Cascade fragmentation: deviation from power law in primary radiation damage. Supplementary material.*

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An estimate of the number of loops trapped in a foil

In this appendix, an estimate is made for the lower bound of the number of loops which would remain trapped in a foil at time \( t \) after a cascade, if the assumption is made that the loops are very mobile but interact strongly with each other and with images of themselves through elastic interactions. No account is taken for the effect of immobile residual cascade debris or impurities which might pin an otherwise mobile loop. The expression is derived by finding the expected distribution for the minimum separation between loop pairs, and using this minimum separation to find an inter-loop interaction strength. The variation of the interaction is then found as one loop is moved towards the surface of the foil, and a barrier for the loop to escape is hence found. If this barrier is large compared to \( k_B T \), a loop is trapped.

Consider a pair of loops generated within a single subcascade. The probability that a pair of loops, one generated at \( \vec{r}_1 \) with respect to the cascade origin, and the other at \( \vec{r}_2 \), are separated by distance \( R \) in 3-d space is

\[
4\pi R^2 P(R) dR \equiv \int \int p(\vec{r}_1, \vec{r}_2) \times \delta (|\vec{r}_1 - \vec{r}_2| - R) d^3\vec{r}_1 d^3\vec{r}_2.
\] (1)

We start by assuming the generating function is spherically symmetric and separable, \( p(\vec{r}_1, \vec{r}_2) = p(r_1)p(r_2) \), with normalisation \( \int 4\pi r^2 p(r)dr = 1 \). This yields

\[
P(R) = \frac{2\pi}{R} \int_{r_1=0}^{\infty} \int_{r_2=|R-r_1|}^{R+r_1} p(r_1)p(r_2) r_1 r_2 dr_1 dr_2.
\] (2)

If these two loops move on skew glide paths, the minimum distance between them is \( R_0 = |\vec{n} \cdot (\vec{r}_1 - \vec{r}_2)| \), where \( \vec{n} \) is the unit vector between the loops at

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minimum separation. If we further assume there is no correlation between the Burgers vector of a loop and its initial position, we find \( R_0 = R/\sqrt{3} \). Equation 2 can be solved analytically for some simple \( p(r) \) distributions. For \( p(r) \sim \exp(-r^2/2\sigma^2) \) we find

\[
P(R_0) = \frac{3\sqrt{3}}{8\pi^{3/2}\sigma^4} \exp\left(-3R_0^2/4\sigma^2\right).
\]  

Ignoring the complex angular dependence, the functional form for the elastic interaction between two circular loops containing \( N_1, N_2 \) defects respectively and separated by \( R_0 \) is [1, 2]

\[
E(R_0) \sim \frac{\mu a_0^6}{16\pi(1-\nu)} \frac{N_1 N_2}{R_0^4},
\]  

where \( \mu \) and \( \nu \) are elastic constants, here with values of 1000 eV/nm\(^3\) [1]. If a loop is at its minimum energy a distance \( L \) from the surface of a foil, and its glide direction is at an angle \( \theta \) to the surface normal, then as it moves to a depth \( z \) below the surface

\[
E(z|R_0, L) \sim -\frac{\mu a_0^6}{16\pi(1-\nu)} N_1 \left( \frac{N_2 \cos^3 \theta}{((L-z)^2 + R_0^2 \cos^2 \theta)^{3/2}} + \frac{N_1}{8z^3} \right).
\]  

