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Master-equation for cascade damage modeling

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Abstract

This paper is a continuation of our effort to understand and model irradiation effects under cascade damage. The conventional master equation for the evolution of a void ensemble is reformulated to include the stochastic effects due to the random cascade initiation. Numerical solution of the modified master equations to model the evolution of an ensemble of voids explicitly shows that stochastic fluctuations due to random cascade initiation produce important effects that cannot be accounted for by the conventional mean-field rate theory approach. The results are in good agreement with those derived previously using the Fokker–Planck equation.

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1. Introduction

Due to the stochastic nature of point-defect fluxes, the growth of a void proceeds like a random-walk process in the one-dimensional space of void sizes. Indeed, Mansur et al. [1] were among the first authors to show that the concentrations of point-defects generated during cascade irradiation undergo large fluctuations that affect the rates of point-defect absorption by sinks. Under such circumstances, the growth of an individual void is not monotonic, but fluctuates, even in the absence of vacancy emission.

Since very small vacancy clusters are mobile [2,3], a small region near the origin of the space of void sizes can be considered as a 'sink', where a shrinking void disappears, i.e., ceases to exist as a separate entity of the void ensemble. It is clear from this picture that a 'random-walking' void always has a finite probability to disappear into the sink, i.e., shrink away, even if the ensemble-averaged size is dictated to increase with time, due to the operation mechanisms such as dislocation or production bias [4]. This is allowed by a compensating portion that grows faster than the ensemble average. It is hardly surprising then, when stochastic effects are taken into account, the description of the evolution of the void ensemble, such as its number density, may be substantially different from that based on the standard rate theory, in which all voids are intrinsically assumed to be the same, i.e., all grow as the ensemble average.

In their investigation of void nucleation at elevated temperatures under cascade-damage irradiation, Semenov and Woo [4] found that the probability of shrinkage of the small void embryo is strongly dependent on the ratio between the void drift velocity and the void

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diffusion coefficient in the size space. The latter has its origin from fluctuations due to the stochastic nature of the point-defect migratory jumps, as well as that of the cascade initiations. The effects of the two different types of fluctuations are additive. However, the contribution from the cascade-induced fluctuations becomes dominant as the total sink strength and the sink absorption radius increases [5]. Thus, the fluctuations may not only play a role in void nucleation, where they are conventionally taken into account, at least partially, but also in the evolution of small voids of experimentally observable sizes.

The production bias [6], a simplified model proposed to treat complexities introduced by the intra-cascade formation of point-defect clusters, is closely related to the evolution of small clusters and their effects on the microstructure development. As a necessary sequel to the production bias model, the effects of cascade-induced fluctuation on irradiation-damage modeling has been considered in detail via a formulation using the Fokker–Planck equation (see [7] for a review). Though rigorous, the analytic approach is usually not easily applicable to the general problem of damage accumulation under cascade irradiation. To take into account the effects of stochastic fluctuations in processes such as nucleation and growth of defects, a set of kinetic equations, commonly known as master equations, has also been used [8–14]. This route sometimes offers a more convenient alternative than the Fokker–Planck equation approach. The numerical solution of the set of master equations, often numbered in the millions or even billions, is achievable using a grouping method first proposed by Kiritani [9] and subsequently improved [13,14]. Despite all indications of its importance, a version of the master equations, in which the effects of the cascade-induced fluctuations are taken into account, is not available.

In the present paper the conventional master equations are reformulated to include the stochastic effects due to random cascade initiation. Applying the modified master equations, the random cascade initiations are explicitly shown to have a large effect on the evolution of a void ensemble. We consider the reduction in void-number density with increasing dose in molybdenum at temperatures below 1000 K under neutron irradiation [15–17]. In this case, vacancy emission from voids is insignificant and is unlikely to cause the shrinkage of the voids. The results will be compared with those derived from the Fokker–Planck equations.

