Supplementary Materials for

A model for dose dependence of the void swelling in electron-irradiated alloys

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1. Detailed derivation of our model

The diffusion equations for interstitial and vacancy are

$$\frac{\partial c_i}{\partial \tau} = G_i - R_{iv} c_i c_v - S_i c_i, \tag{1}$$

$$\frac{\partial c_v}{\partial \tau} = G_v - R_{iv} c_i c_v - S_v c_v. \tag{2}$$

And the bias for the total sink absorption rate ($S_{i,v}$) can be expressed as $b = \frac{S_i}{S_v}$.

If $S_i \neq S_v$, no analytical solution exists for the diffusion equations. But, when it comes to quasi-steady state (τ is long enough), with the assumption $G_i = G_v = G$, there is a relation between interstitial concentration and vacancy concentration,

$$\frac{\partial c_i}{\partial \tau} = \frac{\partial c_v}{\partial \tau} = 0 \implies S_i c_i = S_v c_v \implies c_i = \frac{S_v}{S_i} c_v, \tag{3}$$

which can be used as an approximation for semi analytical solution,

$$c_v(\tau) = \frac{-S_v + \sqrt{-4GR_{iv}\frac{S_v}{S_i} - S_v^2} \tan(\frac{-\sqrt{-4GR_{iv}\frac{S_v}{S_i} - S_v^2}\tau + 2\tan^{-1}\frac{S_v}{\sqrt{-4GR_{iv}\frac{S_v}{S_i} - S_v^2}}}{2})}{2R_{iv}}, \tag{4}$$

$$c_i(\tau) = \frac{S_v}{S_i} \frac{-S_v + \sqrt{-4GR_{iv}\frac{S_v}{S_i} - S_v^2} \tan(\frac{-\sqrt{-4GR_{iv}\frac{S_v}{S_i} - S_v^2}\tau + 2\tan^{-1}\frac{S_v}{\sqrt{-4GR_{iv}\frac{S_v}{S_i} - S_v^2}}}{2})}{2R_{iv}}. \tag{5}$$

The quasi-steady state limitations for interstitial and vacancy concentration are

$$\lim_{\tau \to \infty} c_i(\tau) = c_i = \frac{S_v}{S_i} \frac{2G}{S_v + \sqrt{4GR_{iv}\frac{S_v}{S_i} + S_v^2}}, \tag{6}$$

$$\lim_{\tau \to \infty} c_v(\tau) = c_v = \frac{2G}{S_v + \sqrt{4GR_{iv}\frac{S_v}{S_i} + S_v^2}}. \tag{7}$$

Insert c_i and c_v into void swelling model $\frac{dr}{dt} = \frac{\Omega}{r}[D_v c_v - D_i c_i]$, where r is the average void size, so the growth rate becomes

$$\frac{dr}{dt} = \frac{\Omega}{r}\left[D_v - D_i\frac{S_v}{S_i}\right]c_v = \frac{\Omega}{r}\left[D_v - D_i\frac{S_v}{S_i}\right]\frac{2G}{S_v + \sqrt{4GR_{iv}\frac{S_v}{S_i} + S_v^2}} = \frac{\Omega}{r}(D_v S_i - D_i S_v)\frac{\sqrt{\frac{4GR_{iv}}{S_v S_i} + 1} - 1}{2R_{iv}} \tag{8}$$

As mentioned above, $\frac{S_i}{S_v} = b$, the growth rate becomes

$$\frac{dr}{dt} = \frac{\Omega}{r}\left[D_v S_i - \frac{D_i S_i}{b}\right]\frac{\sqrt{\frac{4GR_{iv}}{S_v S_i} + 1} - 1}{2R_{iv}} \tag{9}$$

With the $r(0) = 0$ constraint, the solution is

$$r = \left\{ t\frac{\Omega}{R_{iv}}\left(\sqrt{1 + \frac{4GR_{iv}}{S_v S_i}} - 1\right)(D_v S_i - \frac{D_i S_i}{b})\right\}^{\frac{1}{2}} \tag{10}$$

For sink dominant regime, $\frac{4GR_{iv}}{S_i S_v} \ll 1$, then

$$\sqrt{1 + \frac{4GR_{iv}}{S_v S_i}} - 1 \approx 1 + \frac{1}{2}\frac{4GR_{iv}}{S_v S_i} - 1 = \frac{2GR_{iv}}{S_v S_i} \tag{11}$$

$$r = \left\{ t\frac{2G\Omega}{S_v S_i}(D_v S_i - \frac{D_i S_i}{b})\right\}^{\frac{1}{2}} = \left\{ t\frac{2G\Omega}{S_v}(D_v - \frac{D_i}{b})\right\}^{\frac{1}{2}} \tag{12}$$

