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NOTICE

N. M. Ghoniem¹, J. Alhajji² and F. A. Garner³

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HARDENING OF IRRADIATED ALLOYS DUE TO THE SIMULTANEOUS FORMATION OF VACANCY AND INTERSTITIAL LOOPS

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ABSTRACT: Clustering of irradiation produced point defects is recognized to impede dislocation motion and hence influence mechanical-deformation characteristics. In this paper, a model is presented for the simultaneous nucleation and growth of vacancy and interstitial loops in irradiated metals. The model is based on the homogeneous time-dependent rate theory. Conservation equations are developed for single defects as well as defect clusters. Defect-conservation equations include production by irradiation and thermal sources; and destruction by mutual recombination, migration to sinks as well as clustering into loops. Interstitial clustering is assumed to occur by diffusion of interstitial atoms. Vacancy loops, on the other hand, are assumed to form by an athermal cascade-collapse process. The density of such loops is determined as a result of the production of cascades and the finite loop lifetime. Cascade overlap and coalescence are also included in the model.

The calculations are extended to the analysis of the radiation-induced changes in tensile properties due to formation of interstitial and vacancy loops. A simple hardening model relates the microstructural calculations to predictions of changes in tensile strength. The results of this study show good agreement with hardening data for copper irradiated in RTNS-II at room temperature. The results also provide insight on differences in microstructural results observed in various experimental studies on copper.

KEY WORDS: vacancy, interstitial, dislocation, dislocation loop, irradiation, yield strength, hardening, rate theory, copper.

INTRODUCTION

Experimental investigations over the last two decades have established that exposure of metals at relatively low temperatures to neutron irradiation results in an increase in the yield strength. However, this strengthening is not necessarily beneficial. Radiation-induced strengthening has been directly linked to a loss of ductility in austenitic steels, and to a shift in the ductile-to-brittle transition temperature (DBTT) in ferritic steels.

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¹Professor, University of California, Los Angeles, CA 90024²Research assistant, University of California, Los Angeles, CA 90024³Fellow scientist, Westinghouse Hanford Company, Richland, WA 99352

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MASTER

The confident design of structural components that must withstand the rigors of an irradiation environment requires that irradiation-induced changes in properties be included in the design process. For example, the anticipated low temperature failure of the first wall in conceptual designs of Tandem Mirror Fusion Reactors has been predicted to arise from the irradiation shift of the DBTT.[1] It is technologically important, therefore, to study the response of alloys to irradiation hardening. Recent experimental work using the Rotating Target Neutron Source (RTNS-II) has been directed toward the study of this phenomena in a fusion-relevant spectrum.[2]

Neutron irradiation leads to the production of single vacancies, interstitials and impurity atoms. Vacancy aggregates formed in collision cascades may also collapse athermally to form depleted zones or vacancy loops. The subsequent interactions and agglomeration of these defects are now recognized to be the primary cause of irradiation hardening. Figure 1 shows typical irradiation-induced microstructures and the associated hardening that is observed in copper irradiated in RTNS-II at 25°C.

In this paper, we develop a model for the simultaneous formation of vacancy and interstitial aggregates at low temperatures. The model is not a comprehensive microstructural description applicable under all irradiation conditions. The formation of precipitates, cavities and dislocation networks at higher temperatures are excluded.

The microstructural evolution at higher temperatures is much more complex and microstructurally-based mechanical property correlations are largely phenomenological in nature.[3-4] The phenomenological approach is useful for interpolation or extrapolation beyond the range of existing data. However, for low temperature irradiation where the goal is to study fundamental atomistic processes, a different approach can be employed. Therefore, the first objective of this work is to investigate the simultaneous nucleation and growth of both vacancy and interstitial loops in irradiated materials at low temperatures ($T < T_m/3$). The second objective will be to apply the microstructural insight gained in this study to the description of the irradiation-induced hardening phenomenon.

