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Risø-R-1186(EN)

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On Recoil Energy Dependent Void Swelling in Pure Copper: Theoretical Treatment

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Abstract Over the years, an enormous amount of experimental results have been reported on damage accumulation (e.g. void swelling) in metals and alloys irradiated under vastly different recoil energy conditions. Unfortunately, however, very little is known either experimentally or theoretically about the effect of recoil energy on damage accumulation. Recently, dedicated irradiation experiments using 2.5 MeV electrons, 3.0 MeV protons and fission neutrons have been carried out to determine the effect of recoil energy on the damage accumulation behaviour in pure copper and the results have been reported in Part I of this paper (Singh, Eldrup, Horsewell, Ehrhart and Dworschak 2000).

The present paper attempts to provide a theoretical framework within which the effect of recoil energy on damage accumulation behaviour can be understood. The damage accumulation under Frenkel pair production (e.g. 2.5 MeV electron) has been treated in terms of the standard rate theory (SRT) model whereas the evolution of the defect microstructure under cascade damage conditions (e.g. 3.0 MeV protons and fission neutrons) has been calculated within the framework of the production bias model (PBM). Theoretical results, in agreement with experimental results, show that the damage accumulation behaviour is very sensitive to recoil energy and under cascade damage conditions can be treated only within the framework of the PBM. The intracascade clustering of self-interstitial atoms (SIAs) and the properties of SIA clusters such as one-dimensional diffusional transport and thermal stability are found to be the main reasons for the recoil energy dependent vacancy supersaturation. The vacancy supersaturation is the main driving force for the void nucleation and void swelling. In the case of Frenkel pair production, the experimental results are found to be consistent with the SRT model with a dislocation bias value of 2%.

ISBN 87-550-2705-9
ISSN 0106-2840

Information Service Department, Risø, 2000

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1 Introduction

In the past, it has not been possible to treat explicitly the effect of recoil energy on defect accumulation in the form, for example, of voids. A close examination of literature in this field helps to identify two main reasons for this limitation. Until relatively recently, the vital information regarding the details (e.g. nature, efficiency and morphology) of defect production as a function of recoil energy was simply not available. The second reason is related directly to the fact that there existed no theoretical framework within which the main features of the damage production at higher recoil energies such as intracascade clustering of both self-interstitial atoms SIA_s and vacancies, thermal stability and one-dimensional glide of SIA clusters could be treated properly.

The experimental observations showing the athermal formation of vacancy loops at higher recoil energies (for review, see English and Jenkins 1987) led Bullough, Eyre and Krishan (1975) to propose a model commonly known as BEK model to account for the formation of vacancy loops at higher recoil energies. The BEK model is an extension of the standard rate theory model and uses the dislocation bias as the only driving force for the damage accumulation. The so-called "composite" model proposed by Stoller and Odette (1987) is similar to the BEK model except for the fact that the vacancy clusters are assumed to be microvoids instead of collapsed vacancy loops. The BEK type of models neither consider the intracascade clustering of SIAs nor do they include a treatment of the properties of SIA clusters such as their thermal stability and their ability to glide one-dimensionally.

In recent years, however, a considerable amount of effort has been spent on establishing a new model called the Production Bias Model (PBM) (Woo and Singh 1990, 1992, Singh and Foreman 1992) in which all the main features of the damage production at higher recoil energies including the effect of one-dimensional glide of small SIA clusters (Trinkaus, Singh and Foreman, 1992,1993, Trinkaus, Singh and Woo 1994, Singh, Golubov, Trinkaus, Serra, Osetsky, and Barashev 1997) are included. The PBM is formulated such that the problem of damage accumulation can be properly treated at any recoil energy (see Section 2). The main objective of the present paper is to calculate the effect of recoil energies in the range covering the production of isolated Frenkel pairs, cascades and subcascades. The physical basis of the present calculations is described in Section 2, whereas the details of theoretical treatments are presented in Section 3. Results of the numerical calculations are compared with the results of irradiation experiments (Singh, Eldrup, Horsewell, Ehrhart and Dworschak 2000) with 2.5 MeV electrons, 3 MeV protons and fission neutrons with a damage rate of $\sim 5\times 10^{-8}$ dpa/sec at 523 K in section 4. Section 5 presents the main conclusions of the present work.

2 Physical Considerations

Before presenting the theoretical framework for treating the effects of recoil energy on defect accumulation, it is important to identify the main parameters which may be responsible for controlling the nature and the magnitude of the effect. First of all, it should be appreciated that the relevant parameter for the accumulation of radiation damage is the fraction of defects (i.e. SIAs and vacancies) surviving subsequent to the collision event and not the number of displacements produced during the collision (Zinkle and Singh 1993, Singh and Zinkle 1993). Another fundamental aspect of the damage production is as to whether or not at a given primary knock-on atom (PKA) energy the damage is produced as isolated single Frenkel pairs (e.g. by 1 MeV electrons) or as multi-displacement cascades, where a significant fraction of defects survives as defect clusters (see below for details). As shown by molecular dynamics (MD) simulations, multi-displacement cascades begin to form, for example, in copper already at a PKA energy of ~0.5 keV (e.g. Diaz de la Rubia and Guinan 1990, 1992, Foreman, English and Phythian 1992, Phythian, Stoller, Foreman, Calder and Bacon 1995). At still higher recoil energies cascades break-up into subcascades (Heinisch 1990, Heinisch and Singh 1993, Stoller, Odette and Wirth 1997). The cascade break-up energy increases with atomic mass density of metals and varies, for example, from about 2 keV in aluminium to about 250 keV in tungsten (see Table 2 in Heinisch and Singh 1993). In addition to intracascade clustering, a substantial fraction of the displacement damage is annihilated via SIA-vacancy recombination during the cooling-down phase of the cascades.

Thus, an increase in the PKA energy leads to changes, not only in the fraction of the surviving defects but also in the defect morphology and dispositions varying from homogeneously distributed Frenkel pairs to heterogeneously distributed clusters of SIAs and vacancies.

The results of MD simulations have established the following salient features of the damage production as a function of PKA energy:

(a) At PKA energies of ~0.5 keV and above the damage production occurs in the form of multi-displacement cascades,

(b) Intracascade recombination of SIAs and vacancies during the cooling-down phase leads to a decrease in the fraction of surviving defects (i.e. damage efficiency) with increasing PKA energy and reaches a value of ~10% of the NRT value at the PKA energy of ~10 keV at void swelling temperatures. Beyond this energy level, the decrease in the damage efficiency is not very significant,

(c) Intracascade clustering of both vacancies and SIAs occur already during the cooling-down phase of the cascades,

(d) Clustering occurs in a segregated form such that the vacancy clusters are formed at cascade centre, whereas clusters of SIAs are formed at the cascade periphery,

(e) Size and number of clusters produced per cascade increase with increasing PKA energy.

It should be noted that the MD results showing intracascade recombination and decrease in the damage efficiency, formation of clusters of SIAs and vacancies in the cascades and glide of small SIA clusters are consistent with experimental results obtained using resistivity measurements, diffuse X-ray scattering experiments and transmission electron microscopy (for review see, for example, Zinkle and Singh 1993, English and Jenkins 1987, Trinkaus, Singh and Foreman 1993).

3 Theoretical Treatment

As described in Part I of this paper (Singh et al. 2000), the median recoil energy during irradiation of copper with 2.5 MeV electrons, 3.0 MeV protons and fission neutrons are expected to be about 0.05, 1 and 60 keV. In other words, both the nature and disposition of the damage produced by these recoils with vastly different energies are expected to be substantially different. The irradiation with 2.5 MeV electrons, for example, is expected to generate practically all displacements in the form of isolated Frenkel pairs homogeneously distributed in the crystal. In contrast, the irradiation with fission neutrons will generate damage predominantly in the form of multi-displacement cascades and subcascades with a rather segregated and inhomogeneous spatial distribution of the surviving defects and their clusters. The irradiation with 3 MeV protons with the median recoil energy of 1 keV represents an intermediate case where both multi-displacement cascades and Frenkel pairs are likely to be generated.

Thus, the main objective of the present work is to establish a theoretical framework within which the results of these irradiation experiments with electrons, protons and fission neutrons can be adequately described. Clearly, the results of 2.5 MeV electron irradiation can be treated in terms of the standard rate theory (SRT) whereas the microstructure evolution in the cases of 3 MeV proton and fission neutron irradiations can be described properly only within the framework of the PBM (see Section 2). Before presenting the results of numerical calculations of various aspects of the damage accumulation, it is not only useful but also necessary to outline, first of all the main features, scope and limitations of the SRT and PBM.

3.1 Standard Rate Theory Model

The SRT model was formulated within the framework of the mean-field type chemical rate theory approach (e.g. Brailsford and Bullough 1972, Wiedersich 1992) in which the defects are assumed to be produced randomly in space and time in the form of single interstitials and vacancies. Furthermore, the model is exclusively based on the concept of sink bias such as dislocation bias. The bias difference between sinks, such as between dislocations and voids, creates a difference in the absorption rate of vacancies and interstitials at such sinks. In the SRT model, this is the only driving force for the microstructural evolution.

