CONF-761027--14

EFFICIENCY OF DEFECT PRODUCTION IN CASCADES

R.S. Averback, R. Benedek, and K.L. Merkle

MASTER

International Conference
on the Properties of Atomic Defects in Metals
Argonne National Laboratory
Argonne, Illinois
October 18-22, 1976

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

UWIC-AUA-USERDA

DISTRIBUTION OF THIS REPORT

ARGONNE NATIONAL LABORATORY, ARGONNE, ILLINOIS

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

The facilities of Argonne National Laboratory are owned by the United States Government. Under the terms of a contract (W-31-109-Eng-38) between the U. S. Energy Research and Development Administration, Argonne Universities Association and The University of Chicago, the University employs the staff and operates the Laboratory in accordance with policies and programs formulated, approved and reviewed by the Association.

MEMBERS OF ARGONNE UNIVERSITIES ASSOCIATION

The University of Arizona	Kansas State University	The Ohio State University
Carnegie-Mellon University	The University of Kansas	Ohio University
Case Western Reserve University	Loyola University	The Pennsylvania State University
The University of Chicago	Marquette University	Purdue University
University of Cincinnati	Michigan State University	Saint Louis University
Illinois Institute of Technology	The University of Michigan	Southern Illinois University
University of Illinois	University of Minnesota	The University of Texas at Austin
Indiana University	University of Missouri	Washington University
Iowa State University	Northwestern University	Wayne State University
The University of Iowa	University of Notre Dame	The University of Wisconsin

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. Mention of commercial products, their manufacturers, or their suppliers in this publication does not imply or connote approval or disapproval of the product by Argonne National Laboratory or the U. S. Energy Research and Development Administration.

EFFICIENCY OF DEFECT PRODUCTION IN CASCADES*

R.S. Averbach, R. Benedek, and K.L. Merkle
Materials Science Division
Argonne National Laboratory
Argonne, Illinois 60439

ABSTRACT

In copper and silver, the defect production by energetic ions has been investigated for projectile masses between 1 and 209 in the energy range between 10^4 and 10^6 eV. Thin-film residual-resistivity measurements were used to determine the defect production below 10K. Calculations of the number of Frenkel pairs produced by various projectiles as a function of energy were performed, based on Lindhard's cross sections and a modified Kinchin-Pease expression. A comparison of measured and calculated damage rates shows that the defect-production efficiency decreases with ion mass for light projectiles, whereas at masses >20 the cascade efficiency remains rather constant and assumes a value of $\xi \approx 0.3$ for both Ag and Cu. The decrease in defect efficiency indicates a transition from isolated Frenkel-pair formation to the production of energetic displacement cascades.

*Work supported by U.S. Energy Research and Development Administration.

EFFICIENCY OF DEFECT PRODUCTION IN CASCADES*

R.S. Averbach, R. Benedek, and K.L. Markle
Materials Science Division
Argonne National Laboratory
Argonne, Illinois 60439

1. Introduction

The interest in the development of controlled thermonuclear fusion reactors has given considerable importance to the defect production associated with the implantation of He and other light ions as well as to the production of damage in very energetic recoil cascades in the range above 100 keV. In addition to providing information on the defect production by such projectiles, the present work is part of a systematic investigation of defect production as a function of incident particle mass and energy, aimed at elucidating and quantifying defect production in cascades.

2. Calculation of the number of Frenkel pairs produced in stopping an energetic projectile

The number of Frenkel pairs N_F produced over its range by a projectile of initial energy E_0 is calculated from the relation

$$N_F^t = \int_0^{E_0} dE \int_{E_d^{av}}^{T_{max}} \frac{d\sigma(T,E)}{dT} (S_n(E) + S_{el}(E))^{-1} \nu_F(T) \quad (1)$$

which integrates over the Frenkel pairs produced by the host recoils of energy T along the path of the incident projectile. In numerical evaluations, Lindhard's formulation [1] of both the differential scattering cross section $d\sigma(T,E)/dT$ and the nuclear and electronic stopping powers, $S_n(E)$ and $S_{el}(E)$, respectively, was used. The number of Frenkel pairs $\nu_F(T)$ produced by a recoil of energy T was calculated from a modified Kinchin-Pease expression

*Work supported by the U.S. Energy Research and Development Administration

$$v_F(T) = \begin{cases} 0 & T < E_d^{av} \\ 1 & E_d^{av} \leq T \leq 2.5 E_d^{av} \\ \frac{0.8 E_D(T)}{2 E_d^{av}} & T \geq 2.5 E_d^{av} \end{cases} \quad (2)$$

where the damage energy $E_D(T)$ is calculated using Robinson's formula [2]. The average threshold energies E_d^{av} (29 eV for Cu and 39 eV for Ag) are taken from Lucasson's [3] tabulation of electron threshold data. Figs. 1 and 2 show the results of calculations for a number of projectiles. The defect production increases rapidly with the mass of the projectile, reflecting the decrease in the fraction of energy lost to electronic excitations.

