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Linear stability analysis of helium-filled cavities in SiC *

Hanchen Huang and Nasr Ghoniem
Mechanical, Aerospace and Nuclear Engineering Dept., University of California, Los Angeles, CA 90024, USA

In this paper, we present a theoretical analysis of the stability of cavities in SiC under fusion irradiation conditions. Nucleation and growth of helium-filled cavities is modeled by dynamical equations. The growth/shrinkage of a cavity is given in terms of two equations representing the rates of change of the net number of vacancies and helium atoms inside the cavity. The equations describe the drift motion of cavities in a two-dimensional phase under the influence of point defect and helium absorption. First the linear stability of these equations is performed to identify the nature of singular points in phase space. The directions of trajectories around the saddle point are also found. The effects of dislocation density and void density on the nature of the singular points are considered. The effect of helium atom generation rate is also investigated. It is found that in the case of high helium generation, as in SiC under fusion conditions, the critical cavity size is relatively small (about 30 Å), and one saddle point is found between two stable critical points. This is shown to correspond to a bimodal cavity distribution.

1. Introduction

Many experimental observations of irradiation effects on the microstructure of SiC have been made in a number of irradiation facilities. However, the successful development of composite SiC/SiC materials for fusion applications must rely on a fundamental understanding of this data base. In fact, specific experiments must be planned to explore critical physical phenomena.

Swelling of SiC under neutron irradiation is known to be a result of the condensation of helium and vacancies to form cavities. However, in order to simulate or extrapolate the data to fusion conditions, an understanding of the factors which influence the swelling phenomenon is required. We focus our attention in this paper on a fundamental question in the study of swelling, that is, the stability of cavities under irradiation.

The concept of critical radius for cavity growth was developed first for the study of the swelling of nuclear fuels [1–4]. It was later extended by several investigators for the analysis of void swelling in irradiated alloys [5–8]. This concept has proved to be useful in the development of radiation resistant alloys [9–10].

We wish to add to these studies of the critical radius, and analyze the details of cavity stability under neutron or ion irradiation. Although the previous efforts have considered many of the factors which influence the critical growth radius, they were not analyze in terms of the stability theory of dynamical systems. Inclusion of the effects of continuous helium generation and further resolution back into the matrix can be accomplished within this framework.

In the following, we present a theoretical analysis of the linear stability of average size cavities under irradiation. This includes a rigorous study of the critical points in the phase space which describes cavity stability. The nature of the critical points and the factors which influence their dimension are discussed. Approximate analytical expressions are derived for the size of the critical cavity in the phase plane. Phase space trajectories around critical points are also presented.

2. Theoretical model

The concentration of point defects and mobile helium atoms during irradiation described by the standard rate theory [11]

$$dC_v/dt = K - D_v C_v(\rho + 4\pi RN), \qquad (1)$$

$$dC_i/dt = K - D_i C_i(Z\rho + 4\pi RN), \qquad (2)$$

$$C_{He}/dt = G_{He} - D_{He} C_{He}(\rho + 4\pi RN) + hNbK\Omega, \qquad (3)$$

where Cs are concentrations of various defects, K and G_{He} are production rates of point defects and helium atoms, respectively, subscripts i, v, He denote interstitial, vacancy and helium atoms respectively, Z is the bias factor for interstitial–dislocation interaction, ρ is the dislocation density, N is the concentration of cavities, R is the radius of the cavity and b is the resolu-

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Table 1
Physical parameters

Parameter	Value	Unit	Reference
Point defect production rate $K\Omega$	10^{-6}	dpa/s	11
Helium atoms generation rate $\xi = G_{He}/K$	2 and 20	appm/dpa	Estimated
Preexponential diffusion coefficient D_v^0	8.4×10^9	cm^2/s	13
Self-diffusion energy $E_s = E_m + E_f$	8	eV/atom	Estimated
Dislocation density ρ	10^9–10^{10}	cm^{-2}	11
Void density N	10^{15}–10^{16}	cm^{-3}	11
Dislocation bias factor ΔZ	0.1	-	Estimated
Surface energy γ	1000	$erg cm^2$	11
Irradiation temperature T	1000	°C	Estimated
Resolution parameter b	1	-	Estimated
Atomic volume Ω	2.07×10^{-21}	cm^3	13

tion probability of He from cavities. It is assumed here that the recombination rate of point defects is negligible. We retain the forms of eqs. (1) and (2) for simplicity of algebraic manipulations. Solution of diffusion equations for absorption of point defects and helium on cavities, where the medium is represented as lossy, with homogenized cavity and dislocation sinks, give the following equations [11].

$$dR/dt = \{(\Phi_v - \Phi_i) - \Phi_{vc}[\exp(\Phi(p - 2\gamma/R)/kT) - 1]\}\Omega/R, \tag{4}$$

$$dh/dt = 4\pi R \Phi_{He} - hbK\Omega, \tag{5}$$

where p is the gas pressure inside the cavity, $\Phi = DC$ for every specie, T is the radiation temperature, Ω is the atomic volume, γ is the surface energy, h is the number of helium atoms inside the cavity. All the physical parameters used here are listed in table 1.