The mathematical description of the SRT is based on a set of equations for concentrations of vacancies, C_v, and SIAs, C_i, which can be written as

$$\frac{dC_i}{dt} = G_{NRT} - D_i C_i (Z_i^v k_v^2 + Z_i^d \rho) - \mu_R D_i C_i C_v, \tag{1a}$$

$$\frac{dC_v}{dt} = G_{NRT} - D_v C_v (Z_v^v k_v^2 + Z_v^d \rho) - \mu_R D_i C_i C_v, \tag{1b}$$

where G_{NRT} is the NRT (Norgett, Robinson and Torrens 1975) Frenkel pair generation rate, D_i, D_v are the diffusion coefficients of SIA and vacancies, respectively; $Z_{i,v}^v k_v^2$ with $k_v^2 = 4\pi N_v R_v$ (N_v, R_v are the number density of voids and their mean radius) and $Z_{i,v}^v \rho$ are the sink strength of voids and dislocations for point defect absorption, respectively; μ_R is the recombination coefficient. Note that for the sake of simplicity the thermal emission of vacancies from voids and dislocations is not included in Eqs. (1).

An essential feature of Eq. (1) is that the generation rates of single SIAs and vacancies are equal. At steady state ($dC_v / dt = dC_i / dt = 0$) the effective vacancy supersaturation, $Z_v^v D_v C_v - Z_i^v D_i C_i$, resulting from Eqs. (1) is

$$Z_v^v D_v C_v - Z_i^v D_i C_i = p_d \frac{Z_v^v Z_v^d \rho}{(Z_i^v k_v^2 + Z_i^d \rho)} D_v C_v, \tag{2}$$

where

$$D_v C_v = \frac{2G_{NRT}}{(Z_v^v k_v^2 + Z_v^d \rho)} \left(1 + \sqrt{1 + \frac{4G_{NRT}\mu_R}{D_v (Z_v^v k_v^2 + Z_v^d \rho)(Z_i^v k_v^2 + Z_i^d \rho)}} \right)^{-1}, \tag{3a}$$

$$D_i C_i = D_v C_v \frac{(Z_v^v k_v^2 + Z_v^d \rho)}{(Z_i^v k_v^2 + Z_i^d \rho)}, \tag{3b}$$

$$p_d = (Z_i^d / Z_v^d - Z_i^v / Z_v^v). \tag{3c}$$

For damage accumulation in the form of voids, the most important parameter of the model is the dislocation bias, p_d. In fact, the rate of swelling, dS/dt, which is determined by the difference between total fluxes of vacancies and SIAs to the voids, can be easialy shown (using Eq. (2)) to be given by

$$\frac{dS}{dt} = k_V^2(Z_V^V D_V C_V - Z_i^V D_i C_i) = p_d \frac{Z_V^V k_V^2 Z_V^d \rho}{(Z_i^V k_V^2 + Z_i \rho)} D_V C_V . \tag{4}$$

Thus, Eq. (4) can be used for an accurate and global description of void swelling in the case of pure metals irradiated under the conditions of Frenkel pair production (e.g. 2.5 MeV electrons). It can be seen from Eq. (4) that the intrinsic driving force for the swelling under these conditions is the dislocation bias, p_d.

3.2 Production Bias Model

As indicated already in Section 1, the PBM is fully capable of treating the effects of all salient features of damage production under cascade producing irradiation conditions (see Section 2) including the effect of 1-D diffusional glide of small SIA clusters on damage accumulation. Various aspects of the PBM have been described and discussed in a number of publications (e.g. Woo and Singh 1990, 1992, Singh and Foreman 1992, Trinkaus et al. 1992, 1993, Trinkaus, Singh and Woo 1994, Singh, Trinkaus and Woo 1994, Singh, Foreman and Trinkaus 1994, Trinkaus, Singh and Victoria 1996, Singh et al. 1997). The topic has been briefly reviewed and up-dated recently by Singh (1998, 1999). The most comprehensive and quantitative version of the PBM-based treatment of the damage accumulation has been described recently by Singh et al. (1997) and it is this version which will be used in the present paper to calculate the damage accumulation behaviour of copper under irradiation with 3 MeV protons and fission neutrons.

Taking into account the cascade efficiency and the production of SIA and vacancy clusters in cascades the equations for the SIA and vacancy concentrations may be written as

$$\frac{dC_i}{dt} = (1-\varepsilon_i)G - D_i C_i(k_v^2 + Z_i^d \rho + Z_i^{ic} k_{ic}^2 + Z_i^{vc} k_{vc}^2) - \mu_R D_i C_i C_v, \tag{5a}$$

$$\frac{dC_v}{dt} = (1-\varepsilon_v)G - D_v C_v(k_v^2 + Z_v^d \rho + Z_v^{ic} k_{ic}^2 + Z_v^{vc} k_{vc}^2) - \mu_R D_i C_i C_v + K_{vc}, \tag{5b}$$

where $G = G_{NRT}(1-\varepsilon_r)$; ε_r is the fraction of Frenkel pairs which recombines during cooling-down phase of cascades; ε_i is fraction of interstitials which forms the SIA clusters; $Z_i^{ic} k_{ic}^2, Z_v^{ic} k_{ic}^2$ are the sink strengths of the SIA clusters for absorption of interstitials and vacancies, respectively.

As it was pointed out in Singh et al. (1997) the simplest description of the balance equation for the glissile clusters can be achieved by assuming that all glissile clusters have the same size, $x = x_g$. In this case, the equation for the glissile loop concentration, $C_g(t)$, may be written as

$$\frac{dC_g}{dt} = G_g - D_g C_g k_g^2, \tag{5c}$$

where G_g is the generation rate of glissile loops from all sources, i.e. from cascades and from transformation of sessile to glissile clusters due to vacancy absorption; D_g and k_g^2 are the diffusion coefficients and sink strengths of glissile clusters , respectively. The total sink strength, k_g^2, for the clusters may be written as (see Eq. (2) in Singh et al. 1997)

$$k_g^2 = 2\left(\frac{\pi\rho d_{abs}}{4} + \sqrt{\frac{2}{l(2R_g - l)}} + \sigma_v N_v + \sigma_{vcc} N_{vc} + \sigma_{ic} N_{ic}\right)^2, \tag{6}$$

where $\sigma_v = \pi R_v^2$, d_{abs} is the capture diameter of dislocations for the absorption of the SIA clusters, σ_{vc}, σ_{ic} and N_{vc}, N_{ic} are the mean cross-sections of the sessile vacancy and SIA clusters and number densities of these clusters, respectively; R_g, l are the grain radius and distance from the grain boundary, respectively. The correct value of k_g^2 is a factor 2 larger than that given by Eq. (2) in the paper by Singh et al. (1997). Fortunately this factor cancels out in the partitioning of glissile clusters over sinks.

As mentioned above, 1-D diffusion of glissile clusters and their absorption by sinks leads to an increase in the effective vacancy supersaturation which, in turn, restricts the increase in the number density of sessile SIA clusters. From this standpoint, the accumulation of the sessile SIA clusters occurs in a way similar to that of the vacancy clusters: at relatively low doses, the size distribution function of the sessile SIA clusters achieves a saturation and at higher doses they play a role as the recombination centers for point defects and the glissile SIA clusters. Since the build-up of point defect (PD) clusters is faster than that of dislocations and voids, quasi-steady-state equations for point defect and glissile cluster concentrations can be derived. Taking into account the sessile-glissile transformation, which takes place when the size of a sessile cluster decreases below $x_g + 1$, these steady-state equations can be written as

$$\begin{aligned}(1 - \varepsilon_i^{g,eff})G &= D_i C_i (k_v^2 + Z_i^d \rho) + \mu_R D_i C_i C_v + \\ &D_v C_v Z_v^{ic} k_{ic}^2 + D_i C_i Z_i^{vc} k_{vc}^2 - D_g C_g 2\Lambda x_g \sigma_{ic} N_{ic},\end{aligned} \tag{7a}$$

$$\begin{aligned}G &= D_v C_v (k_v^2 + Z_v^d \rho) + \mu_R D_i C_i C_v + \\ &D_v C_v Z_v^{ic} k_{ic}^2 + D_i C_i Z_i^{vc} k_{vc}^2 + D_g C_g 2\Lambda x_g \sigma_{vc} N_{vc},\end{aligned} \tag{7b}$$

$$\varepsilon_i^{g,eff} G / x_g = D_g C_g k_g^2, \tag{7c}$$

where $\varepsilon_i^{g,eff}$ is the effective fraction of the glissile component ($\varepsilon_i^{g,eff} = \varepsilon_i^g + \varepsilon_i^s x_g / \prec x_i^s \succ$); $\varepsilon_i^s, \varepsilon_i^g$ $(\varepsilon_i^s + \varepsilon_i^g = \varepsilon_i)$ are the fractions of sessile and glissile SIA clusters, respectively; $\prec x_i^s \succ$ is the mean size of sessile SIA clusters generated by the cascades and $\Lambda = \sqrt{k_g^2/2}$.

As can be seen from Eqs. (7a) and (7b), the steady state balance equations for point defects within the framework of the PBM have a very specific form since both vacancy and SIA concentrations depend on the concentration of the glissile clusters. In addition, it has to be emphasized that: (i) the left hand sides of these equations are not equal and, consequently, glissile SIA clusters play a key role in production of vacancy supersaturation at the steady-state; (ii) the effective fraction of the glissile loops $\varepsilon_i^{g.eff}$ defined by $\varepsilon_i^s, \varepsilon_i^g$ is incorporated in these equations explicitly, (iii) the third and forth terms on the right hand sides of the equations describing the absorption of PDs by the sessile clusters of both types are equal. This is related to the conservation of vacancies and SIAs when the concentration of vacancy and sessile SIA clusters reach saturation. Note that the previously presented steady-state balance equations for vacancies and SIAs (Singh et al., 1997, see Eqs. (20)) do not include the sessile-glissile SIA cluster transformation.