SIMULTANEOUS CLUSTERING OF VACANCIES AND INTERSTITIALS

The model presented here is essentially a time-dependent nucleation and growth model for both vacancy and interstitial loops. Conservation equations are developed for single defects as well as defect clusters. Point defect conservation equations include production

by irradiation and thermal sources, and destruction by mutual recombination, migration to sinks as well as clustering into loops. Interstitial clustering is assumed to result from diffusional migration of interstitial atoms. Vacancy loop formation, on the other hand, is assumed to result from the athermal collapse of collision cascades. In other words the nucleation of vacancy loops is characterized by collisional rather than diffusional atomistic events. The average sizes of both interstitial and vacancy loops are determined by the competition between defect absorption and vacancy emission. It is also assumed that recently produced vacancy loops may coalesce with existing loops. This mechanism leads to growth of both types of loops (vacancy and interstitial), as will be shown later.

The following rate equations describe the evolution of defect populations and must be solved simultaneously. The notation employed in these equations is defined in Table 1, with the exceptions of concentrations C, diffusivities D and rate constants K. P_d is the damage production rate in dpa/sec, Q_{vl} is the fraction of vacancies in loops, and F_{el} is the loop line tension in eV/cm².

$$\begin{aligned}
 \frac{dC_v}{dt} = & (1 - \epsilon) P_d - Z_{vd}^n \rho_d^n D_v (C_v - C_v^e) \\
 & - Z_{vd}^{i1} \rho_d^{i1} D_v \left\{ C_v - C_v^e \exp \left(- \frac{[\gamma_{sf} + F_{el}(\bar{R}_{i1})] b^2}{kT} \right) \right\} \\
 & - Z_{vd}^{v1} \rho_d^{v1} D_v \left\{ C_v - C_v^e \exp \left(\frac{[\gamma_{sf} + F_{el}(\bar{R}_{i1})] b^2}{kT} \right) \right\} \\
 & - \alpha C_v C_i - K_v^{2i} C_v C_{2i} - K_v^{3i} C_v C_{3i}
 \end{aligned} \tag{1}$$

$$\begin{aligned}
 \frac{dC_i}{dt} = & P_d + K_v^{2i} C_v C_{2i} + 2\gamma_{2i} C_{2i} - K_i^1 C_i^2 - \alpha C_v C_i \\
 & - K_i^{2i} C_i C_{2i} - K_i^{3i} C_i C_{3i} - Z_{id}^k D_i C_i (\rho_d^k + \rho_d^{i1}) - Z_{id}^n D_i C_i \rho_d^n
 \end{aligned} \tag{2}$$

$$\begin{aligned}
 \frac{dC_{2i}}{dt} = & \frac{1}{2} K_i^1 C_i^2 + K_v^{3i} C_v C_{3i} - K_i^{2i} C_i C_{2i} \\
 & - K_v^{2i} C_v C_{2i} - \gamma_{2i} C_{2i}
 \end{aligned} \tag{3}$$

$$\frac{dC_{31}}{dt} = K_i^{21} C_i C_{21} + K_v^{41} C_v C_{41} - K_i^{31} C_i C_{31} - K_v^{31} C_v C_{31} \quad (4)$$

$$\frac{dN_{11}}{dt} = K_i^{21} C_i C_{21} \quad (5)$$

$$\frac{d\bar{R}_{11}}{dt} = \frac{1}{b} \left\{ Z_i^l D_i C_i - Z_v^l D_v C_v + D_v C_v^e \exp\left(-\frac{[\gamma_{sf} + F_{e1}(\bar{R}_{11})]}{kT} b^2\right) \right\} \quad (6)$$

$$\frac{dN_{v1}}{dt} = \frac{\epsilon P_d \Omega}{\pi \bar{R}_{v1}^2(0) b} \left\{ 1 - \left(\frac{v}{\lambda}\right) N_{v1} \right\} - \frac{N_{v1}}{\tau} \quad (7)$$

$$\frac{dQ_{v1}}{dt} = \epsilon P_d + Z_v^l \rho_d^{v1} D_v C_v - Z_i^l \rho_d^{v1} D_i C_i - \rho_d^{v1} D_v C_v^e \exp\left(\frac{[\gamma_{sf} + F_{e1}(\bar{R}_{v1})]}{kT} b^2\right) \quad (8)$$

$$\tau = \frac{-\bar{R}_{v1}(0)}{\left[\frac{d\bar{R}_{v1}}{dt}\right] \bar{R}_{v2}(0)} \quad (9)$$

$$\frac{d\bar{R}_{v1}}{dt} = \frac{1}{b} \left\{ Z_v^l D_v C_v - Z_i^l D_i C_i - D_v C_v^e \exp\left(\frac{[\gamma_{sf} + F_{e1}(\bar{R}_{v1})]}{kT} b^2\right) \right\} \quad (10)$$

$$\bar{R}_{v2} = \left[\frac{Q_{v1} \tau}{\pi b N_{v1}}\right]^{1/2} \quad (11)$$

