parameters are $D_{lv} = 8.5 \times 10^{-13} \text{ cm}^2/\text{sec}$, $D_i = 3.6 \times 10^{-2} \text{ cm}^2/\text{sec}$, $E_{lv}^m = 0.85 \text{ eV}$, $E_i^m = 0.13 \text{ eV}$, $T = 23^\circ\text{C}$, sink density of $3.5 \times 10^{-6} \text{ atom fraction}$, displacement rate of $8 \times 10^{18} \text{ cm}^{-3} \text{ sec}^{-1}$, film thickness of 1200 Å.

Fig. 7. Same as Fig. 6 except $T = 125^{\circ}\text{C}$. The times up to steady state and the near surface peak positions are here comparable to that associated with the self ion irradiations.

Fig. 8. Theoretical and experimental dechanneled fraction versus depth for 2 MeV He⁺ dechanneling from 2 MeV random damage in 5000 Å gold film with $f = \text{constant}$ in the theory of Section 5.

Fig. 9. Same as Fig. 8 except $f_d = Q \exp \left\{ - \left[\frac{\epsilon_{\perp}^* - \epsilon_{\perp}}{\epsilon_{\perp}} \right]^2 \right\}$.

Fig. 10. Relative rate of change of transverse energy versus total transverse energy for thermal, electronic, and defect dechanneling of 2 MeV He^+ in gold. Also presented as rate of change of transverse energy versus closest approach distance to channeling walls as described in Section 5.