2. Reformulation of the mater equations

The general kinetic equation for the microstructure evolution under cascade-damage irradiation, with full statistics, has been derived in [18]. In the absence of the cascade induced fluctuations, this equation can be reduced to the conventional master equation [18]:

$$\frac{\partial f(x,t)}{\partial t} = J(x-1,t) - J(x,t), \tag{1}$$

where x measures the void size in terms of the number of vacancies in the void, $f(x,t)$ is the void distribution function in the size space, and $J(x,t)$ is the flux of voids in the size space, which is given by

$$J(x,t) = P(x,t)f(x,t) - Q(x+1,t)f(x+1,t). \tag{2}$$

The kinetic coefficients $P(x,t)$ and $Q(x,t)$ are, respectively, the rates of increase and decrease of the number density of voids of size x. When vacancy emission from voids is negligible, they are just the rates of vacancy and interstitial absorption and have the following conventional form:

$$P(x,t) = \frac{3x^{1/3}}{a^2} D_v C_v(t), \tag{3}$$

$$Q(x,t) = \frac{3x^{1/3}}{a^2} D_i C_i(t), \tag{4}$$

where D_j and C_j ($j = i, v$) are the diffusion coefficient and the atomic concentration of point-defects, respectively, $a = (3\Omega/4\pi)^{1/3}$ and Ω is the atomic volume.

On the other hand, in the simplest approximation, which still keeps the effect of the cascade-induced fluctuations, the general kinetic equation also takes the form of the Fokker–Planck equation [5,18]:

$$\frac{\partial f(x,t)}{\mathrm{d}t} = -\frac{\partial}{\partial x}\left\{P(x,t) - Q(x,t) - \frac{\partial}{\partial x}\left(\frac{P(x,t)+Q(x,t)}{2} + D^c(x,t)\right)\right\} f(x,t), \tag{5}$$

with

$$D^c(x,t) = \frac{3x^{2/3} G\langle N_d^2\rangle}{4aN_d k_v(t)}\left[1 + \frac{k_v(t)}{k_i(t)}\right]. \tag{6}$$

Here G is the effective generation rate of point-defects, N_d and $\langle N_d^2\rangle$ are the average number and the average square number of point-defects generated in a single cascade, respectively, and k_j^2 is the total sink strength for point-defects of the type j.

The diffusivity D^c governs the 'diffusive spread' of the void distribution function in the size space due to the random cascade initiation. Since the term $D^s(x,t) = (P(x,t) + Q(x,t))/2$ represents the diffusivity due to the random migratory jumps of point-defects, in Eq. (5) it can be seen that the effects of both types of fluctuations on the void evolution are additive.

The Taylor's expansion of Eq. (1) up to the second term also gives Eq. (5), but without the corresponding contribution of cascade-induced fluctuations. Thus, to the same order of approximation as the Fokker–Planck equation (5), the kinetic equation for the void distribution function can be rewritten in the form of the conventional master equation (1), with the kinetic coefficients $P(x,t)$, $Q(x,t)$ replaced by

$$P^{c}(x,t) = P(x,t) + D^{c}(x,t), \tag{7}$$

$$Q^{c}(x,t) = Q(x,t) + D^{c}(x,t). \tag{8}$$

The evolution of the void number density $N(t)$ and the swelling $S(t)$ is then governed by the following equations:

$$\frac{dN(t)}{dt} = \sum_{x=x_0}^{\infty}\left(\frac{\partial f(x,t)}{\partial t}\right) = J^{c}(x_0-1,t), \tag{9}$$

$$\frac{dS(t)}{dt} = \sum_{x=x_0}^{\infty}\left(x\frac{\partial f(x,t)}{\partial t}\right) = x_0 J^{c}(x_0-1,t) + \sum_{x=x_0}^{\infty} J^{c}(x,t), \tag{10}$$

where x_0 is the minimum size of the vacancy cluster, below which a void changes into a mobile vacancy cluster and ceases to be a void embryo. The flux $J^{c}(x,t)$ can be written as

$$J^{c}(x,t) = P^{c}(x,t)f(x,t) - Q^{c}(x+1,t)f(x+1,t), \quad x \geqslant x_0. \tag{11}$$