TABLE 1
DEFINITION OF TERMS

<u>Symbol</u>	<u>Definition</u>	<u>Units</u>
V	Capture volume of a vacancy loop	cm^3
Z_v^i	Interstitial/vacancy loop bias factor for vacancies	-
Z_i^i	Interstitial/vacancy loop bias factor for interstitials	-
γ_{sf}	Stacking fault energy	eV/cm^2
ν	Poisson's ratio	-
$\nu_{i,v}$	Interstitial/vacancy vibrational frequency	s^{-1}
Ω	Atomic volume	cm^3
ρ_d^n	Network dislocation density	cm/cm^3
ρ_d^{il}	Line dislocation density, interstitial loop	cm/cm^3
ρ_d^{vl}	Line dislocation density, vacancy loop	cm/cm^3
α	Point defect recombination coefficient	s^{-1}
γ_{2i}	Di-interstitial dissociation rate	s^{-1}
ϵ	Fraction of vacancies produced directly in vacancy loops	-
τ^{vl}	Lifetime of an individual vacancy loop	s^{-1}
$\Delta\sigma_{SR}$	Increase in the shear stress due to short range interaction	ksi
$\Delta\sigma_{LR}$	Increase in the shear stress due to long range interaction	ksi
$\Delta\tau$	Total increase in shear stress	ksi
$\Delta\sigma$	Total increase in yield stress	ksi

Equations (1-11) were numerically solved using standard numerical methods for stiff ordinary differential equations.[5] These equations are obtained by simply describing the balance between processes for production and destruction using homogeneous rate theory, as described in References [6] and [7].

Self-interstitial atoms are considered to migrate randomly between trapping sites. Their diffusion coefficient is determined by an effective migration energy such that

$E_{\text{eff}}^{\text{m}} = E_{\text{i}}^{\text{m}} + E_{\text{i}}^{\text{c}}$, where E_{i}^{m} is the migration energy and E_{i}^{c} is the trap binding energy. This was shown by Mansur [8] to be a reasonable approximation to describe trapping, providing the trapping is not particularly strong. The trap-hindered motion of self-interstitials results in agglomeration due to the increased formation of di-interstitials, as described in equation (2). Since di-interstitials can be destroyed by thermal dissociation or vacancy impingement, [7] the critical nucleus size for interstitial loops is therefore taken as three atoms. A time-dependent rate equation is therefore developed for the total number of interstitial loops by integrating the nucleation current for clusters that grow past the critical nucleus size. This current is described in equation (5). The size distribution of interstitial loops is approximated by an average radius \bar{R}_{il} given in equation (6). The interstitial loop of average size grows by interstitial absorption and vacancy emission, and shrinks by vacancy absorption.

The description of formation and growth of vacancy loops is treated differently. Since vacancies diffuse too slowly at low temperature to allow agglomeration, the formation of vacancy loops must arise from collisional events and cascade collapse. The rate equation for vacancy loop concentration therefore represents a balance between direct production by irradiation and evaporation of loops both thermally or by irradiation. Moreover, as the density of cascades increases, an increasing fraction of crystal space will not be available for further production $\{1 - (V/\Omega)N_{\text{vl}}\}$ without overlap of cascades occurring. V is an effective loop volume for coalescence, Ω is the atomic volume and N_{vl} is the fractional loop concentration. This is a mechanism by which loops can grow, not by diffusional processes, but due to collisional events. The vacancy loops are essentially unstable, however. Their lifetime, τ , is determined by the net flux of interstitials to them and their rate of vacancy emission. These processes tend to reduce the lifetime of the loop, in complete contrast to the behavior of loops of interstitial character. When a vacancy loop is formed, it immediately acts as a net interstitial sink because of the dislocation character of its perimeter. Si-ahmed and Wolfer [9] proposed that both vacancy and interstitial loops can grow in coexistence if the non-linear elasticity effects on the strain field are factored into the bias calculations. In the present model, this is not a necessary condition, and simultaneous loop growth can proceed by cascade overlap for vacancy loops. For cascade collapse modeling, the coalescence volume is chosen to be a sphere with a radius that is three times the