Note that we neglect image interactions with the bottom surface of the foil, which we assume distant, and assume only one loop is moving. The barrier which the loop must overcome to be detrapped and be lost to the surface is approximately given by the difference of the stationary points of this function--i.e. \( \Delta E(R_0, L) = E(z_{max}|R_0, L) - E(z_{min}|R_0, L) \). A good estimate for the low energy point is \( z_{min} = L \), and a good estimate for the highest energy point is \( z = L/2 \). A better estimate for the high energy point is to use a single Newton-Raphson refinement,

\[
z_{max} = \frac{L \left( \frac{5}{4} (4R_0^2 \cos^2 \theta + L^2)^{7/2} N_1 - 2L^5 \cos \theta (4R_0^2 \cos^2 \theta - 3L^2) N_2 \right)}{2 \left(4R_0^2 \cos^2 \theta + L^2\right)^{7/2} N_1 - 8L^5 \cos \theta (R_0^2 \cos^2 \theta - L^2) N_2}. 
\]  

An estimate for the time taken to overcome this barrier is [3]

\[
\Delta t \sim \frac{L^2}{4D} \exp\left(\frac{\Delta E(R_0, L)}{k_B T}\right),
\]  

where \( D \) is the effective diffusion coefficient, with a value of \( 3.23 \times 10^{-7} \) m\(^2\)/s [1]. The probability that a loop of size \( N_1 \) is trapped elastically at time \( t \) after cascade initiation in a foil at temperature \( T \) is then

\[
p_{\text{self-trap}}(N_1, t|T) = \int_{R_0=0}^{\infty} \int_{L=0}^{\infty} \int_{N_2} P(R_0) P(L) P(N_2) \times \Theta\left(\exp\left(\frac{\Delta E(R_0, L)}{k_B T}\right) - \frac{4Dt}{L^2}\right) \, dR_0 dL dN_2,
\]  

where \( \Theta(x) \) is the Heaviside Theta function, and \( P(L), P(N_2) \) are respectively the probability of producing a loop a distance \( L \) from the surface of a foil, and the probability that a loop generated in a cascade is of size \( N_2 \),
An estimate of the number of invisible spots

In this appendix, an estimate is made for the number of spots on a TEM micrograph which are invisible due to their intensity falling below a measurable threshold [4]. We will start by assuming that a spot with diameter \( d \) will appear with an intensity \( I \) above background drawn at random from a distribution \( f_d(I) \), but that only spots which have an intensity \( \Delta I \) above the background level have a chance of being recorded. For our micrographs we compare the maximum of a 2-d Gaussian intensity profile fit to the spot intensity with \( \Delta I \) equal to three times the background intensity standard deviation. We need to estimate \( f_d(I) \) from the observed spots, and from this compute the true number of spots of diameter \( d \), i.e.

\[
  n_{\text{true}}(d) = \int_0^\infty n_0 f_d(I) \, dI > n_{\text{obs}}(d) = \int_{\Delta I}^\infty n_0 f_d(I) \, dI.  \tag{9}
\]

The intensity distribution \( f_d(I) \) will be a function of many factors, including loop depth, orientation, and Burgers vector as well as any post-process image corrections. It is not practical to attempt a derivation here, but nor is it necessary- our purpose is to determine an error bar only. Examination of histograms of the intensities of spots on many micrographs suggests a simple form for \( d > 3 \text{nm} \),

\[
  f_d(I) \sim \frac{1}{\sqrt{2\pi} \sigma_d} \exp \left( -\frac{(I - I_d)^2}{2\sigma_d^2} \right).  \tag{10}
\]

Hence the ‘true’ number of loops is

\[
  n_{\text{true}}(d) = n_{\text{obs}}(d) \left( \frac{1 - \text{erf} \left( \frac{-I_d}{\sqrt{2\sigma_d^2}} \right)}{1 - \text{erf} \left( \frac{\Delta I - I_d}{\sqrt{2\sigma_d^2}} \right)} \right).  \tag{11}
\]

In our micrographs we find \( I_d \) and \( \sigma_d \) are approximately linear in \( d \) for small \( d \). We fit the constant of proportionality using all spots \( 3 < d < 7 \text{nm} \) in all micrographs. The possibility of this large number of unseen faint spots in the micrographs up to \( n_{\text{true}}(d) \) is shown as a large (positive) error bar on the small loops in Figure 4 of the main article.

References

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