The flux $J^{c}(x_0-1,t)$ is the net rate of production of the smallest embryos. It is determined by the difference between the rate of their formation from mobile vacancy clusters, $\dot{n}_{v}(x_0)$, and that of shrinkage of the existing embryos below the minimum size x_0 i.e.,

$$J^{c}(x_0-1,t) = \dot{n}_{v}(x_0) - Q^{c}(x_0,t)f(x_0,t). \tag{12}$$

Note that, since there are no voids in the size range $x = x_0 - 1$, $f(x_0-1,t) = 0$. The flux of void embryos shrinking below the minimum size can be calculated from the Fokker–Planck equation (5), and is given by the derivative $\partial/\partial x[D(x,t)f(x,t)]$ at $x = (x_0-1)$. Here $D(x,t) = D^{s}(x,t) + D^{c}(x,t)$ is the total diffusivity in the size space. Written in terms of finite difference for the discrete value of the variable $\Delta x = 1$, this flux is approximated by $D(x_0,t)f(x_0,t)$. The difference between $Q^{c}(x_0,t)$ and $D(x_0,t)$ arises when the Poisson distribution is approximated by the Gaussian one, during the derivation of the Fokker–Planck equation (5) [18]. When $(D_{v}C_{v} - D_{i}C_{i}) \ll D_{i}C_{i}$, which is the case we actually consider in the present paper, $Q^{c}(x_0,t) \cong D(x_0,t)$. Within the validity of this approximation, both approaches based on the modified master equation or the Fokker–Planck equation, would give the same results.

From Eqs. (7), (8) and (10)–(12), the rate of accumulation of vacancies in voids can also be written as

$$\frac{dS(t)}{dt} = [x_0\dot{n}_{v}(x_0) - (x_0-1)Q^{c}(x_0,t)f(x_0,t)] + \sum_{x=x_0}^{\infty}(P(x,t) - Q(x,t))f(x,t). \tag{13}$$

In Eq. (13), the terms in square brackets describe the difference between the number of vacancies that have been immobilized to form void embryos, and that which becomes mobile due to the void shrinkage. Since $V(x,t) = (P(x,t) - Q(x,t))$ represents the conventional average void growth rate, the second term is just the average net vacancy flux received by the void ensemble. This means that the foregoing modification does not affect the form of balance equations for the concentrations of vacancies C_{v} and interstitials C_{i}. Thus,

$$\frac{dC_{v}}{dt} = (G - x_0\dot{n}_{v}(x_0) + (x_0-1)Q^{c}(x_0,t)f(x_0,t)) - D_{v}C_{v}\left[Z_{v}\rho_{d} + \frac{3}{a^2}\sum_{x=x_0}^{\infty}x^{1/3}f(x,t)\right], \tag{14}$$

$$\frac{dC_{i}}{dt} = G - D_{i}C_{i}\left[Z_{i}\rho_{d} + \frac{3}{a^2}\sum_{x=x_0}^{\infty}x^{1/3}f(x,t)\right], \tag{15}$$

where ρ_{d} is the dislocation density, and Z_{j} is the reaction constant between dislocations and point-defects.

3. Low temperature evolution of voids in Mo

The reduction of void number density with increasing dose is often observed in neutron or ion irradiated molybdenum at low temperatures [15–17]. The disappearance of the voids was originally attributed to the segregation to the void surfaces of the transmutation impurities (technetium) [15]. Evidently, this explanation cannot be applied to the case of ion irradiation [16,17]. Using an analytical approach based on the Fokker–Planck equation, it is found that cascade-induced fluctuations may lead to a large increase in void shrinkage. Indeed, changes in void densities of several hundred per cent in not uncommon [4,19]. Thus, under the proper experimental conditions, voids with a diameter of 5 nm may shrink away with a probability of more than 50%, while for voids with diameters $\cong$3 nm, the calculated shrinkage probability may reach 80% [4]. This is consistent with the observation that the overall density drop during the medium-dose irradiation was due to the reduction in the number of voids having diameters $\leqslant$3 nm [15]. Using the modified master equation derived in the foregoing section, we calculate in the following the evolution of the size distribution function (SDF) of voids, and study void shrinkage and its dependence on the cascade morphology and other microstructure features.