vacancy loop radius. Input parameters chosen to represent relatively pure copper are listed in Table 2.

TABLE 2
MATERIAL PARAMETERS FOR COPPER

<u>Parameter</u>	<u>Definition</u>	<u>Numerical Value</u>	<u>Reference</u>
<u>FIXED PARAMETERS</u>			
E_1^m	Migration energy of single interstitial	0.12 eV	[28]
E_v^m	Migration energy of single vacancy	0.72 eV	[29]
E_{2i}^B	Binding energy of di-interstitials	1.19 eV	[30]
$R_{v1}(o)$	Radius of the newly born vacancy loop	15 Å	[6]
<u>ASSUMED PARAMETERS</u>			
ϵ	Fraction of vacancies produced directly in vacancy loops	10%	
E_1^t	Trap binding energy	0.28	
Z_i^l	Loop bias factor for interstitials	1.02	
Z_i^n	Network bias factor for interstitials	1.02	

IRRADIATION HARDENING AT LOW TEMPERATURE

It is traditional to describe the effects of irradiation hardening with models that account for the interactions of various defects which act as barriers that resist the motion of dislocations. The resistance forces have been classified as either long-range (LR) or short-range (SR). The long-range forces are due to the repulsive interaction between moving dislocations and the dislocation network. The long-range interaction of the stress fields of dislocation loops is significant when the loops are large. In this study, loops were considered large when their average radius exceeds ~ 25 Å.

Short-range forces arise from the interaction between moving dislocations and small defects lying in the slip plane. Such defects impose pinning forces on the moving dislocations at points of contact. Solution hardening by solute atoms functions in this manner. Since the temperature of interest for this study is low, the small defects which contribute to solution hardening are only those abundant in this temperature range. We therefore include single vacancies, single interstitials, di- and tri-interstitials and small vacancy and interstitial disks.

The total increase in the shear stress, $\Delta\tau$, due to irradiation is given by:

$$\Delta\tau = \Delta\tau_{SR} + \Delta\tau_{LR} . \quad (12)$$

Solution hardening by tetragonal distortions was first investigated by Fleischer.[10] He classified the hardening process as being either gradual or rapid. Gradual hardening was attributed to substitutional impurities, and is caused by an elastic mismatch between solute atoms and the alloy matrix. On the other hand, small atomic disks or single defects tend to cause a highly asymmetrical lattice distortion, which is deemed responsible for the rapid hardening observed under irradiation.

The maximum force per unit length on the moving dislocation is F^{\max}/ℓ , where F^{\max} is the maximum force exerted by the defect and ℓ is the inter-defect spacing. Hence, the increase in shear stress, τ , to move the pinned dislocation is

$$\tau = \frac{F^{\max}}{b} , \quad (13)$$

where b is the slip vector of the dislocation, and ℓ is defined by

$$\ell = (dN)^{-1/2} , \quad (14)$$

where d is the defect diameter and N is its volumetric concentration.

In the case of a tetragonal distortion, the maximum force is calculated using a method suggested by Cochardt, et al.[11] By calculating the interaction energy and maximizing its derivative, the maximum force was shown to be

$$F^{\max} = G\Delta\epsilon b^4 / \alpha y_{\min}^2 , \quad (15)$$

where y_{\min} is the distance of the closest defect to the slip plane, and α is a numerical factor for the different slip planes in a face-centered cubic lattice. $\Delta\epsilon$ is a measure

of the strain due to tetragonality distortion, and has been assigned a value of 0.55 for an interstitial atom, 0.08 for a divacancy and 1.00 for a vacancy or interstitial loop. It was also concluded by Westbrook [12] in an experimental study of the NiAl intermetallic compound, that single vacancies are more potent hardeners than are single self-interstitial atoms.

