Investigation of the radiation growth of single Zr crystal by means of rate theory incorporating with the loop nucleation model

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Abstract

This report depicts the hybrid model between the mean field rate theory and the loop nucleation theory, to characterize the irradiation growth in single Zr crystal.

Keywords:

1. Model description

The model is implemented with following assumptions:
1. Initial microstructure consists of a- and c-type edge dislocations, homogeneously lying in the prismatic planes and the basal plane. It means that the density of the prismatic dislocation lines with the Burgers vectors along different $\boldsymbol{a1}$, $\boldsymbol{a2}$ and $\boldsymbol{a3}$ directions are equal. Then we can simplify the model by summing up these three directions together.
2. The primary damage produced in displacement cascades is mobile point defects, vacancy pyramids and SIA clusters with the Burgers vector along $\boldsymbol{a}$ directions.
3. The point defects present 3D isotropic diffusion, while SIA clusters migrate 1D along their Burgers vectors. Sessile vacancy pyramids are only formed in the basal plane and will collapse to vacancy loop beyond a critical dose (or loop size $r_{vl}^{c} \sim$ 3nm, see Christean). *[How about di-interstitials and tri-interstitials? immobile? SIAs-crowding should present 1D motion.]*
4. Prismatic vacancy-type loops are not considered in this work (see Fig. 1 and Choi paper), whereas the basal interstitial loops are not formed (in

agreement with the experimental observations). The basal vacancy-loops are only formed at high dose.

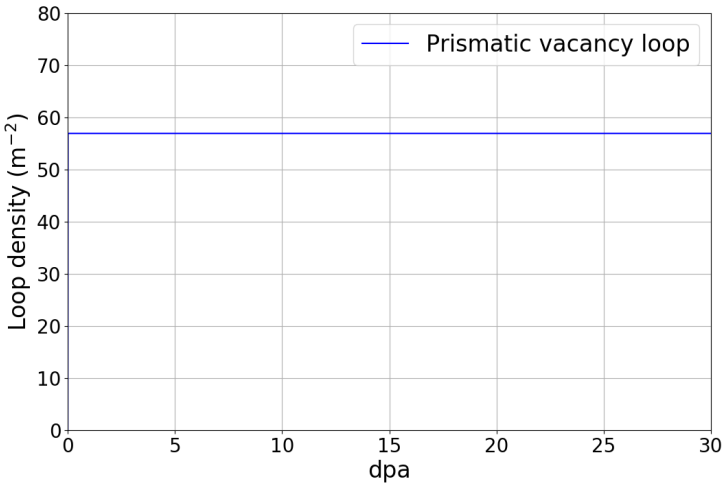

Figure 1: Density of prismatic vacancy-type loops versus irradiation dose.

5. The critical nucleus size for interstitial loops is taken as three, and di-interstitial can be destroyed by dissociation or vacancy impingement.
6. The SIA clusters interact with dislocations of the same Burgers vector only. *[The di-interstitials and tri-interstitials react with mobile point defects only. Maybe we should modify this.]*
7. The dislocation bias factor for point defects, mutual recombination of point defect and thermal vacancies are ignored.

The density of initial dislocation lines are set as constant, and the sessile loops evolve with the radiation dose. The total dislocation density of the system is therefore written as:

$$\begin{aligned} \rho_{tot} &= \rho_d^a + \rho_d^c + \rho_{il}^a + \rho_{vl}^c \\ &= \rho_d^a + \rho_d^c + 2\pi r_{il}^a N_{il}^a + 2\pi r_{vl}^c N_{vl}^c \end{aligned} \tag{1}$$

where rho_d^a and ρ_d^c are the edge dislocation density with Burgers vectors along $\boldsymbol{a}$ and $\boldsymbol{c}$ directions, respectively. And ρ_{il}^a, ρ_{vl}^c are corresponding densities of SIAs-type loops and vacancy-type pyramids/loops. r_{il}^a, N_{il}^a are the mean radius and number density of SIAs-type loops.

The radiation growth is directly associated with the microstructure evolution in crystals involving the diffusion of mobile defects, the sessile loops growth and shrinkage. The concentration C of mobile defects, i.e. single vacancies, single SIAs, di-interstitials, tri-interstitials and SIA clusters are obtained from the stead-state balance equations:

$$\frac{dC_v}{dt} = G^{NRT}(1-\epsilon_r)(1-\epsilon_v) - \rho_{tot} D_v C_v - \beta^v_{2i} C_v C_{2i} - \beta^v_{3i} C_v C_{3i} \tag{2a}$$

$$\begin{aligned}\frac{dC_i}{dt} &= G^{NRT}(1-\epsilon_r)(1-\epsilon_i) + \beta^v_{2i} C_v C_{2i} + 2\alpha^i_{2i} C_{2i} \\ &\quad - \rho_{tot} D_i C_i - 2\beta^i_{1i} C_i C_i - \beta^i_{2i} C_i C_{2i} - \beta^i_{3i} C_i C_{3i}\end{aligned} \tag{2b}$$

$$\frac{dC_{2i}}{dt} = \beta^i_{1i} C_i C_i + \alpha^i_{3i} C_{3i} + \beta^v_{3i} C_v C_{3i} - \alpha^i_{2i} C_{2i} - \beta^i_{2i} C_i C_{2i} - \beta^v_{2i} C_v C_{2i} \tag{2c}$$

$$\frac{dC_{3i}}{dt} = \beta^i_{2i} C_i C_{2i} - \alpha^i_{3i} C_{3i} - \beta^i_{3i} C_i C_{3i} - \beta^v_{3i} C_v C_{3i} \tag{2d}$$