To avoid ambiguity, we consider the low-temperature regime, in which vacancy emission from voids can be neglected, and which can be estimated from the conventional mean-field equation. Thus, the growth rate of the average void radius R is given by

$$\frac{dR}{dt} = \frac{Z_v \rho_d}{R(\rho_s + Z_v \rho_d)} \left\{ \frac{(Z_i/Z_v - 1)G}{(\rho_s + Z_i \rho_d)} - D_v (C_s^e(R) - C_\infty) \right\}, \tag{16}$$

where $\rho_s = 4\pi NR$ is the void sink strength and C_∞ is the equilibrium vacancy concentration. Using Eq. (16), the range of temperatures T, for which vacancy emission is negligible, can be estimated. Thus, the mean equilibrium concentration $C_s^e(R)$ of vacancies in the neighborhood of a void of radius R can be written as

$$C_s^e(R) = C_\infty \exp\left(\frac{2\gamma_s \Omega}{k_B T R}\right), \tag{17}$$

where γ_s is the surface tension and k_B is the Boltzmann constant. The temperature dependence of the critical emission rate K_{cr}, which is equal to the damage rate, is given by

$$K_{cr} = \frac{D_v(\rho_s + Z_i \rho_d)}{(Z_i/Z_v - 1)\varepsilon} (C_s^e(R) - C_\infty), \tag{18}$$

where $\varepsilon = G/K$ is the fraction of point-defects surviving the intra-cascade recombination, with K being the nominal NRT dpa rate [20]. The material parameters of Mo used in the present calculation are listed in Table 1. In Fig. 1, K_{cr} is plotted as a function of temperature for different values of void concentration and radius, assuming a value of 1.05 for Z_i/Z_v. Thus, for a typical neutron dose rate of 10^{-6} NRT dpa/s and a temperature $T < 1000$ K, the void radius, above which vacancy emission can be neglected, is less than 0.21 nm, corresponding to a critical void size of $x = 4$. For a typical ion dose rate of 10^{-3} NRT dpa/s, the corresponding temperature range is $T < 1200$ K.

In applying the master equations, it should be noted that small vacancy clusters are usually mobile. In such cases, equations for the mobile vacancy clusters have to be added, and the master equation (1) must be modified to include interactions between the mobile and immobile clusters. In the present application, we neglect the mobility of all vacancy clusters, and only consider the $x_0 = 2$ case. The flux $J(x,t)$ on the right hand side of Eq. (1) is replaced by the flux $J^c(x,t)$ (see Eq. (11)). As void nucleation is beyond our present scope, the kinetics of small vacancy clusters is not considered in detail. Instead, we focus on the difference between the evolution of a void ensemble, with and without the stochastic effects of random cascade initiation taken into account. For this purpose, we take $\dot{n}_v(x_0)$ to be zero for simplicity and solve the modified master equation Eq. (1) together with the conservation Eqs. (14) and (15), using the computer code developed previously [14].

Table 1
Material parameters for molybdenum

Parameter	Value
Atomic volume, Ω	1.017×10^{-29} m^3
Vacancy migration energy	1.5 eV
Vacancy formation energy	3.0 eV
Vacancy diffusivity pre-exponential	3.0×10^{-6} m^2/s
Interstitial migration energy	0.085 eV
Interstitial diffusivity pre-exponential	1.6×10^{-5} m^2/s
Surface free energy, γ_s	2.05 J/m^2
Melting temperature, T_m	2898 K

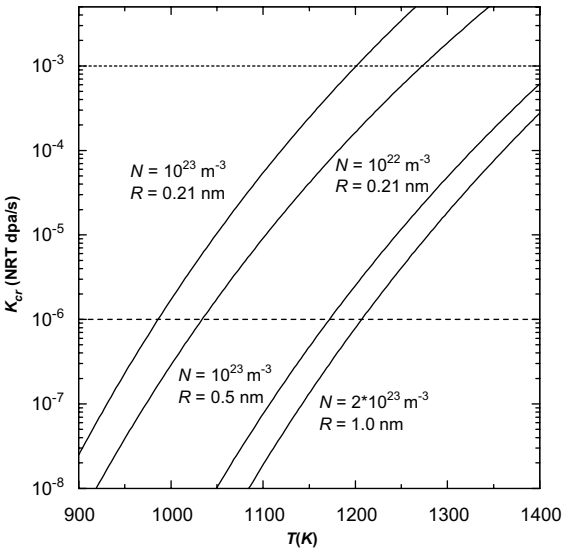


Fig. 1. Temperature dependence of the emission parameter K_{cr} given by Eq. (18) at different values of void concentration and void radius ($\varepsilon = 0.3$, $\rho_d = 2 \times 10^{13}$ m^{-2}, $Z_i/Z_v - 1 = 0.05$).