Assuming additive contributions to the increase in the shear stress, the total contribution for short-range interaction is

$$\Delta\tau_j = \frac{Gb}{\beta} (\sum N_i d_i)^{1/2}, \quad (16)$$

where the subscript j describes a particular defect, i refers to the size class of the same defect, and β is a numerical factor ranging from 1.0 to 4.0. [13-17] In this study, we adopt Fleischer's value for small loops of $\beta = 3.7$. [10]

Network dislocations contribute to long-range hardening [18] according to the expression

$$\Delta\tau = \alpha Gb \sqrt{\rho_d^n}, \quad (17)$$

where ρ_d^n is the network dislocation density. The coefficient α has been measured at values of 0.15 to 0.3. [18] This effort employs Johnson's value $\alpha = 0.2$, [19] which was confirmed recently. [4]

The elastic interaction between prismatic dislocation loops and network dislocations is only significant when the loops are large. Loops were considered large at an arbitrary radius of 25 Å. The interaction of the stress fields between dislocation loops and network dislocations has been investigated by Kroupa and Hirsch. [20] Using Friedel's estimate [21] of the average distance between interacting loops, Kroupa and Hirsch [20] show that

$$\Delta\tau_{LR} = \frac{Gb d N^{2/3}}{\eta} \quad (18)$$

where η is a numerical factor ranging from 1.45 to 16. [20-23] Experimental results by Holmes [23] suggest a value of 1.45 for 316 stainless steel. Since the incremental increase in the shear stress caused by short-range barriers is proportional to $\langle l \rangle^{-1}$, where $\langle l \rangle$ is the average distance between obstacles, $\Delta\tau_{SR}$ can be described by

$$\Delta\tau_{SR} \sim (\sum (n_j d_j))^{1/2} \quad (19)$$

where the sum is over defect type j . The total short-range hardening must therefore be expressed as

$$\Delta\tau_{SR} = \{\Delta\tau_v^2 + \Delta\tau_I^2 + \Delta\tau_{2I}^2 + \Delta\tau_{3I}^2 + \Delta\tau_{vI}^2 + \Delta\tau_{IL}^2\}^{1/2} . \quad (20)$$

According to the Von Mises criterion, the relation between the incremental changes in shear and yield stresses is

$$\Delta\tau_Y = \sqrt{3} \Delta\tau \quad (21)$$

Hence, the irradiated tensile strength, σ_1 , is expressed by

$$\sigma_1 = \sigma_0 + \Delta\sigma_Y \quad (22)$$

where σ_0 is the unirradiated yield strength.

During the early stages of irradiation, both vacancy and interstitial loops are known to be small and function as short-range barriers. The yield strength at low fluence for well-annealed material is therefore

$$\sigma_1 = \sigma_0 + \frac{1}{2} Gb \{ (Nd)_{vI} + (Nd)_{IL} + (Nd)_v \}^{1/2} \quad (23)$$

At higher fluences, the interstitial loop density tends to saturate while the loops continue to grow. Therefore,

$$\sigma_1 = \sigma_0 + 1.2 Gb (N^{2/3} d)_{IL} + \frac{1}{2} Gb \{ (Nd)_{vI} + (Nd)_v \}^{1/2} \quad \text{for } d_{IL} > 50 \text{ \AA} . \quad (24)$$

RESULTS AND DISCUSSION

Recent room temperature irradiations of copper and other metals in RINS-II are aimed at identifying the nature of displacement damage produced by 14 MeV neutrons.[2,24] In such experiments, the accumulated displacement dose is correlated with changes in mechanical properties. Both microhardness [2] and tensile tests [24] have been employed in these studies. In this section, the model developed in the previous section is applied to copper irradiated in RINS-II at room temperature. Values chosen for relevant model parameters are listed in Table 2. The aim of the analysis in this section is to

The average radius of a vacancy loop that forms during a cascade collapse event stays roughly constant up to $\sim 5 \times 10^{17}$ n/cm², and then starts to decrease due to absorption of interstitial atoms. All vacancy loops are assumed to be produced at an average radius of 15 Å. At a given time, there is a mixture of freshly produced loops and older ones. Due to the absorption of excess interstitials, the average size is reduced as irradiation proceeds. At higher fluences ($>10^{19}$ n/cm²) significant cascade overlap commences, and vacancy loops start growing again.

