NERS521

Calculating dpa Cheat Sheet

Displacement cross section integrals

For simple, hard sphere elastic interactions the maximum energy transfer, $\hat{T}$, is given as,

$$\hat{T} = \gamma E_i$$

where,

$$\gamma = \frac{4M_1 M_2}{(M_1 + M_2)^2}$$

See Chapter 1.1.1 of Was, 2nd Edition for derivations. We then need to compare $\hat{T}$ with the displacement energy, E_d and the electronic cutoff energy, E_c. Based on where $\hat{T}$ lands within these ranges, we can determine the displacement cross section, $\sigma_d(E_i)$. For simple calculations assuming isotropic, elastic scattering using the [Kinchin-Pease model](#) we can use simple "if-then" logic to determine the displacement cross section:

If $\hat{T} < E_d$, then

$$\sigma_d(E_i) = \frac{\sigma_s(E_i)}{\gamma E_i} \int_{\check{T}}^{\hat{T}} v(T)\, dT = \frac{\sigma_s(E_i)}{\gamma E_i} \int_{\check{T}}^{\hat{T}} 0\, dT = 0$$

$$\therefore \ \sigma_D(E_i) = 0$$

If $E_d < \hat{T} < 2E_d$, then

$$\sigma_D(E_i) = \frac{\sigma_s(E_i)}{\gamma E_i}\left(\int_0^{E_d} v(T)\, dT + \int_{E_d}^{\hat{T}} v(T)\, dT \right) = \frac{\sigma_s(E_i)}{\gamma E_i}\left(0 + \int_{E_d}^{\hat{T}} 1\, dT \right)$$

$$\sigma_D(E_i) = \frac{\sigma_s(E_i)}{\gamma E_i}\left(\hat{T} - E_d \right) = \frac{\sigma_s(E_i)}{\gamma E_i}(\gamma E_i - E_d) = \sigma_s(E_i)\left(1 - \frac{E_d}{\gamma E_i} \right)$$

$$\therefore \; \sigma_D(E_i) = \sigma_s(E_i) \left(1 - \frac{E_d}{\gamma E_i} \right)$$

If $2E_d < \hat{T} < 2E_c$, then

$$\sigma_D(E_i) = \frac{\sigma_s(E_i)}{\gamma E_i} \left(\int_0^{E_d} \upsilon(T) \, dT + \int_{E_d}^{2E_d} \upsilon(T) \, dT + \int_{2E_d}^{\hat{T}} \upsilon(T) \, dT \right)$$

$$\sigma_D(E_i) = \frac{\sigma_s(E_i)}{\gamma E_i} \left(\int_0^{E_d} 0 \, dT + \int_{E_d}^{2E_d} 1 \, dT + \int_{2E_d}^{\hat{T}} \frac{T}{2E_d} \, dT \right)$$

$$\sigma_D(E_i) = \frac{\sigma_s(E_i)}{\gamma E_i} \left(0 + E_d + \frac{\hat{T}^2 - (2E_d)^2}{4E_d} \right) = \frac{\sigma_s(E_i)}{\hat{T}} \left(\frac{\hat{T}^2}{4E_d} \right)$$

$$\therefore \; \sigma_D(E_i) = \sigma_s(E_i) \left(\frac{\gamma E_i}{4E_d} \right)$$

If $2E_d < \hat{T} < 2E_c$, then

$$\sigma_D(E_i) = \frac{\sigma_s(E_i)}{\gamma E_i} \left(\int_0^{E_d} \upsilon(T) \, dT + \int_{E_d}^{2E_d} \upsilon(T) \, dT + \int_{2E_d}^{E_c} \upsilon(T) \, dT + \int_{E_c}^{\hat{T}} \upsilon(T) \, dT \right)$$

$$\sigma_D(E_i) = \frac{\sigma_s(E_i)}{\gamma E_i} \left(\int_0^{E_d} 0 \, dT + \int_{E_d}^{2E_d} 1 \, dT + \int_{2E_d}^{E_c} \frac{T}{2E_d} \, dT + \int_{E_c}^{\hat{T}} \frac{E_c}{2E_d} \, dT \right)$$

$$\sigma_D(E_i) = \frac{\sigma_s(E_i)}{\gamma E_i} \left(0 + E_d + \frac{E_c^2 - (2E_d)^2}{4E_d} + \frac{E_c}{2E_d} \left(\hat{T} - E_c \right) \right)$$

$$\sigma_D(E_i) = \frac{\sigma_s(E_i)}{\gamma E_i} \left(0 + E_d + \frac{1}{2E_d} \frac{E_c^2 - (2E_d)^2}{2} + \frac{E_c}{2E_d} (\gamma E_i - E_c) \right)$$

$$\therefore \; \sigma_D(E_i) = \sigma_s(E_i) \left(\frac{E_c}{2E_d} \right) \left(1 - \frac{E_c}{2\gamma E_i} \right)$$

The Kinchin-Pease model for displacements

The Kinchin-Pease (K-P) model is a simplified estimate of the number of displaced atoms (N_d) per PKA[^2] by means of the simple set of proposed relationships:

$$
N_d = \begin{cases} 0 & \text{for } 0 < E < E_d \\ 1 & \text{for } E_d < E < 2E_d \\ \frac{E}{2E_d} & \text{for } 2E_d < E < E_c \\ \frac{E_c}{2E_d} & \text{for } E_c < E \end{cases}
$$

Where E is the energy of the PKA and E_d is the threshold energy. At energies above E_c, the recoils lose energy only by electron excitation, while below E_c the energy transfer and loss is controlled by hardsphere elastic interactions (e.g. scattering). Note, the simplified model does not account for the effects due to the crystal lattice (e.g. crystal structure effects) for either single interactions or more complex damage cascades.