Snapshots of the calculated void size distribution functions are presented in Fig. 2(a) and (b), for different values of N_d, which measures the average number of free defects generated per cascades, and total dislocation density ρ_d. The calculated average void size ($R(0) \cong 2$ nm) and void number density ($N(0) \geqslant 10^{23}$ m^{-3}) of the initial void distribution are typical for experimental void ensembles in molybdenum after a few NRT dpa, within the temperature range under consideration [16,21,22]. The voids can also be considered as the major point-defect sinks in our calculation, because the sink density ratio ρ_d/ρ_s at the corresponding temperatures is on the order of 1% experimentally [16,21,22]. In this regard, similar to other pure metals, typical steady-state dislocation density in molybdenum is just above 10^{13} m^{-2} [7,16,21,22].

Fig. 2, together with Fig. 3 for the total void number density, clearly shows substantial increase of the coarsening effect on the void ensemble when stochastic fluctuations due to the random cascade initiation are taken into account. Indeed, even for a relatively high dislocation density of 10^{14} m^{-2}, up to half of the initial voids may dissolve (see Fig. 3(a)), due to the cascade-induced fluctuations. On the other hand, the size of the surviving

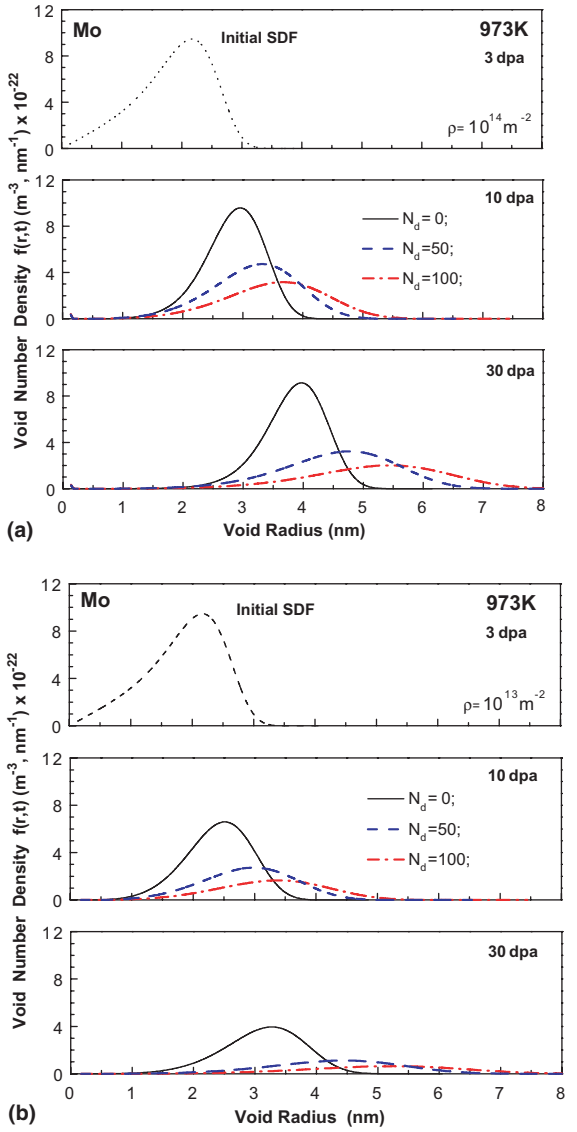


Fig. 2. Snapshots of the void size distribution at different values of the total dislocation density ρ_d and the average number of point-defects generated in a single cascade.