Subtracting Eq. (7a) from Eq. (7b) the vacancy supersaturation can be written as

$$D_v C_v - D_i C_i = p_d \frac{Z_v^d \rho}{k_v^2 + Z_i^d \rho} D_v C_v + \frac{\varepsilon_i^{g.eff} G}{k_v^2 + Z_v^d \rho}\left(1 - \frac{\sigma_{vc} N_{vc} + \sigma_{ic} N_{ic}}{\Lambda}\right). \tag{8}$$

The first and second terms on the right hand side of Eq. (8) correspond to the effect of the dislocation bias and cascade production bias, respectively. It can be seen that the first term depends on the vacancy concentration and consequently on the sink strength for PDs of all traps including PDs clusters. In contrast, the second term depends on the PDs sink strength in the form of voids and dislocation only. On the other hand, the absorption of the glissile SIA clusters by both vacancy and SIA types of sessile clusters (see the expression in the brackets) plays an important role in determining the effective value of the production bias.

Having determined the vacancy supersaturation, we can now describe the void swelling rate in the following form:

$$\frac{dS}{dt} = k_v^2 (D_v C_v - D_i C_i) - D_g C_g 2\Lambda x_g \sigma_v N_v. \tag{9}$$

Taking Eqs.(7c) and (8) into account, the swelling rate can be finally written as

$$\begin{aligned} \frac{dS}{dt} &= p_d \frac{k_v^2 Z_v^d \rho}{k_v^2 + Z_i^d \rho} D_v C_v \\ &+ \varepsilon_i^{g.eff} G \left[\frac{k_v^2}{k_v^2 + Z_v^d \rho} \left(1 - \frac{\left(\sigma_{vc} N_{vc} + \sigma_{ic} N_{ic}\right)}{\Lambda} \right) - \frac{\sigma_v N_v}{\Lambda} \right]. \end{aligned} \tag{10}$$

As can be seen from Eq. (10), the swelling rate under cascade damage conditions is a complicated function of a number of parameters. These include the elastic bias for dislocations, the dislocation density ρ and densities and sizes of voids and PD clusters. Furthermore, Eq. (10) also demonstrates the dependence of swelling rate on the recoil energy via the production parameters such as $\varepsilon_r, \varepsilon_i^s, \varepsilon_i^g, x_g$. Thus Eq. (10) describes the swelling behaviour under cascade damage condition in a realistic and comprehensive manner. In other words, the PBM as formulated by Singh et al. (1997) can be considered as a proper basis for studying the effect of recoil energy on defect accumulation in the form of voids, which is the main objective of the present paper.

4 Numerical Calculations and Comparison with Experiments

The evolution of size distribution functions of PD clusters and voids has been calculated using a new grouping method developed by Golubov, Ovcharenko, Barashev and Singh (2000) for the numerical solution of kinetic equations of the type used by Singh et al. (1997). The cascade production of both vacancy and SIA types of sessile clusters in the case of proton and neutron irradiations has been assumed to be the only mechanism for their nucleation. In contrast, a semi-empirical homogeneous nucleation model based on effective energetics of voids (adjusted to experimental observations) is used to describe the evolution of the void size distribution function. The main set of material parameters for copper used in the calculations, except for the grain size, is the same as given in Table 1 of Singh et al. (1997). The damage parameters used in the calculations for electron, proton and neutron irradiations are given in Table 1.

4.1 Electron Irradiation

Since all displacements generated under 2.5 MeV electron irradiations are expected to result in Frenkel pairs, we use the SRT model to determine the magnitude of damage accumulation in the form of voids. Since practically no defect clusters in the form of loops or SFT were observed (see Singh et al. 2000) only voids and dislocations are considered to be the sinks for point defects. The fraction of Frenkel pairs recombining spontaneously during their production has been taken to be zero, i.e. $G = G_{NRT}$.

The dose dependence of void swelling (Fig.1) in copper irradiated with 2.5 MeV electrons was calculated numerically using SRT (see section 3.1) and a dislocation bias of 2%. Since the dislocation density both in unirradiated and electron irradiated copper was found to be very low ($<10^{12}$m^{-2}) (see Singh et al. 2000) it is almost impossible to determine experimentally an accurate value of dislocation density. It was therefore decided to calculate the swelling for two values of dislocation density (i.e. 1×10^{11} and 5×10^{11}m^{-2}). The results are shown in Fig. 1.

In these calculations, the dose dependence of the void density between the dose levels of 2.3×10^{-3} and 1.3×10^{-2} dpa was estimated using a semi-empirical homogeneous nucleation model and the void energetics adjusted to describe the experimentally observed void size distributions. The terminal void density at 1.3×10^{-2} dpa is known both from transmission electron microscopy (TEM) and positron annihilation spectroscopy (PAS) whereas at the low dose level of 2.3×10^{-3} dpa, the void density could be estimated only from the PAS results. An analysis of the PAS results (Singh et al. 2000) suggested that at 2.3×10^{-3} dpa voids of mean diameter <d> of 8-10 nm would be consistent with the void density of about $2\times10^{18}\mathrm{m}^{-3}$. Therefore the swelling was calculated using these two different sizes of voids at 2.3×10^{-3} dpa and the results are shown in Fig. 1.

As can be seen in Fig. 1, the results calculated with dislocation bias of 2% are in a good agreement with the experimental data. This value of the dislocation bias is consistent with the value estimated by Konobeev and Golubov (1992) from the swelling results for 1 MeV electron irradiated copper reported by Glowinski (1976). From the void swelling results on 1 MeV electron irradiated copper, Barlow (1977) also obtained a value of 2% for the dislocation bias. It is interesting to note in this context that the swelling results on 1 MeV electron irradiated pure Fe-Cr-Ni alloys have also yielded a dislocation bias of about 2% (Walters 1985). Thus, the SRT model is fully capable of explaining the swelling results in copper obtained under the condition of Frenkel pair production with a dislocation bias of 2%.

4.2 Proton and Neutron Irradiations

As indicated in section 3, the irradiations with 3.5 MeV protons and fission neutrons are expected to generate multi-displacement cascades. The damage accumulation in both cases, therefore, can be appropriately treated only within the framework of the PBM. The production of displacement cascades and intracascade clustering introduce a number of damage production parameters (i.e. $\varepsilon_r, \varepsilon_i^s, \varepsilon_i^g, x_g$, (see section 2 and 3)) and parameters describing properties of clusters (e.g. thermal stability and mobility) that will have to be taken into account in the treatment of damage accumulation in terms of the PBM. In the following, we shall consider the case of neutron irradiation first since the available experimental results in this case make it possible to estimate reasonable values of some of these parameters. The mean size of the glissile clusters, x_g, which does not affect the damage evolution very much, can be reasonably fixed at $x_g = 5$ without losing the sense of generality. The recombination parameter, ε_r, can be estimated for both proton and neutron irradiations on the basis of experimental data and the results on recoil energy dependence of ε_r obtained by MD calculations by taking the mean PKA energies for proton and neutron irradiations to be 1 keV and 30 keV, respectively (see Table 1). The magnitude of parameters, such as the fractions $\varepsilon_v, \varepsilon_i^s, \varepsilon_i^g$ and the binding energy of vacancies to vacancy clusters, E_b, have been estimated by fitting them to the experimental data.

It should be noted that the values of various parameters quoted in Table 1 are the same as given by Singh et al. (1997) except for the value of ε_v. This value of ε_v was earlier fixed arbitrarily at a level of 0.5 since the calculation of void swelling and its dose dependence was not sensitive to this value. However, in the present work, the value of ε_v is fitted to experimental results on the size and density of stacking fault tetrahedra (SFTs) and on void swelling, and represents the global average of the fraction of vacancies contained in SFTs.

The kinetics of the evolution of SFTs under neutron irradiation is rather complicated and is not fully understood yet. In the present calculations we have chosen a specific function to describe the size dependence of the binding energy, E_b, of a vacancy to SFT. This function yields a rather unconventional size dependence of E_b first increasing but beyond a certain size range decreasing with size. Such "abnormal" behaviour of SFT energetics has been recently demonstrated by MD calculations (Osetsky et al. 2000). The chosen function, however, allows us to calculate the density and size distribution in agreement with experiments (see later).

The main parameter controlling the rate of accumulation of SFT at low doses is the fraction ε_v. The accumulation of the sessile SIA clusters is mainly controlled by the fraction ε_i^s. On the other hand, as shown in section 3 (see Eq. 10), the production bias and, consequently, the swelling rate at low doses when the trapping of the glissile SIA clusters by voids is negligibly small, is determined by the effective fraction of the glissile component $\varepsilon_i^{g,eff}$. Thus, the magnitude of $\varepsilon_i^{g,eff}$ can be fixed by comparing the calculated results for void swelling with the experimental data using $\varepsilon_i^{g,eff} = \varepsilon_i^g + \varepsilon_i^s x_g / \prec x_i^s \succ$. In other words, the damage parameters used in the present calculations, can be reasonably fixed by fitting the calculated results to experimental ones for the dose dependence of void swelling concurrently with the accumulation of the sessile SIA clusters.

To complete the input parameters for the calculations, the cross-sections $\sigma_v, \sigma_{vc}, \sigma_{ic}$ have to be specified as well. For voids, with a rather weak stress field, the cross-section can be approximated by the geometrical one, $\sigma_v = \pi R^2$, where R is the void radius. Unfortunately, very little is known about interaction between the glissile SIA clusters and sessile ones of both types (i.e. vacancy and interstitial) and, therefore, it is difficult to quantify the cross-sections σ_{vc}, σ_{ic}. In the present paper, the trapping cross-section for SFTs, σ_{vc}, is assumed to be of the form $\sigma_{vc} = \pi R_{eff}^2$, i.e. similar to voids, where R_{eff} is taken to be equal to the radius of inner sphere of a SFT, which can be considered as a lower limit for the cross-section σ_{vc}.