On the other hand, interstitial loops grow continuously by diffusion of point defects and their average radius is a monotonically increasing function of neutron fluence. This behavior is shown in Figure 3.

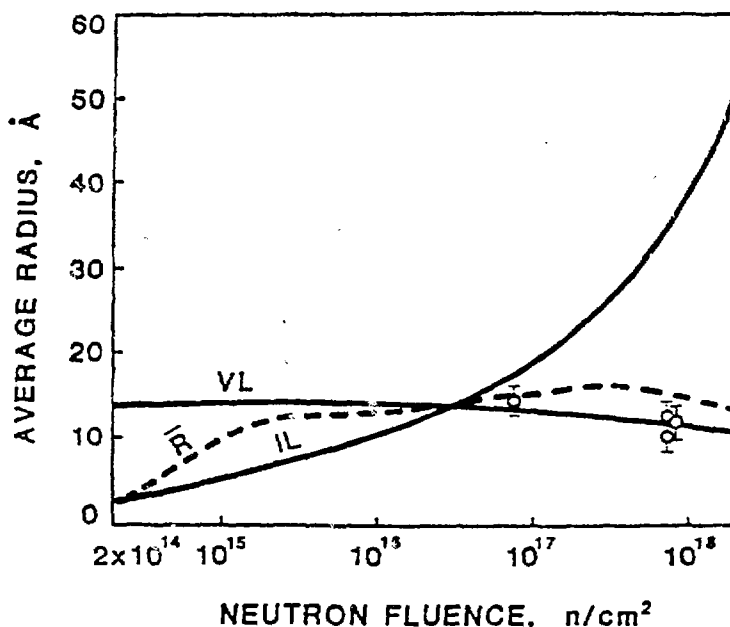


Fig. 3 - Calculated fluence dependence of average radius for vacancy and interstitial loops in copper irradiated in RTNS-II at 25°C. The radius for the combined population is also shown in comparison with measurements.[2]

Various experimental observations have been made regarding the distribution of irradiation-produced clusters of vacancies and interstitials in copper.[2,25-27] Roughly equal numbers of vacancies and interstitials in their respective clusters were reported by Brager, et al.,[2] and by Larson and coworkers. [25] However, other investigators reported a range of twice as many vacancies as interstitials to less than half as many vacancies as interstitials in loops.[26-27] While the differences

may arise from resolution problems in the microscope, the present model predicts a partitioning of point defects into loops that is fluence and temperature dependent. Therefore, these experimental observations may not be inconsistent. In order to study the distribution of produced point defects, we define the following:

$$\begin{aligned}
 f_1 &= \text{fraction of defects in clusters} \\
 &= \frac{\text{number of clustered defects}}{\text{irradiation dose}} \\
 &= \frac{N_{vl} \cdot R_{vl}^2 \cdot b + N_{il} \cdot R_{il}^2 \cdot b}{\text{dpa}} \quad (25)
 \end{aligned}$$

$$\begin{aligned}
 f_2 &= \text{interstitial fraction of defects in clusters} \\
 &= \frac{\text{number of interstitial atoms in clusters}}{\text{total number of defects in clusters}} \\
 &= \frac{N_{il} \cdot R_{il}^2}{(N_{vl} \cdot R_{vl}^2 + N_{il} \cdot R_{il}^2)} \quad (26)
 \end{aligned}$$

$$\begin{aligned}
 f_3 &= \text{fraction of loops of vacancy character} \\
 &= \frac{N_{vl}}{N_{il} + N_{vl}} \quad (27)
 \end{aligned}$$

