By acceptance of this article, the publisher or recipient acknowledges the U. S. Government's right to retain a nonexclusive, royalty-free license in and to any copyright covering the article.

75-38

DEPTH DISTRIBUTION OF DAMAGE IN COPPER IRRADIATED Conf - 7510Cb - 4

J. Narayan, T. S. Noggle and O. S. Oen Solid State Division, Oak Ridge National Laboratory Oak Ridge, Tennessee 37830

#### ABSTRACT

Transmission electron microscopy has been used to study radiation damage as a function of depth caused by 58 MeV and 4 MeV Ni<sup>58</sup> and 1 MeV He ions in copper single crystals at ambient temperature. The experimental damage density vs. penetration depth distributions have been compared with calculations which are based on the atomic collision theory of Lindhard et al. (LSS). For 58 MeV Ni<sup>58</sup> ions, the calculated damage profile using the theoretical LSS value of the electronic stopping parameter (k = 0.167) agrees well with experiment. However, for 4 MeV Ni<sup>58</sup> ions it is necessary to use k = 0.12 to get agreement with the experimental data. In the case of 1 MeV He, the depth location of the calculated damage peak is in good agreement with experiment when the electronic stopping determined by Chu and Powers is used whereas it is about 15% too close to the surface using the tables of Northcliffe and Schilling.

INTRODUCTION

This report was prepared as an account of work sport-web by the United States Government. Neither United States are the United States from the United States are the United States from the United States from

The simulation of fast neutron damage in reactor materials by heavy ion irradiation is motivated mainly by the large "equivalent" doses that can be achieved in a short period of time. Such ion experiments can help quide the selection of reactor materials once a detailed understanding of the similarities and inherent differences of fast neutron and ion produced damage is established. One of the problems in the use of ions for these simulation studies is due to the large variation in the damage rate with ion penetration depth. Accurate information is required as to this depth variation of the damage and its equivalence to fast neutron damage.

MASTER

In the present investigation, the depth variation of the damage in copper due to 58 MeV and 4 MeV Ni<sup>53</sup> and 1 MeV He<sup>4</sup> ions irradiations at ambient temperature has been studied by electron microscopy. The experimental results have been compared with calculated theoretical damage energy profiles and it has been found that parameters in the theoretical treatment of the electronic stopping must be modified to fit the experimental data. The justification for using modified stopping power parameters will be discussed.

# EXPERIMENTAL

High purity (99.999%) copper single crystals were used in this study. Subsequent to irradiation, specimens were electroplated with copper and sectioned perpendicular to the original irradiated surface. Thinning of these sections was carried out such that the thin region suitable for electron microscope study contained the original surface and the full penetration depth of the ions. This technique has been described in detail previously with the present modification that the plated brass layer originally thought necessary to define the original surface is not required and is no longer used. The specimens were studied in a Hitachi 200 E electron microscope. The density and size distributions of the damage clusters (dislocation loops) were determined as a function of distance from the original surface. For comparison with the theoretical calculations, the experimentally measured values were converted into the equivalent point defect densities assuming circular loops.

### CALCULATIONS

The theoretical model developed previously to calculate the depth distribution of the damage is based largely on the theory of the slowing down of energetic ions in solids developed by Lindhard et al.<sup>2</sup> (LSS). The nuclear scattering between the ion and target atoms was treated using the analytical result of Winterbon et al.<sup>3</sup> which approximates the scattering from a Thomas-Fermi potential. The electronic energy looses, which primarily determine ion ranges for the

energies considered here, were treated using the LSS theory, semi-empirical tables and experimental data. The particular choices made will be discussed in further detail in the section comparing the calculations with the experiment. The calculations did not include the spatial transport of energy by recoiling atoms. This effect, although important for some cases at low ion energies 4,5, is not considered to be significant for the high ion energies treated here. In this respect the model is similar to that of Manning and Mueller.

### RESULTS AND DISCUSSION

Figure 1 shows a transmission election micrograph of the dislocation loop damage in Cu using 58 MeV Ni ions. In the micrograph, the ions were incident from the left side and the marked increase in the damage density near the end of range is clearly visible. In the upper graph of Fig. 1 the experimental point defect density (histogram), obtained from the density and loop size distributions, is plotted against penetration depth. The smooth curve in this graph is the calculated damage energy (right hand ordinate) as a function of penetration depth using the LSS theory for the electronic stopping (k = 0.167). The overall agreement is fairly good although the calculation predicts the damage peak at a slightly smaller depth than actually observed. It should be mentioned that the vertical scaling is arbitrary and that only about 5% of the defects calculated are observed. The dashed curve is for k = 0.12 which gives a very poor agreement. The reason for calculations with k = 0.12 will become apparent later in the paper.

In Fig. 2, a comparison of experiment and theory is given for 4 MeV Ni ions in copper. The experimental results are represented by the histogram. Again attention is focused on the position of the damage peak. The solid and dashed curves give the calculated deposited damage energy as a function of depth using values of the electronic stopping parameter of k = 0.167 and k = 0.12, respectively.

The dashed curve in which the electronic stopping has been reduced by 28% from that predicted by LSS (k = 0.167) gives quite good agreement with the experimental data. It should be mentioned that a 25% decrease in the nuclear screening length, while keeping the electronic stopping the same, increases the depth of the damage peak by only 5%.