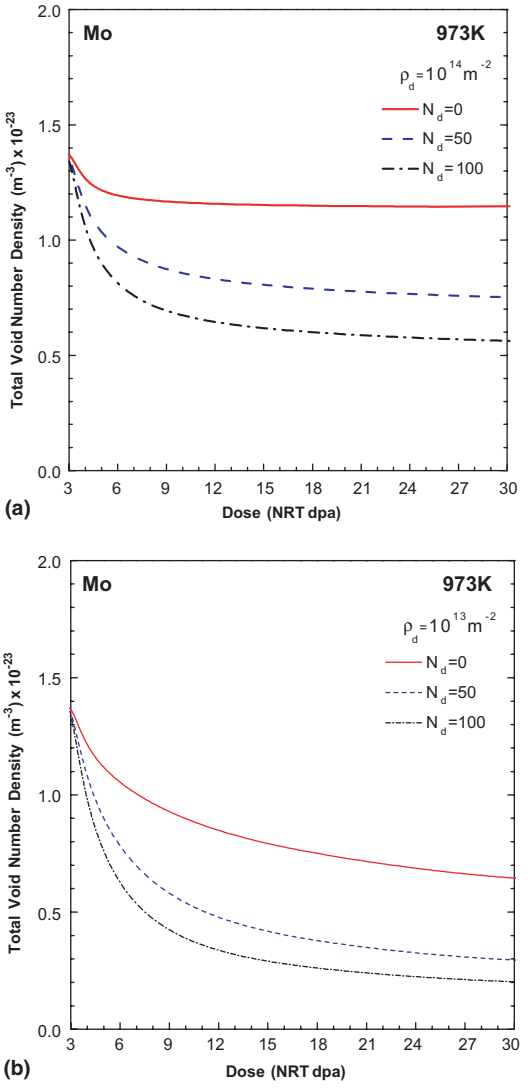


Fig. 3. Void number density as a function of dose at different values of the total dislocation density ρ_d and the average number of point-defects generated in a single cascade.

voids, as well as the average void radius, increase with dose (Figs. 2 and 4). When the voids are the major sinks for mobile defects, lower dislocation density also causes a decrease of the average void growth rate (Eq. 16 and Fig. 4). As a result, the number of surviving voids decreases even more dramatically when the total dislocation density drops from 10^{14} to 10^{13} m^{-2} (Fig. 3(b)). In agreement with the analytical calculations [4] and experimental results [15], about 80% of voids may have disappeared when the void swelling rate is about 2×10^{-4} (NRT dpa)$^{-1}$ (see also Fig. 5).

From Eqs. (8) and (12) the flux of shrinking voids in the size space is given by $(Q(x_0,t) + D^c(x_0,t))f(x_0,t)$. The ratio of the first two terms can be approximately written as

$$\frac{D^c(x_0,t)}{Q(x_0,t)} \cong \frac{a x_0^{1/3} k_v N_d}{2}. \tag{19}$$

According to Eq. (19), for $N_d = 100$, $k_v^2 = 10^{15}$ m^{-2} (see Fig. 6) the ratio $D^c(x_0,t)/Q(x_0,t) \cong 0.27$ ($x_0 = 2$), i.e., $D^c(x_0,t) < Q(x_0,t)$. At first sight, the effect of cascade fluctuations does not appear to be significant. However, comparing with the case for $N_d = 0$, i.e., no intra-cascade clustering, the void number density see a reduction of up to several hundred percent, when cascade-induced

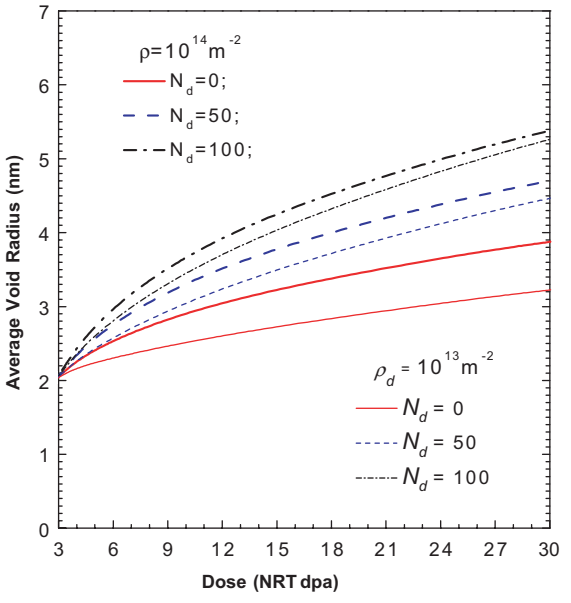


Fig. 4. Average void radius as a function of dose at different values of the total dislocation density ρ_d and the average number of point-defects generated in a single cascade.

