Illustration

Exercise 4.2-1

Diffusion During Cooling

A (big) crystal cools down from its melting point T_m to room temperature T_r (about 0^o C) with $T = T_m \cdot \exp - (\lambda \cdot t)$. The point defects present have a diffusion coefficient given by $D = D_0 \cdot \exp - (E_m/kT)$.

- **How large is the average distance L that they cover during cooling down from some temperature T to T_r?**

This is not an easy question. What you should do is:

- Use the Einstein relation for the diffusion length (and forget about lattice factors), but consider that the diffusion coefficient is a function of time, i.e.

$$L^2 = 6D \cdot t = \int_{t' = t_0}^{t' = \infty} D(t') \cdot dt'$$

- Proceed by first finding the values of λ for *initial* cooling rates at the melting point of **1 ^{o}C/s**, **10 ^{o}C/s**, **50 ^{o}C/s** and, for fun, **10^4 ^{o}C/s**.
- Using the following substitution will help with the integration

$$u(t) = \frac{E_m \cdot \exp \lambda \cdot t}{kT_m}$$

- The integral now runs from u_0 corresponding to t'_0 to whatever value of u corresponds to $t' = \infty$.
- You will obtain the following integral:

$$L^2 = 2D_0 \int_{?}^{?} \frac{1}{u} \cdot \exp - u \cdot du$$

- This integral cannot be solved analytically. In order to get a simple and good approximation, you may use the linear Taylor expansion for $1/u$ around u_0.
- Show that for realistic u_0 values you can replace $1/u$ by $1/u_0$ in a decent approximation and that you now can do the integral.

Now use typical values for melting temperatures, migration activation energies E_m, and D_0; e.g. from the backbone, two tables or diagrams given here. For missing values (e.g. D_0), make some reasonable assumptions.

- Plot L as a function of T for activation energies E = **1.0 eV**, E = **2.0 eV**, and E = **5 eV** with the four cooling rates given above as parameter.
- Play around a bit and draw some conclusions, e.g. with respect to
  - Average density of precipitates of point defects obtained in big crystals with few internal sinks.
  - Average size of these precipitates for some equilibrium concentration c_0 at T_m.
  - Possible errors made in quenching experiments.
  - Influence of sinks for point defects as a function of the average distance between sinks

Link to the Solution