Figure 4 shows the behavior of the fractions f_1 , f_2 and f_3 as a function of irradiation fluence. It is seen that the fraction of defects in clusters decreases from 28% at 10^{15} n/cm² down to only 10% by a fluence of 10^{18} n/cm². This is reasonably consistent with the observation of Brager and coworkers [2] that at least 9.4% of the defects survive at fluences in the mid- 10^{17} n/cm² range. Within the clustered point defects, there are more interstitials in clusters than vacancies, however. The fraction f_2 is around 60% in the same fluence range. At low fluence, the sink for interstitial atoms has not been completely created, and therefore interstitials continue to form new clusters rather than only annihilate at sinks or with other vacancies. Equilibrium sink conditions are established beyond a fluence of 10^{18} n/cm², and the fraction of interstitials in clusters approaches 50%. The relative number of vacancy loops to total loops, f_3 , is also shown in Figure 4. The fraction of loops of vacancy character increases throughout the irradiation. At higher fluences, the majority of the loops

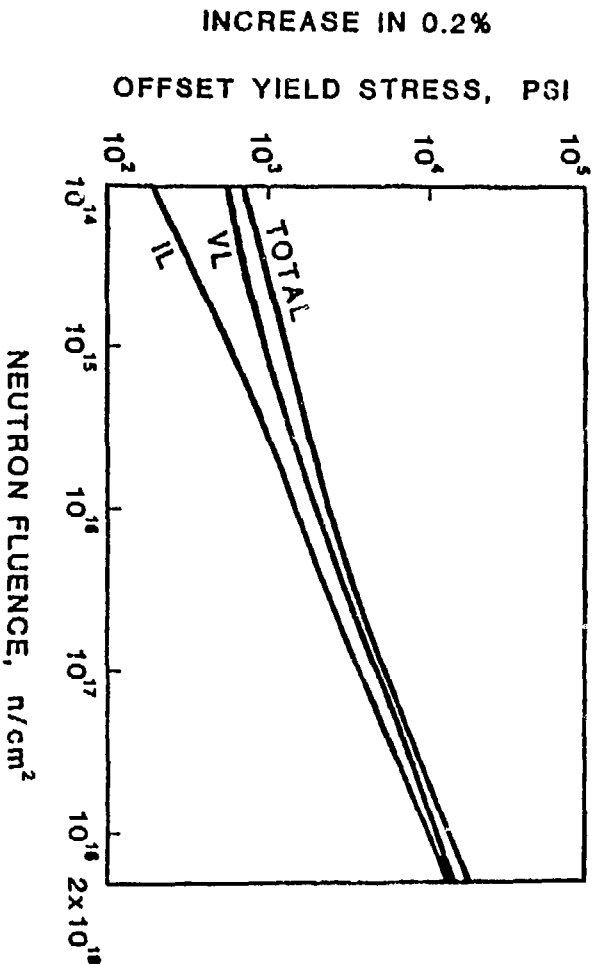


Fig. 5 - Calculated major contributions to the increase in 0.2% offset yield stress of copper at 25°C in RNS-II.

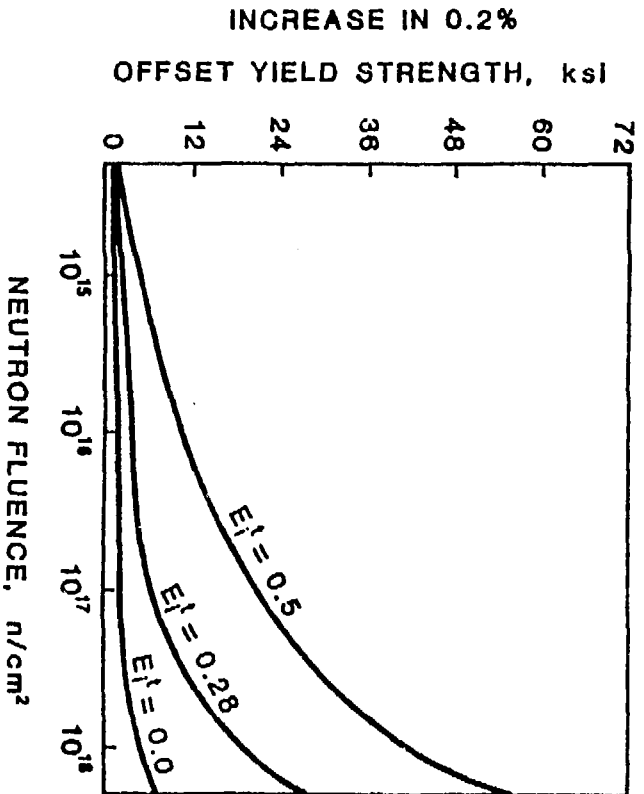


Fig. 6 - Effects of self-interstitial trapping on the predicted increase of yield stress of copper irradiated at 25°C. $E_I^1 = 0.117$ eV.