For dose rate in dpa/s unit, G_{dpa}, is proportional to defect generation rate $G_{dpa} = \eta G$, dose in dpa unit is $\Delta_{\text{dpa}} = G_{dpa}t$, so

$$r = \left\{ 2\Omega(\frac{D_v b - D_i}{bS_v})\frac{\Delta_{dpa}}{\eta}\right\}^{\frac{1}{2}} \tag{13}$$

The swelling's relation with irradiation dose is

$$swelling = \frac{\Delta V}{V_0} = \frac{\frac{4}{3}\pi r^3 - \frac{4}{3}\pi r_0^3}{V_0} = \frac{4\pi}{3V_0}\left\{ 2\Omega(\frac{D_v b - D_i}{bS_v})\frac{\Delta_{dpa}}{\eta}\right\}^{\frac{3}{2}} - \frac{4\pi r_0^3}{3V_0} \tag{14}$$

The swelling relation with dose becomes,

$$swelling = \frac{4\pi}{3V_0}\left\{ 2\Omega(\frac{D_v S_i - D_i S_v}{\eta S_v S_i})\Delta_{dpa}\right\}^{\frac{3}{2}} - \frac{4\pi r_0^3}{3V_0} \tag{15}$$

$$= \alpha[\Delta_{dpa}]^{\frac{3}{2}} - c$$

where r_0 is nucleation radius, $\alpha = \frac{4\pi}{3V_0}\left[2\Omega\frac{D_v S_i - D_i S_v}{\eta S_i S_v}\right]^{\frac{3}{2}}$, $c = \frac{4\pi r_0^3}{3V_0}$.

By letting swelling equals zero,

$$swelling = \frac{4\pi}{3V_0}\left\{2\Omega(\frac{D_v S_i - D_i S_v}{\eta S_v S_i})\Delta_{dpa}\right\}^{\frac{3}{2}} - \frac{4\pi r_0^3}{3V_0} = 0 \tag{16}$$

the incubation dose Δ_0 can be derived as,

$$\Delta_0 = \frac{r_0^2}{2\Omega}\frac{\eta S_i S_v}{D_v S_i - D_i S_v} \tag{17}$$

2. The relation between paramter α and temperature.

For parameter α, $\frac{4\pi\rho_N}{3}\left[2\Omega\frac{D_v S_i - D_i S_v}{\eta S_i S_v}\right]^{\frac{3}{2}}$, temperature affects parameter α by diffusion coefficients D_i and D_v, where diffusion coefficients are in the form of

$$D_v \sim e^{-E_m^v/kT} \tag{18}$$

$$D_i \sim e^{-E_m^i/kT} \tag{19}$$

where E_m^v and E_m^i are migration energy for vacancies and interstitials. Therefore parameter α becomes

$$\alpha = \frac{4\pi\rho_N}{3}\left[2\Omega\frac{D_v S_i - D_i S_v}{\eta S_i S_v}\right]^{\frac{3}{2}} \sim \frac{4\pi\rho_N}{3}\left[2\Omega\frac{be^{-E_m^v/kT} - e^{-E_m^i/kT}}{\eta S_i}\right]^{\frac{3}{2}}. \tag{20}$$

The relation between $\left(be^{-E_m^v/T} - e^{-E_m^i/T}\right)^{1.5}$ and temperature T can be plotted in Figure S1, where biased parameter b equals 1.1 as mentioned in the manuscript, migration energy for interstitial and vacancy of iron are obtain from published paper [1,2], $E_m^i = 0.3\ eV$, $E_m^v = 0.7\ eV$. Accordingly, parameter α also increases with temperature.
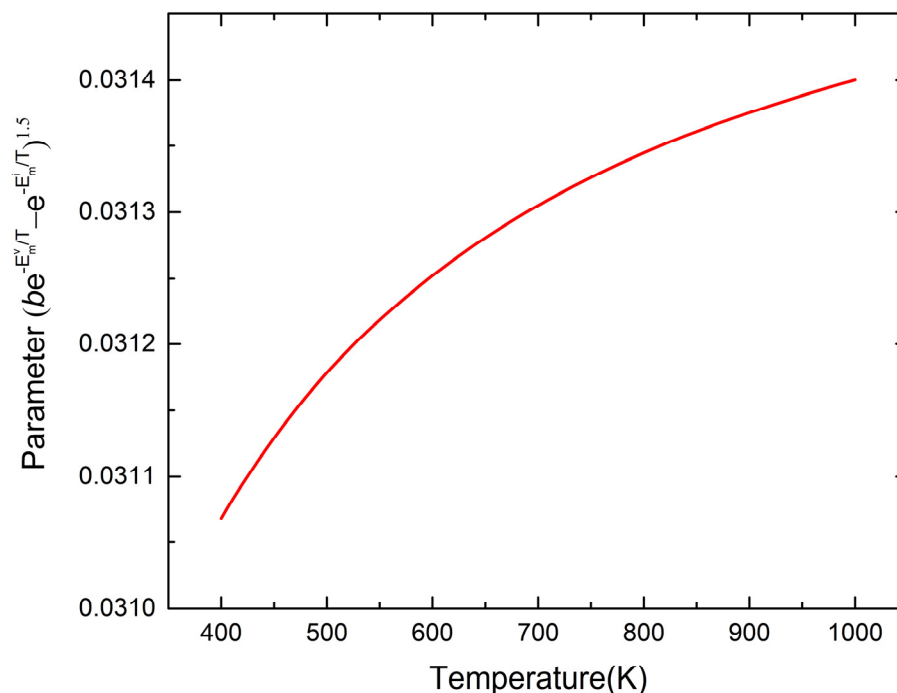
Figure S1. The relation between parameter $\left(be^{-E_m^v/T} - e^{-E_m^i/T}\right)^{1.5}$ and temperature.