3. Measurement of the number of Frenkel pairs produced in monoenergetic cascades

Thin films of Cu and Ag of thickness 2480 and 2215 Å, respectively, were grown by vapor deposition in the shape of resistivity specimens onto cleavage surfaces of rock salt. The films were transferred to anodized aluminum holders and irradiated near 10K with a variety of ions. The ion energy was chosen such that the calculated projected range R_p [4] was approximately one half the film thickness. In this manner, the damage was deposited well into the bulk of the specimen, and, at the same time, essentially all of the ions were stopped within the foil. The measured resistivities were corrected for the electrical size effect. This was accomplished by adjusting the parameters in the Fuchs-Sondheimer theory [5] so that the size-effect-corrected damage-rate, $d\Delta\rho/d\phi$, for 150 keV proton irradiation would be linear in $\Delta\rho$. Our determinations of Frenkel-pair production, however, were made only in the initial part of the damage-rate curve ($< 2 \times 10^{-8}$ Ωcm) to minimize radiation-annealing effects.

The number of Frenkel pairs N_F produced by an incident ion is calculated by the expression [6,7]

$$N_F = \frac{N \cdot t}{\rho_F} \left(\frac{d\Delta\rho}{d\phi} \right)_0, \quad (3)$$

where N is the atomic density, t is the film thickness, ρ_F is the Frenkel-pair resistivity ($\rho_F^{Ag} = 2.1 \times 10^{-4} \Omega\text{cm}$, $\rho_F^{Cu} = 2.0 \times 10^{-4} \Omega\text{cm}$) [3], and $(d\Delta\rho/d\phi)_0$ is the size-effect-corrected initial damage rate. No correction has been made for the resistivity of the implanted ion. This correction is at most $\sim 15\%$ for the proton irradiations and is considerably less for all other projectiles. In this manner, the total number of Frenkel pairs produced by a particle along its entire range is determined. Results are given in table 1 for a wide variety of incident ions. Although results are quoted for only a single specimen in each case, experiments have been performed on films of different thicknesses and residual resistivities. Values of N_F were found to be reproducible to $\sim 10\%$. This reproducibility indicates that errors introduced by inhomogeneities in the defect distribution and by the size effect correction are not overly significant.

In comparing the observed defect production with theory, it is convenient to consider an efficiency factor ξ , defined as

$$\xi = \frac{N_F}{N_F^t}. \quad (4)$$

Table 1 and fig. 3 give values of ξ obtained in the present work.

4. Discussion

In the past, a detailed comparison of measured damage rates with the theory has been hindered by uncertainties in the average threshold energy E_d^{av} . However, recent progress in threshold anisotropy determinations has resulted in a set of recommended average threshold energies for a number of materials [3]. In the present work, these values are used to make quantitative comparisons of the calculated and observed damage production under ion irradiation. Fig. 3 and table 1 show, for both

Cu and Ag, a decrease in efficiency as the projectile mass increases from 1 to 20 amu. Above 20 amu, the cascade efficiencies show only slight variations.

For light ions and particularly for protons, the defect production in principle depends somewhat on the details of the threshold anisotropy. However, the fact that the observed efficiencies for both metals are close to unity for protons tends to justify the use of the proposed threshold energies [3]. An efficiency near $\xi = 1$ has also been found for protons near 100 keV when the beam is transmitted through the specimen [8]. In this instance, the analysis is less sensitive to the detailed form of the threshold function and to the magnitude of the electronic stopping constant.

The initial decrease in efficiency at low ion masses is associated with the transition from isolated Frenkel-pair damage to multiple displacements and cascades. The observed strong decrease in the efficiency as the projectile mass increases seems to be at variance with the results of binary collision computer simulations of cascade events [9,10]. The latter calculations predict only a slight decrease in efficiency as the cascade energy increases.

Some indications, based on theoretical and experimental work, exist that the reduced efficiencies may be primarily due to dynamic close-pair recombination effects which are not taken into account in binary collision models. Recent fully dynamical computer simulations [11] of 2.5 keV cascades in W have shown that recombinations occur between close pairs after the displacement spike has terminated. These recombinations are stimulated by the residual agitation of the lattice in the cascade region. Moreover, recent radiation-annealing experiments have demonstrated that close pairs are unstable in the

vicinity of an energetic cascade [12]. Additional evidence for this is the small amount of Stage I recovery that takes place in energetic displacement cascades [13].