C_{4i} not considered.

$$\frac{dC^a_{cl}}{dt} = G^{NRT}(1-\epsilon_r)\frac{\epsilon_i}{n_{cl}} - \frac{k^2_a}{3} D_{cl} C_{cl} \tag{2e}$$

Interact with dislocation loops and dislocation lines only.

where G^{NRT} is standard dose rate in dpa/s, ϵ_r being the defects recombination fraction, ϵ_i the fraction of SIAs produced in form of 1D mobile clusters and ϵ_v is the fraction of vacancies produced directly in vacancy pyramids/loops. D_j is the diffusion coefficient of j-type monomers ($j = i, v$) and C_{ni} represents the concentration of clusters with n-SIAs ($n = 1, 2, 3$). $\beta^{j'}_{nj} C_{j'}$ is the reaction frequency at which a nj-cluster absorb a defect of type j', α^j_{nj} the j-type defect emission frequency for a nj-size cluster. n_{cl} is the mean number of SIAs in mobile clusters produced from a radiation cascade. k^2_a is the sink strength for the SIA clusters migrating along their Burgers vectors and the factor 1/3 accounts for the sum of all three prismatic directions ($k^2_a = k^2_{a1} + k^2_{a2} + k^2_{a3}$).

The absorption frequency can then be written as

$$\beta^{j'}_{nj} C_{j'} = 2\pi r_n Z^{j'}_{nj} D_{j'} C_{j'} \tag{3}$$

where r_n is the cluster radius (depending on the cluster's shape), and $Z^{j'}_{nj}$ is an efficiency factor that accounts for the defect-dislocation elastic interactions. Similarly, the emission frequency is given by

$$\alpha^j_{nj} = 2\pi r_{n-1} Z^j_{(n-1)j} D_j \frac{\exp\left(-E^b_{nj}/k_B T\right)}{V_{at}} \tag{4}$$

where $E^b_{nj} = E^f_j - (E^f_{nj} - E^f_{(n-1)j})$ is the binding energy of a j-type defect with a cluster, and E^f_j is the formation energy of the corresponding defect. Some analytical expressions for such formation energy are generally adopted to simplify the calculations.

Now it is readily to get the nucleation, growth and shrinkage rates of sessile dislocation loops. Based on the model assumptions, it can be seen that:

$$\Omega \frac{dN_{il}}{dt} = \beta^i_{2i} C_i C_{2i} - \Omega \dot{N}_{cl} \tag{5a}$$

$$\Omega \frac{dN_{vl}}{dt} = \frac{G^{NRT}(1-\epsilon_r)\epsilon_v \Omega}{\pi r^2_{vl}(0)\boldsymbol{b}} \left[1 - \frac{V}{\Omega} N_{vl}\right] \tag{5b}$$

where $\Omega \dot{N}_{cl} \sim G^{NRT}(1-\epsilon_r)\frac{\epsilon_i}{n_{cl}}$ is the contribution from the mobile cluster nucleation. *[Did we over-count or under-count the interstitial loop nucleation rates? N(sessile) = N(3i) - N(cl)?]* Then the last term in Eq. 5b accounts for the overlap effect of vacancy-pyramids/loops during the cascades. *[Shall we change the area expression for the transition from pyramids to loops?]*

Then using the mean-size approximation, the sessile loop radii are writen as

$$\left\langle r^2_{il} \right\rangle \approx \langle r_{il} \rangle^2 = \frac{S^a_i}{\pi \boldsymbol{b} N_{il}} \tag{6a}$$

$$\left\langle r^2_{vl} \right\rangle \approx \langle r_{vl} \rangle^2 = \frac{S^c_v}{\pi \boldsymbol{b} N_{vl}} \tag{6b}$$

where S represents the total number of defects in the loops with different Burgers vectors $\boldsymbol{b}$. And its change rate can be expressed as

$$\dot{S}^a_i = -2\pi r_{il} N_{il} (D_v C_v - D_i C_i) + \frac{k^2_{ila}}{3} n_{cl} D_{cl} C_{cl} \tag{7a}$$

$$\dot{S}_v^c = Q 2\pi r_{vl} N_{vl} (D_v C_v - D_i C_i) \tag{7b}$$

According to the experimental observations, the basal vacancy-type loops are formed at high dose only. Moreover, some recent atomistic simulations have revealed that the agglomeration of vacancies is in the form of pyramids at low dose, which in turn collapse into vacancy loops beyond a critical size/dose resulting in a higher binding energy. In a bid to reproducing such vacancy formation mechanism, we introduce a parameter Q hereof, to characterize the variation of the vacancy absorption efficiency. If the size of the vacancy loop is smaller than a critical value, i.e. $r_{vl} < r_c$, $Q < 1$ is adopted (formation of pyramids). Otherwise, it equals to 1 (formation of loops).

Finally the radiation growth rate can be obtained by computing the net number of SIAs accumulated by dislocations and loops.

$$\dot{E}^a = G_{NRT}(1 - \epsilon_r)\epsilon_i - \rho^a (D_v C_v - D_i C_i) + \dot{E}^a_{nucl} \tag{8a}$$

$$\dot{E}^c = -\rho^c (D_v C_v - D_i C_i) + \dot{E}^c_{nucl} \tag{8b}$$

where the last term in RHS is the contribution of the sessile loop nucleation *[Shall we neglect this term as well?]*.