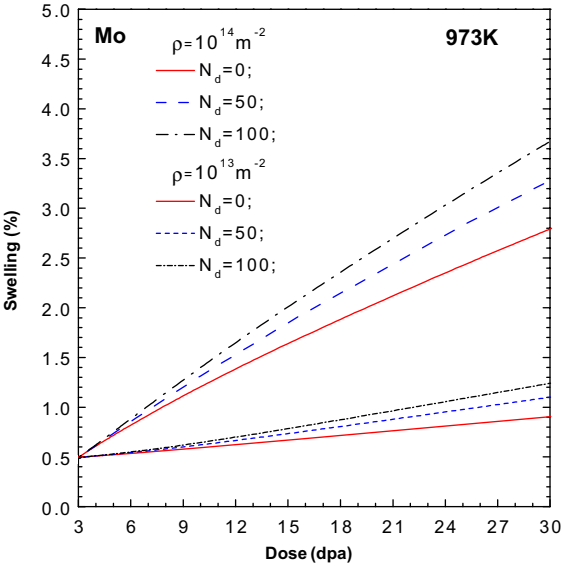
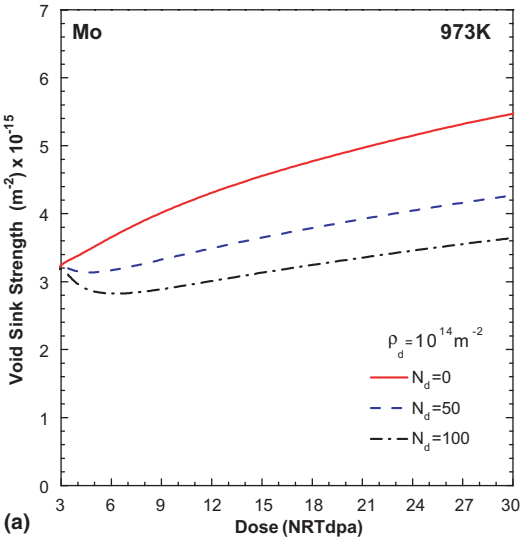


Fig. 5. Void swelling as a function of dose at different values of the total dislocation density ρ_d and the average number of point-defects generated in a single cascade.

fluctuations is taken into account (Fig. 3). Indeed, it follows from Eq. (19) that the ratio $D^c(x,t)/Q(x,t)$ increases with the void size. This size dependence of $D^c(x,t)/Q(x,t)$ results in an additional gradient driving the shrinkage of voids, which is much larger than that induced by a constant increase of $Q(x,t)$.



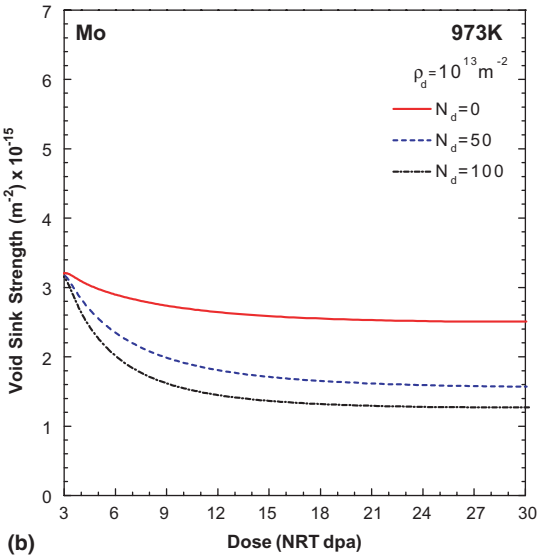


Fig. 6. Void sink strength as a function of dose at different values of the total dislocation density ρ_d and the average number of point-defects generated in a single cascade.

In the presence of a net vacancy flux without vacancy emission, void shrinkage can only occur through the diffusion of voids in the size space. Thus, the time t required for a void of the size x to shrink away can be estimated from the following diffusion relation:

$$x^2 - x_0^2 \approx 2D(x)t. \tag{20}$$

From Eq. (6), the required irradiation dose can be approximated by

$$Gt \approx \frac{xRk_v}{3N_d}, \tag{21}$$

where $R = ax^{1/3}$ and $x \gg x_0$. For $R = 2$ nm ($x^{1/3} = 14.88$), $N_d = 50$, $k_v^2 = 3 \times 10^{15}$ m^{-2} (Fig. 6), Eq. (21) gives a dose of $Gt \approx 2.4$ dpa. Taking into account the intra-cascade recombination, we have $Kt \approx 8$ NRT dpa ($G/K = 0.3$). Evolution of the void number density presented in Fig. 3 also supports this estimation.