The choice of the cross-section σ_{ic} is more problematic. The problem arises since absorption of glissile SIA clusters by the sessile SIA clusters can cause an unlimited increase in the number density of the SIA sessile clusters with increasing dose if no mechanism for the removal of the latter (in addition to the vacancy absorption) is introduced. Since an analysis of this possibility is beyond the scope of this paper we avoid its occurrence by setting σ_{ic} equal to zero.

Neutron Irradiation

The evolution of the size distribution function of voids and PD clusters has been numerically calculated for a constant dislocation density of $\rho = 5*10^{11} m^{-2}$ in the grain interior with $R_g = 10\mu m$ ($l = R_g$, see Eq. (6)). The damage parameters used in the calculations are given in Table 1. The results of the calculations for copper irradiated with fission neutrons are presented in Figs. 2-5.

Fig. 2 shows the dose dependence of the size distribution function of SFT at doses in the range of 10^{-6}-10^{-2} dpa (NRT) obtained by using E_b with the size dependence mentioned earlier (see the inset in Fig. 2). As can be seen in Fig. 2 the calculated maximum size of the SFTs saturates at a level somewhat above 3 nm at doses higher than 10^{-3} dpa which is in a good agreement with experimental results (Singh et al. 1995). Note that the maximum value of the binding energy E_b (see inset in Fig. 2) is about 1.1 eV which is somewhat higher than the effective activation energy of 0.85 eV estimated by Singh and Zinkle (1993) from the temperature dependence of SFT density in copper irradiated with fission neutrons at a damage rate of about $2*10^{-7}$ dpa (NRT)/s. The origin of this difference can be understood on the basis of calculations of the temperature dependence of damage accumulation, which is beyond the scope of the present paper. Such calculations are in progress and the results will be presented elsewhere.

The dose dependence of density and average size of SFTs, sessile SIA clusters and voids calculated using the same parameters as in Fig. 2 are presented in Figs. 3 and 4 together with experimentally measured densities of the clusters and voids and the average sizes of voids. As can be seen from the figures, the calculated results agree well with experimental data in the whole dose range. The calculated mean size of SFTs is found to saturate at about 3 nm which is also in an agreement with experimental observations (Singh et al. 1995).

Fig. 5 shows (a) the calculated dose dependence of sink strength of SFTs, sessile SIA clusters and voids and (b) a comparison of the dose dependence of calculated and measured void swelling. As can be seen from Fig. 5a, the sink strength of SFT is much higher than that of voids and SIA clusters and increases in the whole dose range due to increasing density (see Fig.3). In contrast, the void sink strength increases with increasing void size and the sink strength of SIA clusters follows the sink strength of voids in accordance with the results of the analytical treatment given by Singh et al. (1997) (see Eq. 25a). Note that the calculated results for void swelling agree very well with the measured values.

According to our calculations, the value of ε_i ($\varepsilon_i = \varepsilon_i^s + \varepsilon_i^g$) which is found to be necessary for explaining the experimental results is 0.3 (see Table 1). This value of ε_i is consistent with the results of MD simulations of single cascades in copper for clusters containing four or more SIAs per cluster (see Fig. 9 in Bacon, Gao and Osetsky 2000). Note that our calculations assume a minimum of five SIAs in the clusters formed in the cascades. This agreement, however, should be treated with caution. The reason being that the ε_i value obtained from MD simulations is based on the behaviour of only a few isolated single cascades whereas ε_i value derived from the experimental results refers to a global average value for a very large number of cascades and sub-cascades generated by PKAs with different recoil energies. Finally, it is worth noting that the value of ε_v derived from our experiments is found to be rather low ($\varepsilon_v = 0.06$, Table 1). Unfortunately, it is not possible to corroborate this value of ε_v with MD results since such results are not available at present.

Proton Irradiation

Using the same methodology as for the case of neutron irradiation, the void swelling behaviour of copper irradiated with 3 MeV protons has been calculated numerically. The damage parameters are listed in Table 1 and correspond to a median recoil energy of 1 keV. Note that the damage parameters given in last four lines in Table 1 for the case of proton irradiation have been assumed, for the sake of simplicity, to be the same as for the neutron irradiation; the calculated swelling results are not very sensitive to these parameters. In fact, it can be seen from Eq. (10) that the main parameter determining the swelling rate is the effective fraction of the glissile SIA clusters, $\varepsilon_i^{g,eff}$, which depends only weakly on the size of the glissile and sessile SIA clusters.

Fig. 6 shows the measured and calculated void size distributions in the dose range of $2*10^{-3}$ -$1*10^{-2}$ dpa (NRT). Note that the calculated size distributions are in a good agreement with the measured ones. The dose dependence of calculated and measured densities of SIA clusters, SFT and voids as well as void swelling are given in Fig. 7. As can be readily seen from Fig. 7, the calculated results agree well with the measured ones. Note that the density of SIA clusters is much higher than that of SFTs and is also in agreement with experimental observations. The fractions $\varepsilon_v, \varepsilon_i^s, \varepsilon_i^g$ for the case of proton irradiation (see Table 1) are markedly smaller than that for neutron irradiation. This seems to be reasonable considering the low value of 1 keV estimated for the median PKA energy of 3 MeV protons. It should be pointed out that the value of ε_i derived from the experimental results is reasonably consistent with the value obtained from MD simulations of cascades in copper with a PKA energy of 1 keV and for clusters containing four or more SIAs per cluster (see Fig. 9, Bacon et al. 2000).

4.3 Comparison of Swelling Behaviour in Electron, Proton and Neutron Irradiated Copper

In the preceeding section, various aspects of damage accumulation under electron, proton and neutron irradiations have been calculated and presented separately for each irradiation conditions. At this juncture, it is of interest, however, to make a direct comparison of the swelling behaviour under electron, proton and neutron irradiations which may help identify reason for the recoil energy effect, for example, on void swelling. Fig. 8 shows such a comparison of both calculated and experimentally measured dose dependencies of void swelling.

The results presented in Fig. 8, first of all, demonstrate unambiguously that the increase in recoil energy has a very substantial effect on the swelling behaviour of copper at 523 K. The dose dependence of swelling for 2.5 MeV electron irradiation calculated in terms of SRT model as well as that for 3 MeV proton and fission neutron irradiations calculated within the framework of the PBM agree quite well with the experimental results (Singh et al. 2000). We emphasize here that the experimentally observed swelling behaviour under 3 MeV proton and fission neutron irradiations cannot be rationalized in terms of the SRT model. It should be noted that the deviation of the calculated void swelling from linearity (at $\sim 10^{-2}$ dpa) shown in Fig. 8 for neutron irradiated copper is consistent with experimental results and the prediction of the PBM (Singh and Foreman 1992, Singh et al. 1997). In fact, according to the PBM, the void swelling should come to saturate at some dose level (Golubov, Singh and Trinkaus 2000). The physical reason for this deviation from linearity leading to swelling saturation is the interaction of 1-D diffusing SIA clusters with the void population (see Eq. (10)). Thus, such a behaviour is expected even in the case of 3 MeV proton irradiation. According to the SRT model, on the other hand, such a saturation cannot be expected under irradiation with 2.5 MeV electrons. This implies that at some higher dose level irradiation with 2.5 MeV electrons may lead to even higher swelling than that under neutron irradiation.

On the basis of the experimental results (see Figs. 3 and 7) it has been argued (see Singh et al. 2000) that the effect of recoil energy on void swelling originates from an enhancement of the propensity for void nucleation at higher recoil energies. It was suggested that the main reason for this recoil energy effect is the level of vacancy supersaturation prevailing prior to void nucleation (i.e. at very low doses). In order to test this hypothesis we have calculated the dose dependence of vacancy supersaturation for 2.5 MeV electron (using the SRT model), 3 MeV proton and fission neutron irradiations (using the PBM) and the results are shown in Fig. 9.

Fig. 9 shows the evolution of vacancy supersaturation in the absence of voids which is taken to represent the situation prior to void nucleation. Fig. 9 clearly demonstrates that the recoil energy does have a very significant effect on the prevailing vacancy supersaturation which is, apart from the gas concentration, the primary driving force for the nucleation of voids. In other words, the higher the vacancy supersaturation level, the higher is the propensity for void nucleation (at a given irradiation temperature and gas concentration level). Since the same batch of copper was used in 2.5 MeV electron, 3 MeV proton and neutron irradiation experiments (Singh et al. 2000), it is reasonable to assume that the concentration of residual gas atoms in all specimens was similar if not identical. Therefore, the variation in void density with recoil energy must be due to the differences in the vacancy supersaturation under electron, proton and neutron irradiations. We can therefore conclude that the recoil energy dependent vacancy supersaturation is the main driving force for the effect of recoil energy on void swelling.