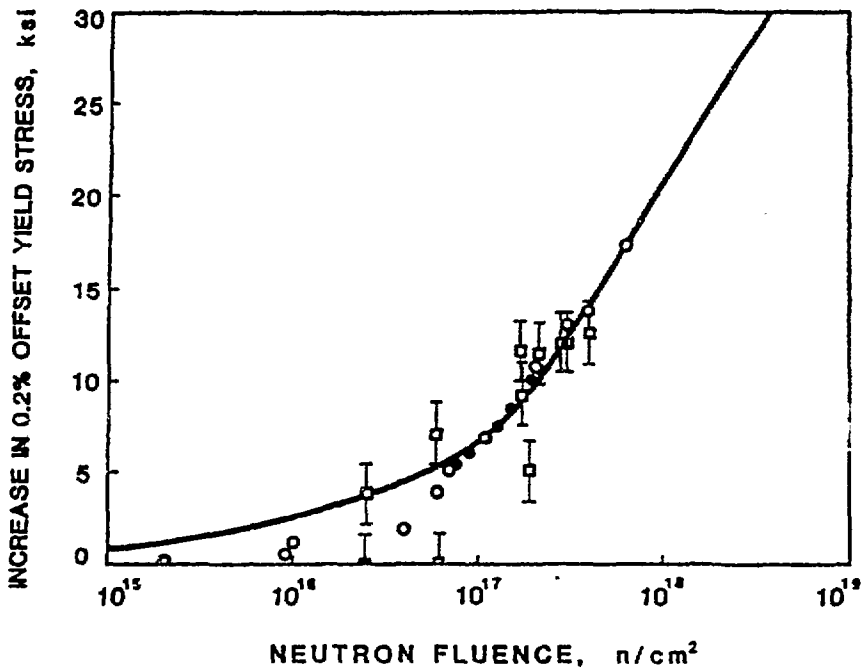


Fig. 7 - A comparison between theoretical calculations and experimental measurements of copper hardening due to RTNS-II irradiation at 25°C. Solid circles = LLL Cu. [24] Open circles = Cominco Cu. [24] Squares = DAFS copper. [2]

formation of interstitial loops with a slow growth rate. Beyond $\sim 2 \times 10^{16}$ n/cm², vacancy loops accumulate to a significant level, and begin to account for the majority of hardening by short-range interactions. Since the average vacancy loop diameter does not drastically change with fluence, the change in yield strength or hardening will increase as $\sim N^{1/2}$, or $\Delta\sigma_y \sim (\phi t)^{1/2}$. This is in agreement with the results shown in Figure 1. However, for high fluences ($> 10^{21}$ n/cm²) saturation will begin to set in due to overlap of cascades.

CONCLUSIONS

The following conclusions can be drawn from this study on irradiation of copper at 25°C in RTNS-II.

- (1) Nucleation and growth of loops occur simultaneously throughout irradiation.
- (2) Below a fluence of approximately 2×10^{16} n/cm², the density of vacancy loops is lower than the density of interstitial loops, while the average radii show the opposite trend.

- (3) During irradiation, the interstitial fraction of total defects in clusters is always larger than the vacancy fraction. The remainder of vacancies exist as single vacancies.
- (4) The fraction of total defects produced that survive in clusters decreases with fluence. Calculations of this fraction agree with measured values in the range where data are available.
- (5) Increased interstitial atom trapping leads to an earlier acceleration of irradiation hardening.
- (6) The measured hardening of copper can be related to the radiation-induced microstructural alterations observed by microscopy. Model-based predictions of those microstructural alterations can be employed in extrapolation of the data and to understanding of the fundamental processes involved.

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