Note also that in the present calculation, void shrinkage occurs when the time-averaged void swelling rate is approximately 2.6×10^{-4} (NRT dpa)$^{-1}$ at $\rho_d = 10^{13}$ m^{-2}, and 1.1×10^{-3} (NRT dpa)$^{-1}$ at $\rho_d = 10^{14}$ m^{-2}, respectively (see Fig. 5). These values are in the typical range of void swelling experimentally observed in molybdenum at the corresponding temperatures [16,21,22]. The higher void swelling for the $N_d \neq 0$ cases can also be readily understood from the foregoing discussions. Indeed, when the voids are the major sinks for the mobile defects ($\rho_s \gg \rho_d$), the conventional expression

$$\frac{dS}{dt} = \frac{(Z_i - Z_v)G\rho_d\rho_s}{(\rho_s + Z_i\rho_d)(\rho_s + Z_v\rho_d)}, \tag{22}$$

gives a swelling rate that increases when the void sink strength is reduced by the cascade-induced stochastic fluctuations. In contrast, when $\rho_s \ll \rho_d$, a similar reduction of the void density will reduce void swelling instead. When $\rho_s \approx \rho_d$, the average void growth rate is usually high and the stochastic fluctuations has no significant effect on the void evolution [4,19].

4. Discussions

It is interesting to note, from our present results, that the void coarsening effect is significant only if the initial void density is sufficiently high. If the initial void density is close to that at the largest dose in Fig. 3, for example, the effect would *not* have been significant. Indeed, it is clear that stochastic fluctuations are generally unfavorable to the nucleation of a void [4], because the probability of stochastic shrinkage is substantially higher for the smaller voids. On the other hand, the shrinkage probability is also strongly affected by the average net vacancy flux $D_vC_v - D_iC_i$ [4]. Thus, referring to Fig. 3, the number of surviving voids is several times higher at $\rho_d = 10^{14}$ m^{-2} than at $\rho_d = 10^{13}$ m^{-2}. Consequently, if the dislocation density is changed slowly from 10^{14} m^{-2} to a steady-state value close to 10^{13} m^{-2}, a significant fraction of the voids nucleated at the higher dislocation density would have shrunk away. This means that for the stochastic void shrinkage to occur, void nucleation must have been completed. Of course, one must be careful that the segregation of the impurities to the void surfaces, causing a reduction of the net vacancy flux received by the voids, may also produce similar effects.

According to the foregoing, a high void-nucleation rate is necessary to bring the ensemble of voids into an inherently unstable state under the action of stochastic fluctuations. This explains why void shrinkage is not always observed, even under very similar irradiation conditions [15,17]. Nevertheless, the present calculations clearly demonstrate that, under the action of stochastic fluctuations, significant void coarsening can occur, for the values of void concentration and void swelling rate, which are typical for molybdenum at the corresponding temperatures.

For temperatures at which vacancy emission from voids is negligible, void coarsening is most often observed experimentally at the initial stage of void-lattice formation. Initially voids are randomly distributed in space. Void coarsening takes place during the ordering process at later stages, resulting in the dissolution of randomly distributed voids, and the nucleation and growth of voids forming a regular lattice [16,23–25]. For the present discussion, it is important to notice the strong correlation between the rate of void nucleation and void-lattice formation [24–27]. Indeed, void-lattice formation is a prominent feature of molybdenum and tungsten, both of which have extremely high void nucleation rates. In other metals, the void lattice formation is observed only occasionally, when conditions for the nucleation of a high void density is created by different means like, for example, by the introduction of impurities, or a preliminary low temperature irradiation.

5. Summary

In this paper, the conventional master equation has been reformulated to include cascade-induced stochastic effects. The modified master equation is applied to investigate the evolution of a void ensemble in the regime of low void growth rate. In agreement with the analytical results derived earlier from a Fokker–Planck equation approach [4,19], the cascade-induced fluctuations are found to play a dominant role in the evolution of a void ensemble, causing the disappearance by shrinkage of the majority of voids, particularly the smaller ones, and the simultaneous growth of the larger ones. This coarsening of the void ensemble is not caused by vacancy emission from the voids, but rather, by the stochastic fluctuations in the point-defect fluxes received by the voids. While this kind of void shrinkage is not expected under the standard theory, it follows from kinetic approaches based on the Fokker–Planck or the master equations, which include the effect of stochastic fluctuations due to the random initiation of cascades.

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