5 Conclusions

The damage accumulation behaviour in copper under 2.5 MeV electron, 3.0 MeV proton and fission neutron irradiations has been studied. The standard rate theory has been applied to the first case whereas the two other cases have been treated within the framework of the PBM. The comparison of these results with the corresponding experimental results reported in Part I of the paper (Singh et al. 2000) leads to the following conclusions:

- The void swelling behaviour observed under 2.5 MeV electron irradiation where defects are produced as Frenkel pairs can be clearly understood in terms of standard rate theory and dislocation bias. The analysis of the void swelling results obtained under 2.5 MeV electron irradiation yields a dislocation bias of $\approx 2\%$.
- Calculations have demonstrated that the observed swelling behaviour under 3 MeV proton and neutron irradiations cannot be rationalized in term of standard rate theory or BEK type models.
- The main components of the irradiation-induced microstructure (i.e. size and density of SFT, SIA clusters and voids) have been calculated in term of production bias model using size distribution functions and are found to be in good agreement with the experimental results for copper irradiated with 3 MeV protons and fission neutrons. Furthermore, the fractions of SIAs contained in the clusters (formed in the cascades) derived from the experimental results for both 3 MeV proton and fission neutron irradiations are found to be reasonably consistent with the results obtained from MD simulations.
- Results presented here confirm that the damage accumulation under irradiation is strongly influenced by the nature of the primery damage production. The generation of even a low fraction of very small cascades (as under 3 MeV proton irradiation) alters the damage accumulation behaviour so substantially (compared to that under electron irradiation) that the results can be rationalized only within the framework of the PBM.
- It is deduced that the recoil energy dependent vacancy supersaturation is the main driving force for the void nucleation and therefore for the effect of recoil energy on void swelling. Thus, the origin of the effect of recoil energy lies in the intracascade clustering of SIAs and the properties of SIA clusters.

Acknowledgements

S.I.G. wishes to thank the Materials Research Department at Risø National Laboratory for the support and hospitality during his visit when this work was completed. The present work was partly funded by the European Fusion Technology Programme.

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Table 1. Values of parameters used in the present calculations

	Electrons	Protons	Neutrons
NRT displacement rate	$1.3*10^{-8}$ dpa/s	$1.3*10^{-8}$ dpa/s	$5.0*10^{-8}$ dpa/s
Recombination fraction, ε_r	0.0	0.75	0.90
Effective displacement rate	$1.3*10^{-8}$ dpa/s	$3.25*10^{-9}$ dpa/s	$5.0*10^{-9}$ dpa/s
Dislocation efficiency for vacancies, Z_v^d	1.0	1.0	1.0
Dislocation efficiency for SIAs, Z_i^d	1.02	1.02	1.02
Fraction of SIAs deposited in sessile clusters, ε_i^s	0.0	0.04	0.10
Fraction of SIAs deposited in glissile clusters, ε_i^g	0.0	0.08	0.20
Fraction of vacancies deposited in SFT, ε_v	-	0.006	0.06
Minimum number of SIAs in sessile clusters	-	6	6
Maximum number of SIAs in sessile clusters	-	25	25
Maximum number of vacancies in SFT	-	30	30
Number of SIAs in glissile clusters, x_g	-	5	5

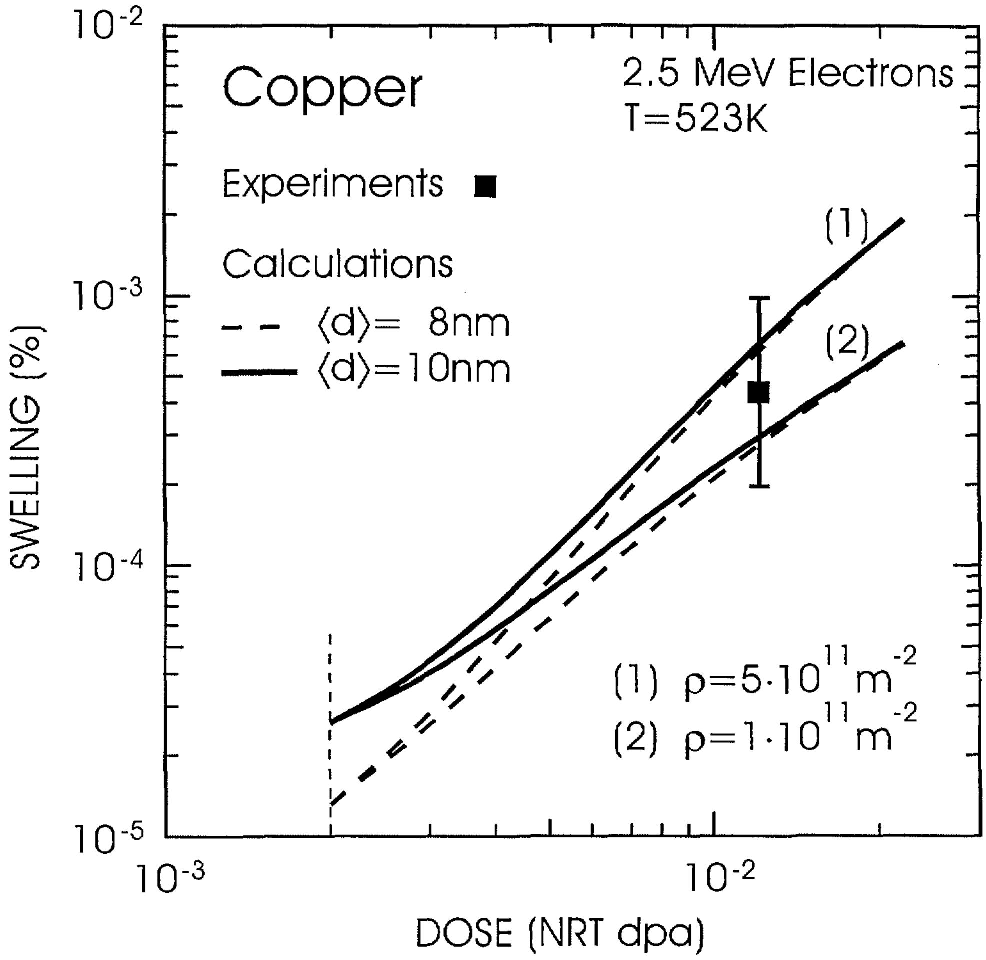

*Figure 1. Dose dependence of void swelling in copper irradiated with 2.5 MeV electrons at a damage rate of 1.3*10^{-8} dpa(NRT)/s using standard rate theory and dislocation bias. Note that a dislocation bias of only 2% is found to be necessary to explain the experimental results.*

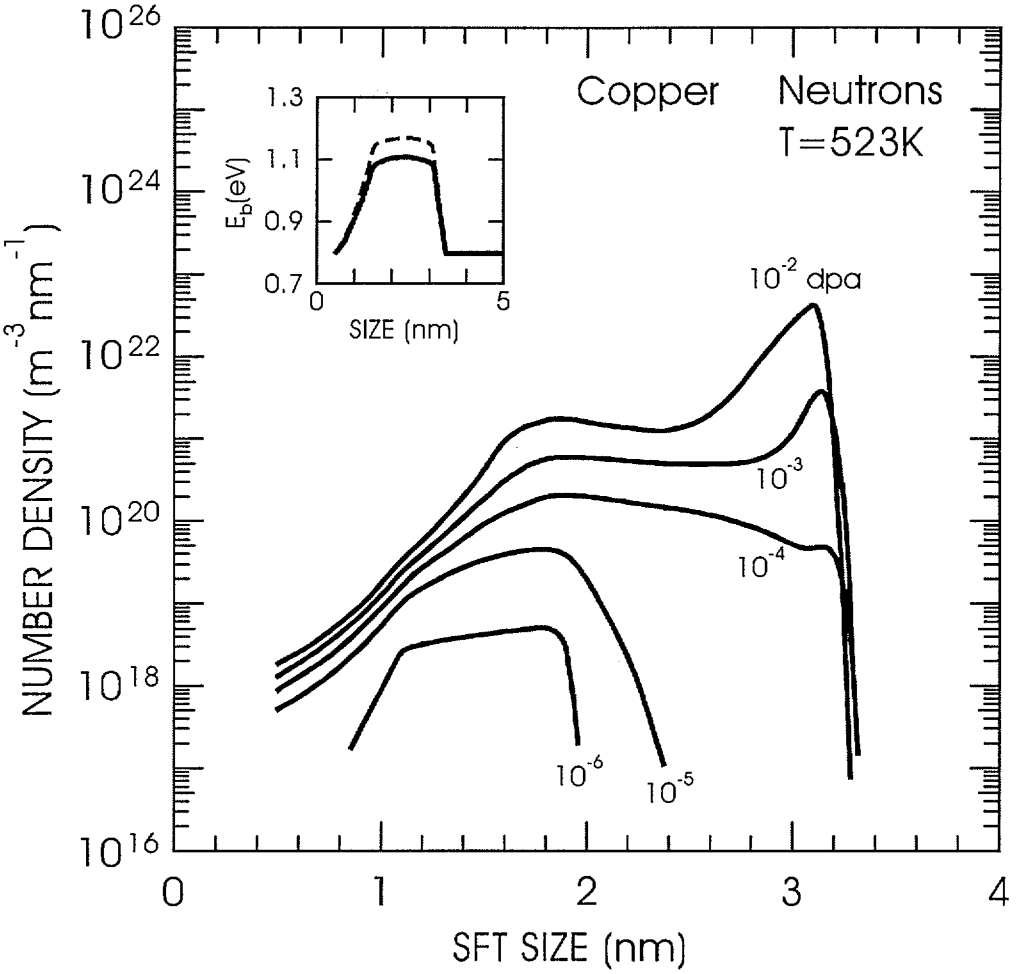

Figure 2. Size distribution function of stacking fault tetrahedra (SFT) for doses in the range of 10^{-6} -10^{-2} dpa (NRT) for copper irradiated at 523K with fission neutrons at a damage rate of $5.0*10^{-8}$ dpa(NRT)/s. These calculations are carried out within the framework of the PBM including a dislocation bias of 2%. The calculated mean sizes are consistent with experimental results.