5. Conclusions

Since efficiency values close to $\xi = 1$ are found, we conclude that no essential discrepancy exists between the calculated and observed damage rates in the cases in which the ion beam produces isolated Frenkel pairs. For irradiations in which multiple displacements and dense cascades, occur, reduced efficiencies are observed. The efficiency for dense cascades in Ag and Cu produced by heavy ion irradiation is found to be ~ 0.3 .

List of figures

- Fig. 1. Calculated number of Frenkel pairs produced along the range of selected ions in copper.
- Fig. 2. Calculated number of Frenkel pairs produced along the range of selected ions in silver.
- Fig. 3. Cascade efficiency as a function of projectile mass in copper and silver.

Fig. 1. Calculated number of Frenkel pairs produced along the range of selected ions in copper.

Fig. 2. Calculated number of Frenkel pairs produced along the range of selected ions in silver.

Fig. 3. Cascade efficiency as a function of projectile mass in copper and silver.

Table 1

Projected range R_p , initial damage rate $(d\Delta\rho/d\phi)_0$, number of Frenkel pairs

N_F , and damage efficiency ξ for a selection of ions incident on silver and copper

Target	Projectile	E_0, keV	R_p, cm	$\left(\frac{d\Delta\rho}{d\phi}\right)_0 \Omega \text{ cm}^3$	N_F	ξ
Ag	H	20	1.40×10^{-5}	5.93×10^{-22}	3.6	1.0
	He	50	1.72×10^{-5}	4.48×10^{-21}	28	.53
	Li	70	1.57×10^{-5}	$.96 \times 10^{-20}$	59	.47
	B	90	1.25×10^{-5}	1.85×10^{-20}	116	.49
	O	150	1.28×10^{-5}	2.94×10^{-20}	182	.40
	Ne	180	1.25×10^{-5}	3.81×10^{-20}	236	.36
	Ar	290	1.15×10^{-5}	7.91×10^{-20}	498	.37
	Ag	540	8.00×10^{-6}	2.04×10^{-19}	1253	.37
	Bi	720	5.95×10^{-6}	2.47×10^{-19}	1533	.33
Cu	H	30	2.00×10^{-5}	6.73×10^{-22}	7.1	1.03
	He	60	1.98×10^{-5}	4.51×10^{-21}	47.5	.61
	Ne	225	1.49×10^{-5}	3.68×10^{-20}	389	.40
	Cu	500	1.14×10^{-5}	1.01×10^{-19}	1059	.31
	Kr	560	1.12×10^{-5}	1.32×10^{-19}	1399	.34
	Ag	560	9.3×10^{-6}	1.35×10^{-19}	1419	.31
	Bi	855	7.0×10^{-6}	2.16×10^{-19}	2276	.32

References

- [1] J. Lindhard, M. Scharff and H. E. Schiøtt, Mat. Fys. Medd. Dan. Vid. Selsk. 33 (1963) 14.
- [2] M. T. Robinson in Radiation Induced Voids in Metals, USAEC Symposium Series 26 (1972) p. 397.
- [3] P. Lucasson, in Fundamental Aspects of Radiation Damage in Metals, eds. M. T. Robinson and F. W. Young, USERDA CONF-751006-P1, Vol. 1, (1975) p. 42.
- [4] H. E. Schiøtt, Rad. Eff. 6 (1970) 107.
- [5] E. H. Sondheimer, Advan. Phys. 1 (1952) 1.
- [6] W. Kesternich and K. L. Merkle, in Applications of Ion Beams to Metals, (Plenum Press, New York, 1976) p. 495.
- [7] K. L. Merkle and R. S. Averback, in Fundamental Aspects of Radiation Damage in Metals, eds. M. T. Robinson and F. W. Young, USERDA CONF-751006-P1 Vol.1 (1975) p. 127.
- [8] K. L. Merkle, R. S. Averback and R. Benedek, to be published.
- [9] M. T. Robinson and I. M. Torrens, Phys. Rev. B 9 (1974) 5008.
- [10] J. R. Beeler, Phys. Rev. 150 (1966) 470.
- [11] M. W. Guinan, private communication.
- [12] R. S. Averback and K. L. Merkle in Fundamental Aspects of Radiation Damage in Metals, eds. M. T. Robinson and F. W. Young. USERDA CONF-751006-P2 (1975) p. 1048.
- [13] R. S. Averback, L. J. Thompson and K. L. Merkle, this conference.