Eqs. (1)–(5) model the dynamical behavior of the concentration of point defects, helium atoms in the matrix, the average cavity radius, and the number of helium atoms in a cavity. It can be shown that the time constants associated with eqs. (1)–93) are much shorter than those in eqs. (4) and (5). An adiabatic elimination procedure can therefore be used, where the time derivatives in eqs. (1)–(3) can be set to zero, and the results are then substituted into eqs. (4) and (5). Under this approximation, we can study the dynamics of cavity evolution in the phase space represented by R and h only.

3. Critical points [12]

If a cavity starts at any position in the phase plane (R, h), its subsequent growth or shrinkage is determined by its position relative to the critical points in the phase plane. Such critical points are obtained by solving for $dR/dt = 0$ and $dh/dt = 0$. This gives

$$K\rho\,\Delta Z/(\rho + 4\pi RN)^2 - \Phi_{vc} \exp[2\gamma\Phi/(kTR) - 3\xi/(\rho b R^2)] - \Omega_{vc} = 0. \tag{6}$$

R is first obtained by solving this equation. The corresponding value of h is then found and are fully determined. However this equation must be solved numerically. For simplicity, helium atoms are described by an ideal gas model. In extreme cases, eq. (6) can be simplified as explained below.

When the dislocation sink strength is much more important than the cavity sink strength, then:

$$[\ln(K\,\Delta Z/\Phi_{vc} + 1)]R^2 - (2\gamma\Omega/kT)R + 3\xi/(\rho b) = 0.$$

Eq. (6) is also satisfied for $R = \infty$.

Solving eq. (6) we can obtain several critical points. For typical fusion and fission irradiation conditions, the critical points and eigenvectors of the saddle point are shown in figs. 1–4.

4. Linear stability analysis [12]

In the near vicinity of the critical points, the growth or decay of perturbations can be studied by expanding R and h as

$$R = R_0 + dR, \tag{7}$$

$$h = h_0 + dh, \tag{8}$$

where R_0 and h_0 are the critical radius and helium atom numbers obtained above and dR and dh are

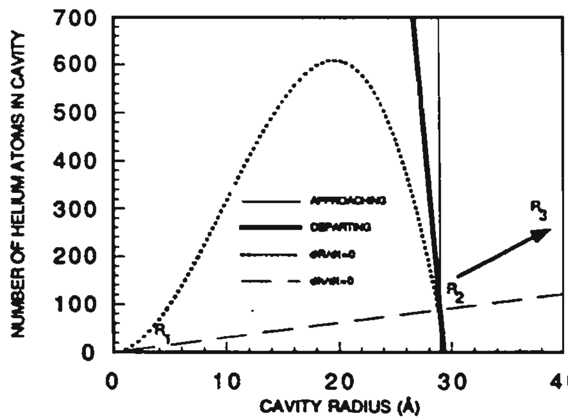

Fig. 1. Phase diagram (h, R) for $\rho = 10^{15}\ cm^{-3}$, $\xi = 50$ appm/dpa.

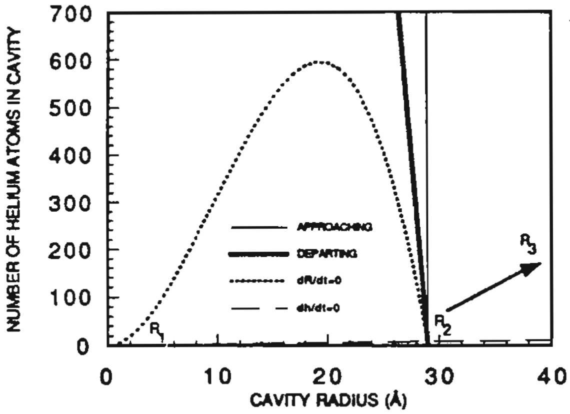

Fig. 2. Phase diagram (h, R) for $\rho = 10^{10}$ cm^{-2}, N $= 10^{15}$ cm^{-3}, $\xi = 50$ appm/dpa.

perturbations. Furthermore, if the perturbations are expressed at $(dR, dh) = e^{\lambda t} = e^{(\eta + i\omega)t}$, eqs. (4) and (5) result in

$$dV/dt = \mathbf{CV}, \text{ or } \lambda\mathbf{V} = \mathbf{CV}, \quad (9)$$

where $\mathbf{V} = [R, h]^T$, $\mathbf{C}$ is the matrix of coefficients composed of C_{ij}.

$$C_{ij} = (\partial/\partial u_j)[du_i/dt], \quad (10)$$

where $u_1 = R$, $u_2 = h$. C_{ij} is evaluated at the critical values.