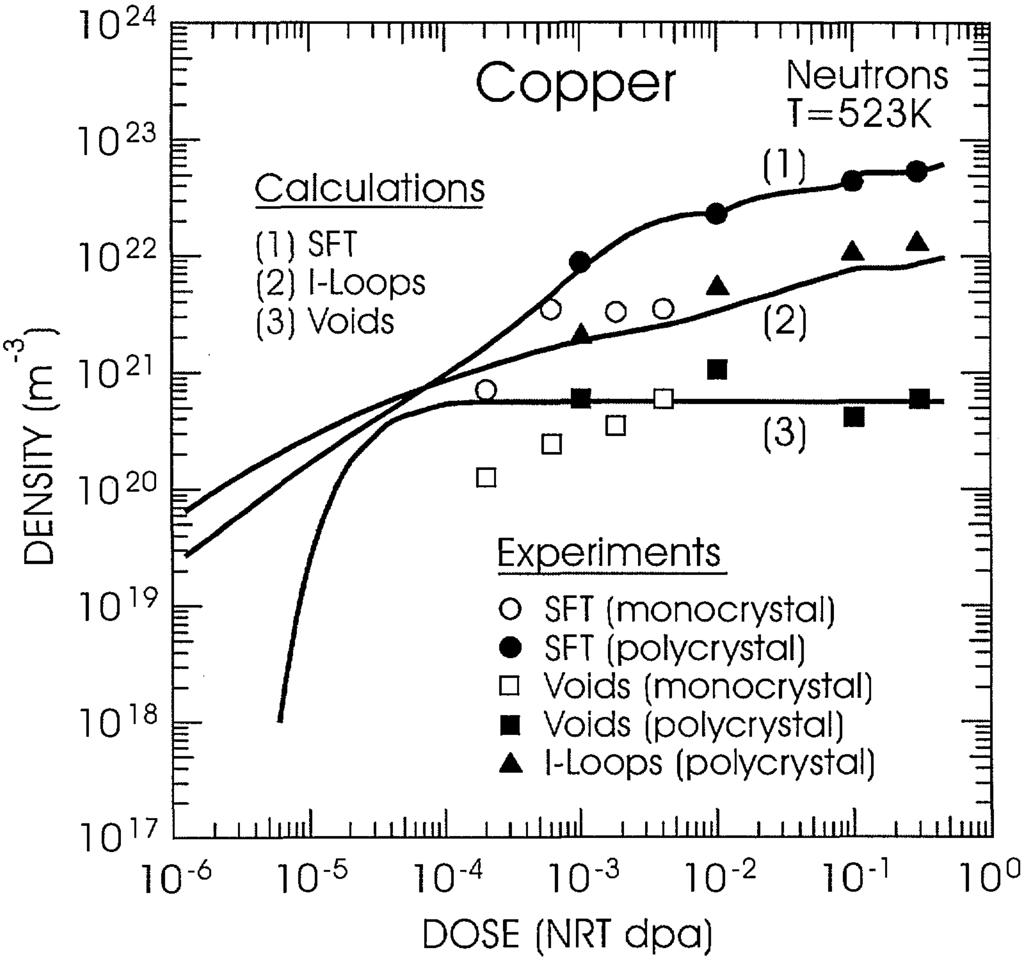

Figure 3. Dose dependence of density of SFTs, sessile SIA clusters and voids calculated within the framework of the PBM using the same damage and material parameters as in Fig. 2. Calculated results agree quite well with the experimental results (●,▲,■, Singh et al. 1995, 2000; O,□, English et al. 1987).

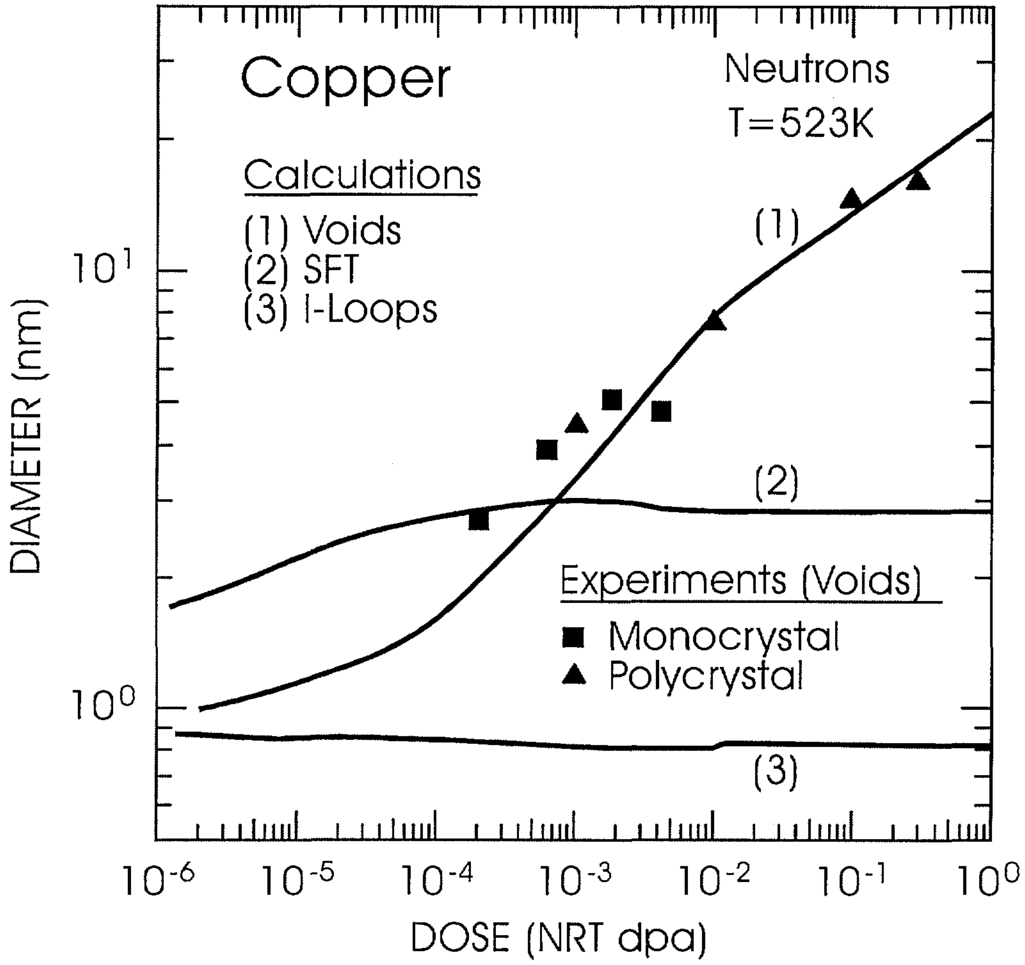

Figure 4. Dose dependence of the average size of voids, SFTs and sessile SIA clusters calculated using the PBM and size distribution function. The same damage and material parameters as in Fig. 2. For comparison, experimentally measured void sizes are also given (▲, Singh et al. 1995, 2000; ■, English et al. 1987).

