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3.21 Kinetics of Materials—Spring 2006

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Lecture 6: The Diffusion Equation.

References

1. Balluffi, Allen, and Carter, *Kinetics of Materials*, Sections 4.1–4.1.2, 4.2.

Key Concepts

- Fick's second law applies *locally* in an evolving concentration field: $\frac{\partial c}{\partial t} = -\nabla \cdot \vec{J} = -\nabla \cdot (-D \nabla c) = D\, \nabla^2 c + \frac{\partial D}{\partial c}\, (\nabla c)^2$.
- The divergence theorem provides a more *global* relation for the accumulation within a volume V bounded by a surface ∂V: $\frac{\partial N}{\partial t} = \int_V (-\nabla \cdot \vec{J})\, dV = -\int_{\partial V} \vec{J}(\vec{r}, t) \cdot \hat{n}\, dA$
- Fick's second law is a second-order partial differential equation. To obtain solutions, one needs *two boundary conditions* and *one initial condition*.
- The equations for conductive heat transport are essentially the same as those for mass transport, giving the relation $\frac{\partial T}{\partial t} = \nabla \cdot \kappa(\nabla T)$ for the evolution of the temperature field. κ is the *thermal diffusivity*.
- When Fick's second law is linearized (by expanding $D(c)$ about the average concentration $\langle c \rangle$), it takes the simple form $\frac{\partial c}{\partial t} = \widetilde{D}_0 \nabla^2 c$, where $\widetilde{D}_0 = D(\langle c \rangle)$ is constant. When this approximation is valid, solutions to simpler problems can be superposed to obtain solutions to more complex problems.
- In one-dimensional diffusion when $D \neq D(c)$, $\frac{\partial c}{\partial t}$ is proportional to the *curvature* of the $c(x)$ profile.
- When a physical situation permits *scaling* by the transformation $\bar{x} = \lambda x$, $\bar{t} = \lambda^2 t$, Fick's second law is transformed to an ordinary differential equation in the variable $\eta \equiv x/\sqrt{4Dt}$.
- Scaling permits a solution for the interdiffusion between two semi-infinite solids, each with initially uniform concentration, for concentration-independent D in terms of a tabulated *error function*, having the form $c(x, t) = A + B\, \mathrm{erf}(x/\sqrt{4Dt})$.
- The principle of superposition of solutions permits derivation of the diffusion field arising from an initial *point source* of diffusant. For one-dimensional diffusion this solution takes the form $c(x, t) = \frac{n_d}{\sqrt{4\pi Dt}} e^{x^2/(4Dt)}$, where n_d is the *source strength*.

Related Exercises in *Kinetics of Materials*

Review Exercise 5.5, pp. 118.