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3.21 Kinetics of Materials—Spring 2006

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Lecture 12: Diffusion in Crystals.

References

1. Balluffi, Allen, and Carter, *Kinetics of Materials*, Section 8.1–8.2.1

Key Concepts

- An understanding of atomistic and molecular *mechanisms* of diffusion enables a more thorough appreciation for the ways in which a material's structure influences the rates at which macroscopic processes such as phase transfomations, diffusional creep, and sintering occur.

- Most of the diffusion mechanisms in crystalline materials depend on *crystal imperfections* such as point defects (vacancies and interstitials), line defects (dislocations), and planar defects (grain boundaries and surfaces). As a result, transport kinetics are often strongly influenced by microstructure.

- Within a given piece of material several diffusion mechanisms can be operative, at different rates. It is not unusual for the dominant mechanism (i.e., the one with the fastest transport kinetics) to be different in different temperature or pressure ranges.

- Fundamental mechanisms for diffusion in crystals include the *ring mechanism*, the *vacancy mechanism*, the *interstitialcy mechanism*, and the *interstitial mechanism*.

- The ring mechanism involves cooperative exchange of a group of neighboring atoms without the aid of vacancies or interstitials (see *KoM* Fig. 8.1). There is no experimental evidence that this mechanism contributes significantly to diffusion in any material.

- The vacancy mechanism involves the exchange of an atom with a neighboring vacant site (see *KoM* Figs. 8.2 and 8.3). Self-diffusion and substitutional solute-atom transport typically occurs by this mechanism.

- The interstitialcy mechanism involves the cooperative motion of an atom with a neighboring interstitial atom (see *KoM* Fig. 8.4). Self-interstitials of varying geometries are known to exist in crystalline materials (see *KoM* Fig. 8.5), and frequently have the form of a "split dumbell" as depicted in *KoM* Fig. 8.6. Although the energy of *formation* for interstitial defects in metals is typically very large, once present these defects move with very low activation energies. Such defects are often in materials that have been heavily irradiated with energetic particles.

- Interstitial components in a crystal are typically smaller than the other components, and the interstitials are generally confined to more open sites in the crystal (e.g., "octahedral" and "tetrahedral" sites in f.c.c. and h.c.p. crystals). Such interstitials may diffuse with realatively low activation energy by direct jumps between interstitial sites (see *KoM* Fig. 8.7).

Related Exercises in *Kinetics of Materials*

Review Exercises 8.1–8.8, pp. 191–197.