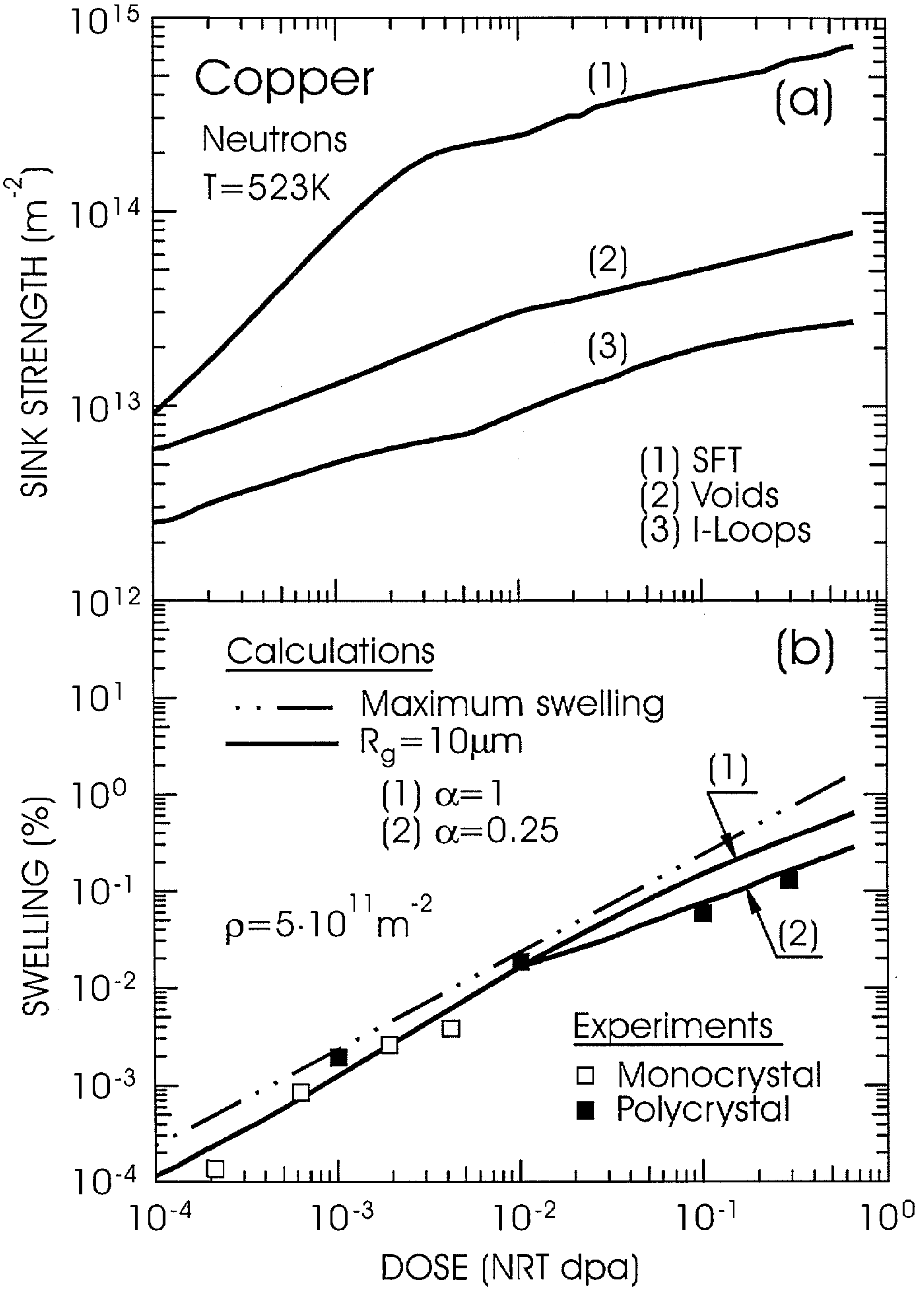

Figure 5. Evolution of (a) sink strength and (b) void swelling as a function of dose for copper under neutron irradiation at 523K calculated using the PBM and size distribution function. Note that the calculated swelling results (solid line 2) agree with the measured values in the whole dose range (■, Singh et al. 1995, 2000; □, English et al. 1987).

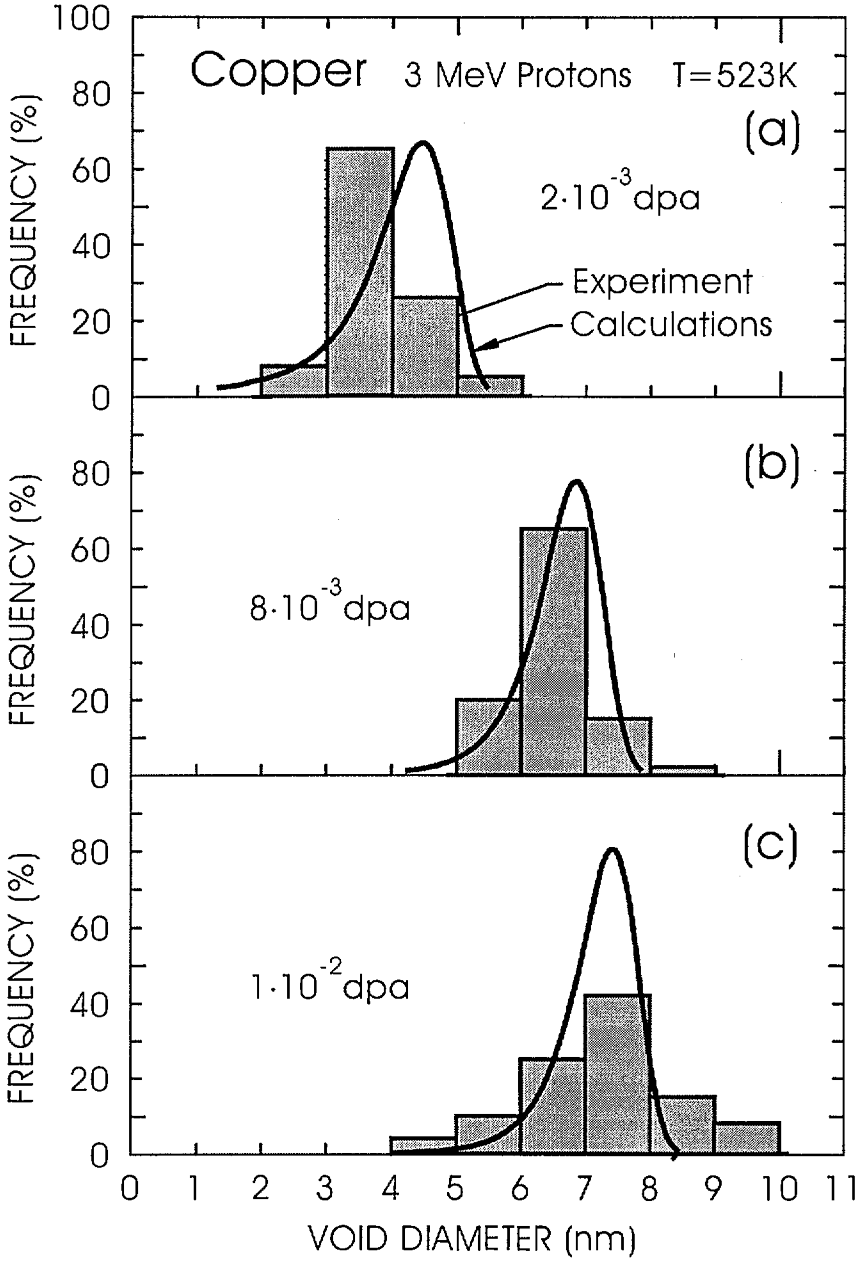

Figure 6. Measured and calculated void size distribution functions for copper irradiated with 3 MeV protons at 523K to different doses at a damage rate of $1.3*10^{-8}$ dpa(NRT)/s. The size distribution functions are calculated using the PBM with the damage parameters appropriate to 3 MeV proton irradiation (Table 1). The material parameters are the same as in the case of neutron irradiation. Calculations include a dislocation bias of 2%. Note that the calculated functions are similar to the measured ones (Singh et al. 2000).

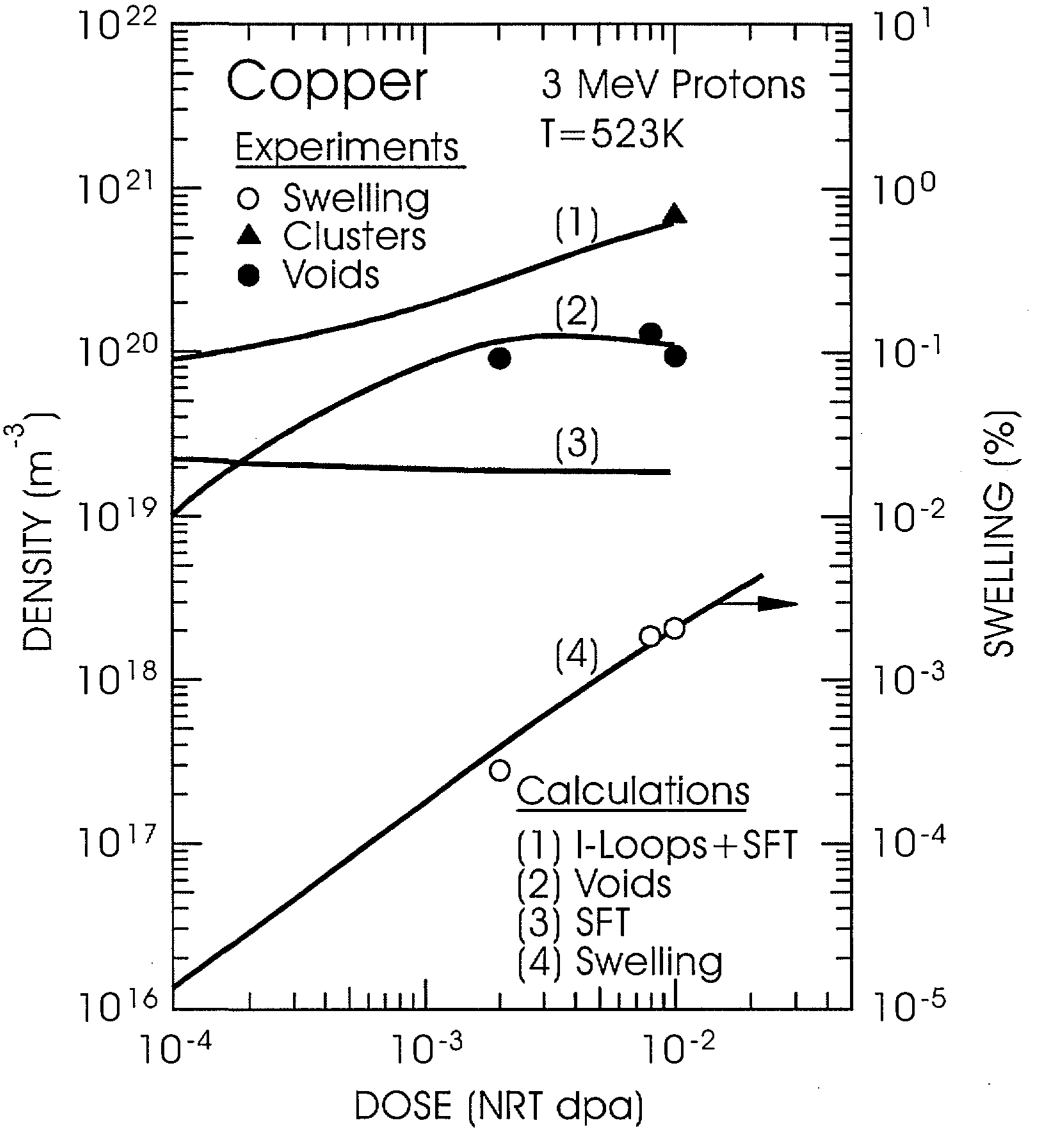

Figure 7. Variations of density of SIA clusters, SFTs and voids and the void swelling with irradiation dose calculated for copper irradiated with 3 MeV protons at 523K at a damage rate of $1.3*10^{-8}$ dpa(NRT)/s. For comparison, the experimental results are also shown (Singh et al. 2000). Note the agreement between the calculated and measured results.

