Massachusetts Institute of Technology
Department of Materials Science and Engineering
77 Massachusetts Avenue, Cambridge MA 02139-4307

3.205 Thermodynamics and Kinetics of Materials—Fall 2003

October 29, 2003

Kinetics Lecture 4A: Solutions to the diffusion/heat equation—II.

Lecture References

1. Balluffi, Allen, and Carter, *Kinetic Processes in Materials*, Chapters 4–5.
2. Poirier and Geiger, *Transport Phenomena in Materials Processing*, 1994. Ch. 13, "Diffusion in Solids," pp. 463–480.

Key Concepts

- Diffusion kinetics generally obey *scaling relationships* — the most important is that the diffusion distance x scales with $\sqrt{t}$. Thus, if a given process takes 100 s in a material of thickness 1 mm, in a material 3 mm thick it will take 900 s.
- A very useful "rule of thumb" in diffusion problems is that for *many* processes, $x^2 = 4Dt$ is a good approximation. Thus, if one knows D and wants to know how long it will take a species to diffuse 100 μm, one can estimate the time by calculating $t = x^2/(4D)$.
- Phase diagrams are often essential in understanding diffusional processes that can be expected to occur in processes like the application of coatings where one material might be joined to something quite different.

  The phase diagram will indicate what, if any, intermediate phases might form, and also provide a very good guide to the compositions of phases that form. Knowledge of the phase diagram allows boundary conditions to the diffusion equation to be specified, and thus enables quantitative modelling of kinetic processes involving multiple phases. A video recording of alloy interdiffusion illustrates examples of phase growth in an interdiffusion zone.
- In general, diffusion problems with time-dependent boundary conditions are difficult to solve with closed-form algebraic expressions. Some solutions are obtainable by *Laplace transform* methods. It is also generally difficult to solve problems with concentration-dependent diffusivities, because this makes the diffusion equation nonlinear. Finally, closed-form solutions generally are available only for the simplest diffusion geometries. In all cases where neat algebraic solutions are lacking, numerical solution methods should be sought.
- There are very powerful and instructive software packages for solving mathematical problems that have "user-friendly" user interfaces. Examples are *Mathematica* and *Maple* which are both available on Athena.

Example Problem 05

A flat surface of pure silicon is exposed to a gas that establishes a constant concentration of 10^{18} atoms of aluminum per cm^{-3} at the surface. The process is carried out at 1200 °C, at which the diffusivity of Al in Si is 10^{-15} m^2 s^{-1}. After 30 min, at what depth below the surface of the Si will the concentration be 10^{16} Al atoms per cm^{-3}?