3. Model application to high-dose irradiation

As shown in Figure S2, S3 and S4, Equation (9) is applied to high irradiation dose data in neutron irradiation experiments [3] and ion irradiation experiments [4], the swelling is also proportional to 1.5 power of the irradiation dose, which, to some extent, can be a validation of our model.
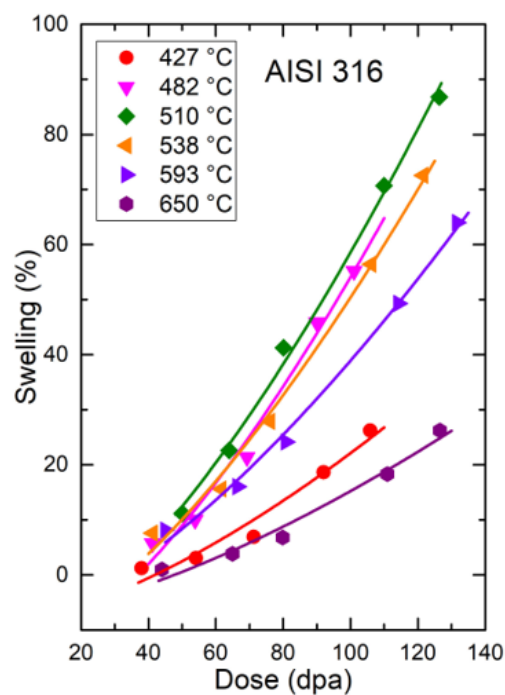

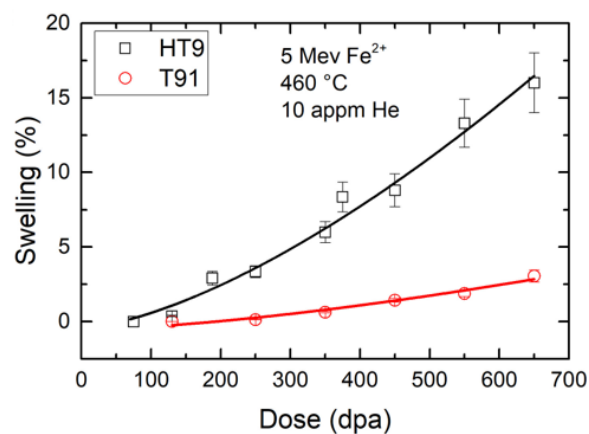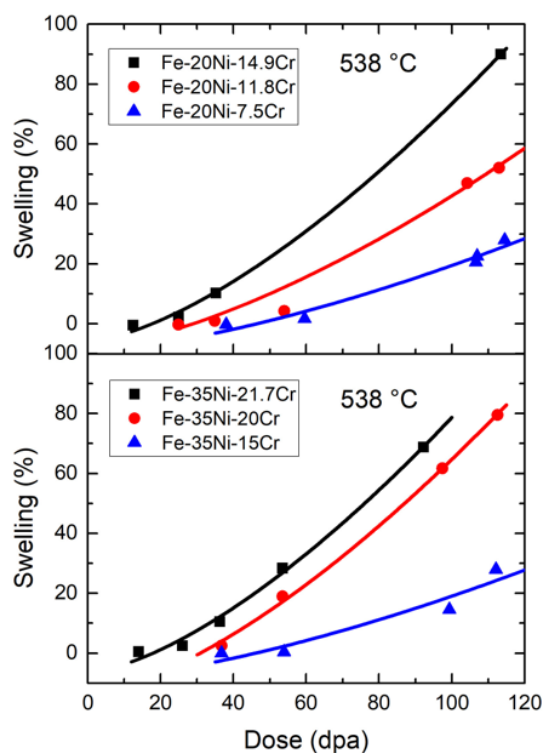**Figure S2.** AISI316 irradiated by neutrons at different temperatures [3].

Figure S3. HT9 and T91 irradiated by 5 MeV Fe++ at 460 °C [4].

Figure S4. Fe-20Ni-xCr and Fe-35Ni-xCr irradiated by neutrons at 538 °C [3].

References

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