Solution of the eigenvalue problem stated in eq. (9) determines λ, which can be found from the characteristic equation:

$$\lambda^2 - T\lambda + D = 0, \quad (11)$$

where $T = C_{11} + C_{22}$, $D = C_{11}C_{22} - C_{12}C_{21}$.

The corresponding eigenvector can be found by

$$V = h/R = (\lambda - C_{11})/C_{12}, \quad (12)$$

where $\mathbf{V} = [V, 1]^T$.

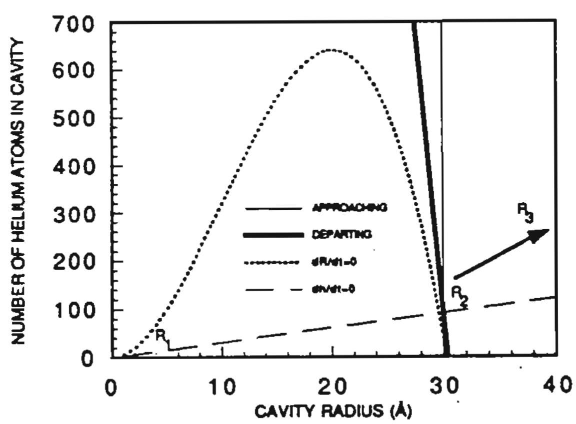

Fig. 3. Phase diagram (h, R) for $\rho = 10^9$ cm^{-2}, N $= 10^{16}$ cm^{-3}, $\xi = 50$ appm/dpa.

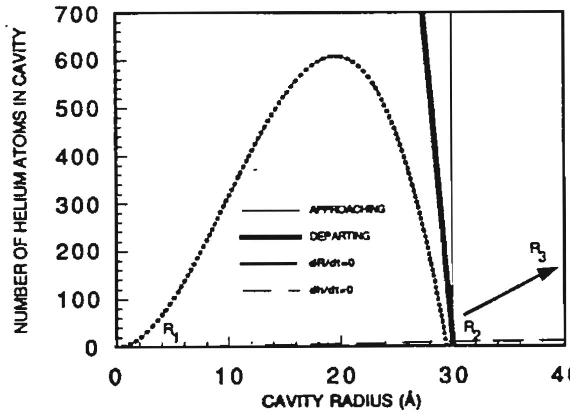

Fig. 4. Phase diagram (h, R) for $\rho = 10^9$ cm^{-2}, N $= 10^{15}$ cm^{-3}, $\xi = 5$ appm/dpa.

The nature and behavior of trajectories around the critical point can be determined by the eigenvalues and corresponding eigenvectors [12]. Usually, there are three critical points. The first critical point, which is very small contains about one vacancy), is found to be a stable node. The second critical point, which is about 30 Å, is a saddle point while the third one, which is almost infinite, is a stable node again. If the state starts from a given point in the phase space (R, h), the trajectory may approach the critical point 1 or 3. If the trajectory approaches critical point 1, the material is stable under irradiation, otherwise, it is unstable (i.e. unbounded swelling takes place).

The trajectories around the saddle point approach the critical point along the direction labeled "APPROACHING" in figs. 1–4 and depart from the critical point along direction labeled "DEPARTING" in the figures. Based on linear stability theory, whether a cavity will grow or shrink is totally determined by the initial cavity dimension. It cannot cross a barrier passing through the second critical point. On the other hand, if there are fluctuations, cavities may overcome the barrier and go to another nucleation regime. From the results shown in figs. 1–4 for different irradiation conditions and material characteristics, it can be seen that:

(1) if the dislocation density is one order of magnitude higher, the number of helium atoms inside the critical cavity is reduced by almost an order of magnitude. So, larger dislocation results in fewer helium atoms required for nucleation;

(2) a change of an order of magnitude in the void density does not appreciably change the critical dimension;

(3) for low helium atom generation rates, the critical cavity includes very few helium atoms (i.e. true void conditions).

5. Conclusions and remarks

Our stability analysis for typical fusion condition (i.e. $P = K\Omega = 10^{-6}$ dpa/s, appm He/dpa = 50) indicates that there exists three critical radii for cavity evolution. The first one, R_1 is nearly zero (i.e. trivial) and the last one, R_3 is almost infinite. The second critical point is a saddle point. we conclude therefore that cavity nucleation will occur by fluctuations overcoming the nucleation energy barrier at R_2. Because R_1 is a stable node, cavities will tend to cluster in its vicinity, unless pushed by fluctuations again past the barrier. If cavities leave the stable regime and get into the unstable regime by fluctuations, they will grow to the third critical point. As the third critical radius is very large, unbounded swelling will take place. We conclude here that the cavity size distribution will invariably be bimodal, and that a degree of swelling reduction can be attained if the cavity transition rate past R_2 is controlled. The role of fluctuations (i.e. cascade effects) can be important in this regard.

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