Figure 3 shows calculated damage energy profiles and the experimental histogram of point defect density vs. depth for 1.0 MeV He ions. The peak in the damage profile was found experimentally at a depth of 1.83 microns from the irradiated surface. The dashed curve was calculated using values for the electronic stopping determined by interpolation from the tables given for He ions in nickel and germanium by Northcliffe and Schilling. The peak in the damage profile in this case is at a depth of 1.58 microns. The solid curve was obtained using the experimental values for the electronic stopping reported by Chu and Powers for He energies between 1000-400 keV, those of White and Mueller for He energies below 125 keV and interpolating for values between 400 and 125 keV. From this, the peak in the damage profile is obtained at 1.85 microns which agrees within 1% of the above experimental values. The reason the electronic stopping determined by interpolating from the widely used tables of Northcliffe and Schilling is particularly poor for He in Cu may be understood from the oscillations in the electronic stopping of He when plotted against the atomic number of the target material. 10 Copper is found to lie at a minimum, which makes interpolation from neighboring elements particularly poor.

The different values of k needed for good agreement with the experimental results for 58.0 and 4.0 MeV Ni ions show that the electronic stopping power of Ni ions in copper is not proportional to the ion velocity. For more discussion on this point see M. T. Robinson 11, this conference. To be consistent with the 4.0 MeV analysis, the 58 MeV analysis should use a smaller k when ion energies get down around 4.0 MeV. This would increase the calculated depth of the damage peak in the 58.0 MeV case, making the agreement even better.

It is believed that the low electronic stopping power for Ni ions at 4 MeV is due to oscillations of the stopping as a function of target atomic number similar to that for He ions 10 and N ions 12 in Cu. These oscillations are related to the electronic charge distribution around the target atoms and are more pronounced at lower energies. At higher energies where the projectile speed is much greater than the target-electron velocities, the target appears as an electron sea and oscillations in the electronic stopping power of projectile ions disappear.

The present results indicate that when accurate stopping power information is available (as in the case of 1 MeV He ions) the theoretical calculations provide an accurate quantitative estimation of the damage peak position. In the case of heavy ions, for which the stopping information is less accurate, substantial differences between the calculated and experimental peak positions can occur. This result is particularly important to those employing heavy ions for simulation studies. Using the 4 MeV Ni ions on copper as an example, the sampling of specimens at the depth predicted by the theoretical LSS calculations would:miss the peak in the damage by 0.25µm and be in a region where the damage energy is changing rapidly with depth and about 25% less than expected. In view of the relatively recently established oscillations in stopping as a function of target material and the departure from the theoretical velocity proportional electronic stopping, ti is to be expected that calculations based on extrapolations in ion energy and/or target material may be subject to appreciable error.

### REFERENCES

- O. S. Oen, J. Narayan and T. S. Noggle, in "Applications of Ion Beams to Metals" ed. by S. T. Picraux, E. P. EerNisse and F. L. Vook, Plenum Press, 1974.
- J. Lindhard, M. Scharff and H. E. Schiott, Kgl. Danske Videnskab. Selskab, Mat.-fys. Medd. 33. No. 14 (1963).
- K. B. Winterbon, P. Sigmund and J. B. Sanders, Kgl. Danske Videnskab. Selskab, Mat.-fys. Medd. 37, No. 14 (1970).
- 4. P. Sigmund, M. T. Matthies and D. L. Phillips, Rad. Eff. 11, 39 (1970).
- 5. D. K. Brice, J. Appl. Phys. 46, 3385 (1975).
- I. Manning and G. P. Mueller, Computer Physics Communications 7, 85 (1974).
- 7. L. C. Northcliffe and R. F. Schilling, Nuc. Data, A7: 233 (1970).
- 8. W. K. Chu and D. Powers, Phys. Rev. 187, 478 (1969).
- W. White and R. M. Mueller, Phys. Rev. 187, 499 (1969).
- J. F. Ziegler and W. K. Chu, Atomic and Nuclear Data Table 13, 463 (1974).
- 11. M. T. Robinson, this conference.
- 12. D. G. Simons, D. J. Land, J. G. Brennan and M. D. Brown in II International Conference on Ion Beam Surface Analysis held at Karlsruhe, Germany, Sept., 1975 (Proceedings to be published).

# FIGURE CAPTIONS

- Fig. 1. Calculated damage energy and experimental histogram of point defect density as a function of penetration depth. Total dose of 58 MeV Ni $^{58}$  is  $1.0 \times 10^{13}$  ions/cm $^2$ . The scale of the abscissa of the graph corresponds directly to dimensions in the micrograph obtained from a specimen irradiated with 58 MeV Ni ions.
- Fig. 2. Calculated damage energy and experimental histogram of point defect density as a function of penetration depth for 4 MeV Ni<sup>58</sup>. The Total dose here is  $5 \times 10^{12} \text{ ions/cm}^2$ . The dashed curve lies above the solid curve at very small penetration depths because the electronic energy losses of the recoiling copper atoms has also been reduced from the LSS value of k = .158 to 0.120.
- Fig. 3. Calculated damage energy and experimental histogram of point defect density depth for 1.0 MeV  $\rm He^4$  ions. The total dose of He ions is 2.0  $\times$   $10^{15}$  ions/cm<sup>2</sup>.

POINT DEFECT DENSITY (cm-3) IN CLUSTERS





