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3.21 Kinetics of Materials—Spring 2006

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Lecture 1: Fields and gradients; fluxes; continuity equation

References

1. Balluffi, Allen, and Carter, *Kinetics of Materials*, Chapter 1.

2. Hildebrand, F. B., *Advanced Calculus for Applications*, Prentice-Hall, (1976). QA303.H642, or other applied math book of your choice.

Key Concepts

- Thermodynamics is precise about equilibrium states, but real materials are rarely at equilibrium.
- The concept of *local equilibrium* is applicable to real materials on a micro-scale.
- The rates of approach to equilibrium in real materials are found experimentally to depend on gradients of thermodynamic potentials.
- A *scalar field* associates a physical quantity with position—e.g., a composition field $c(\vec{x})$.
- The *gradient* of a scalar field is a vector that quantifies how rapidly the field changes with position.
- The *flux* of a substance quantifies the rate at which that substance flows through a unit area. The flux is a vector that is parallel to the local direction of the flow.
- The *rate of accumulation* of a the density of an extensive quantity is *minus* the divergence of the flux of that quantity, plus the rate of production of the substance.
- For conserved quantities like the number of moles of a component in a solution there are no sources or sinks and hence no production of the substance. For non-conserved quantities like entropy there can be production of the quantity during the course of a spontaneous process.
- Numerous kinetic processes are described by systems of linear equations relating fluxes and driving forces. Methods from linear algebra are often used to simplify the description by using coordinates parallel to crystal axes, or by finding principal axes. Matrix eigenvalues, eigenvectors, and similarity transformations are useful tools for describing coupled kinetic processes.

Related Exercises in *Kinetics of Materials*

Review Exercises 1.1–1.4, pp. 16–19.