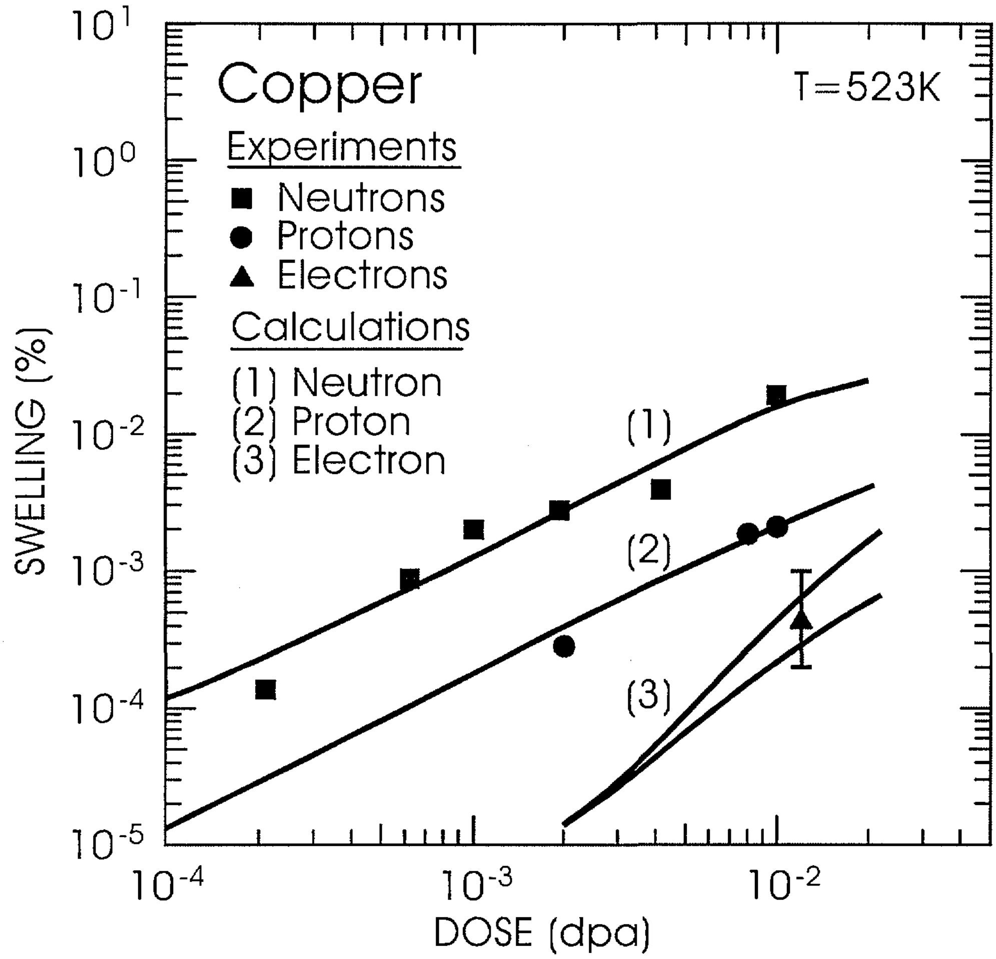

*Figure 8. Comparison of calculated and experimentally measured dose dependence of void swelling for copper irradiated with 2.5 MeV electrons, 3 MeV protons and fission neutrons at 523K at damage rates in the range (1.3-5) *10^{-8} dpa(NRT)/s. The void swelling for proton and neutron irradiation is calculated in terms of PBM, whereas for electron irradiation in terms of SRT. In both cases, the calculated results are in very good accord with the measured values (English et al. 1987, Singh et al. 2000).*

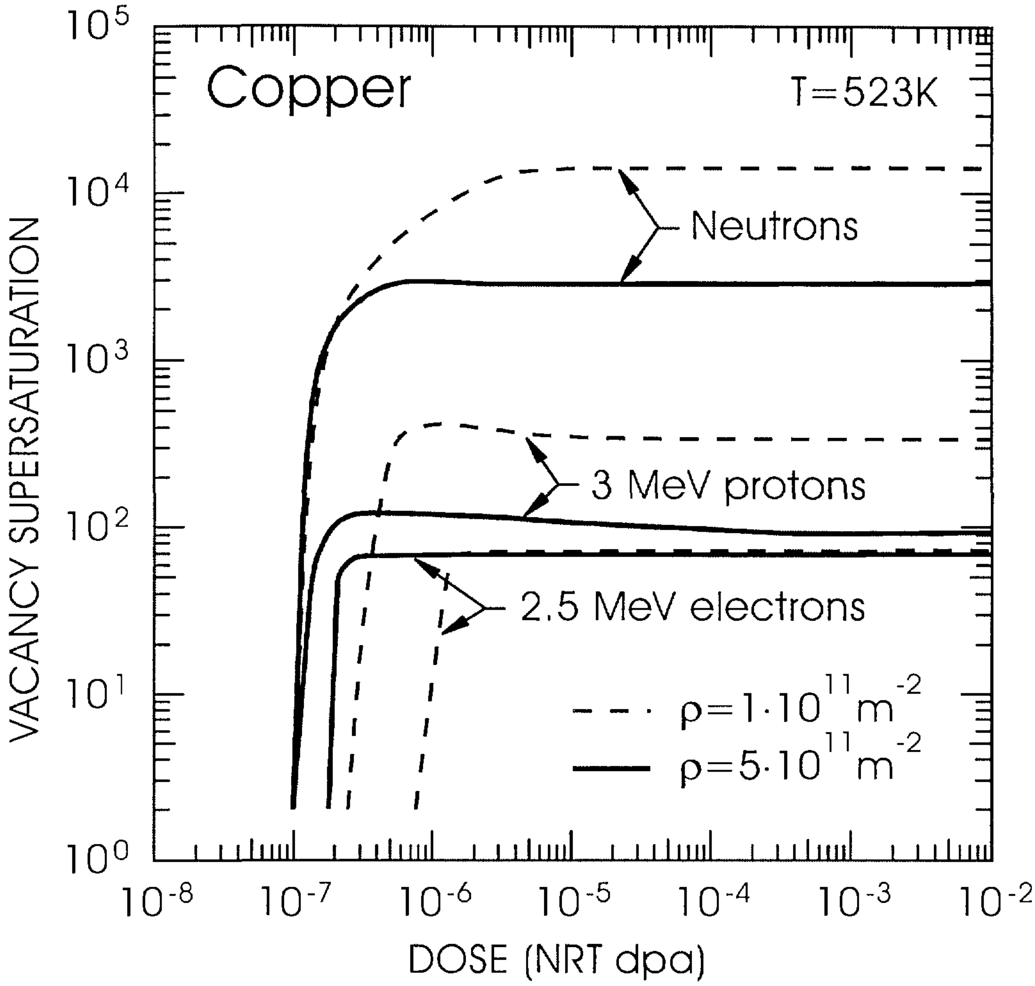

Figure 9. Dose dependence of vacancy supersaturation during 2.5 MeV electron, 3 MeV proton and fission neutron irradiation of copper at 523K for two dislocation densities. These calculations are carried out in the absence of voids (i.e. prior to void nucleation). Note that the level of vacancy supersaturation (i.e. the main driving force for void nucleation) increases with increasing recoil energy.

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Bibliographic Data Sheet **Risø-R-1186(EN)**

Title and authors

On Recoil Energy Dependent Void Swelling in Pure Copper: Theoretical Treatment

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ISBN	ISSN
87-550-2705-9	0106-2840

Department or group	Date
Materials Research Department	June 2000

Groups own reg. number(s)	Project/contract No(s)

Pages	Tables	Illustrations	References
30	1	9	38

Abstract (max. 2000 characters)

Over the years, an enormous amount of experimental results have been reported on damage accumulation (e.g. void swelling) in metals and alloys irradiated under vastly different recoil energy conditions. Unfortunately, however, very little is known either experimentally or theoretically about the effect of recoil energy on damage accumulation. Recently, dedicated irradiation experiments using 2.5 MeV electrons, 3.0 MeV protons and fission neutrons have been carried out to determine the effect of recoil energy on the damage accumulation behaviour in pure copper and the results have been reported in Part I of this paper (Singh, Eldrup, Horsewell, Ehrhart and Dworschak 2000).

The present paper attempts to provide a theoretical framework within which the effect of recoil energy on damage accumulation behaviour can be understood. The damage accumulation under Frenkel pair production (e.g. 2.5 MeV electron) has been treated in terms of the standard rate theory (SRT) model whereas the evolution of the defect microstructure under cascade damage conditions (e.g. 3.0 MeV protons and fission neutrons) has been calculated within the framework of the production bias model (PBM). Theoretical results, in agreement with experimental results, show that the damage accumulation behaviour is very sensitive to recoil energy and under cascade damage conditions can be treated only within the framework of the PBM. The intracascade clustering of self-interstitial atoms (SIAs) and the properties of SIA clusters such as one-dimensional diffusional transport and thermal stability are found to be the main reasons for the recoil energy dependent vacancy supersaturation. The vacancy supersaturation is the main driving force for the void nucleation and void swelling. In the case of Frenkel pair production, the experimental results are found to be consistent with the SRT model with a dislocation bias value of 2%.

Descriptors INIS/EDB

COPPER; IRRADIATION; MICROSTRUCTURE; PHYSICAL RADIATION EFFECTS; RECOILS; THERMONUCLEAR REACTOR MATERIALS; VOIDS

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ISBN 87-550-2705-9
ISSN 0106-2840

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