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3.21 Kinetics of Materials—Spring 2006

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Lecture 7: Solutions to the Diffusion Equation—I.

References

1. Balluffi, Allen, and Carter, *Kinetics of Materials*, Sections 4.3–4.5.

Key Concepts

- When the diffusivity D is concentration-dependent, the diffusion equation is nonlinear and closed-form solutions to practical problems don't exist. The "Boltzmann–Matano" method is a graphical one for using a measured $c(x)$ profile from a diffusion-couple experiment to determine $D(c)$, using the relation $\widetilde{D}(c_1) = -\frac{1}{2\tau}\left(\frac{dx}{dc}\right)_{c_1} \int_{c^R}^{c_1} x(c)\, dc$ after setting the position $x = 0$ such that $\int_{c^R}^{c^L} x\, dc = 0$.

- Examination of asymmetry in an interdiffusion profile $c(x)$ gives useful information about trends in the concentration dependence of $D(c)$: D will be larger on the side with the *shallower* $c(x)$ profile, and D will be smaller on the side with the *steeper* $c(x)$ profile (see *KoM* Exercise 4.2).

- When D is time dependent (e.g., when temperature changes occur during a diffusional process), a simple approach using a *time-weighted* diffusivity defined by $\tau_D = \int_0^t D(t')\, dt'$ allows Fick's second law to be transformed into the alternate linear form $\frac{\partial c}{\partial \tau_D} = \nabla^2 c$. Familiar solution methods to solving the diffusion equation such as error functions and point sources can be readily adapted to cases where D is time dependent.

- In crystals and other anisotropic materials, D is generally anisotropic. Because D relates two vectors, D is a second-rank tensor quantity. Note however that symmetry considerations dictate that for *cubic* crystals, D is *isotropic*.

- The mathematical description of anisotropic diffusion depends on the choice of coordinate axes. Frequently, the most convenient choice is parallel to high-symmetry crystal axes.

- When anisotropic diffusion is described in special coordinate axes termed *principal axes*, the diffusivity tensor is diagonal, and diffusive fluxes along each principal axes are effectively uncoupled.

- Given a diffusivity tensor, finding its *eigensystem* (eigenvalues and eigenvectors) determines its principal axes and the prinicipal values of the diffusivity tensor along the diagonal in the principal axis coordinates.

- Crystal symmetry dictates the form of the diffusivity tensor in the crystal axis system, i.e., where the non-zero terms will be, and which non-zero terms must be equal.

- A scaling transformation, *KoM* Eq. 4.64, permits solutions for isotropic D to be readily adapted to cases in which D is anisotropic (see *KoM* Exercise 5.9).

Related Exercises in *Kinetics of Materials*

Review Exercises 4.1–4.8, pp. 91–97.