Random Walk Calculations in Intermetallic Compounds

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It was recognized some fifty years ago that vacancies do not move randomly in intermetallic compounds but, instead, move on complex correlated sequences. But describing these sequences analytically in tracer and chemical diffusion contexts has necessitated considerable theoretical effort. In this paper, we trace the development of models, diffusion mechanisms and random-walk-based i.e. diffusion kinetics calculations in intermetallic compounds. Models to be discussed will include two and four-frequency models and Ising-type models and their variants and adaptations for different structures. Mechanisms to be discussed include the six-jump cycle, the vacancy-pair mechanism, the antistructural bridge mechanism, the triple-defect mechanism, the antistructural sublattice mechanism, the generalized vacancy mechanism and variants of these. Calculations to be discussed include the Path Probability Method, methods inspired by Manning's random alloy diffusion kinetics theory, and calculations based on the five-frequency model adapted to the six-jump-cycle mechanism. It is emphasized how analytical development is especially enhanced when Monte Carlo computer simulation is done in parallel. It is shown, with examples, that a diffusion kinetics theory should be capable of describing both tracer diffusion *and* chemical interdiffusion in a consistent manner. Unsolved problems are highlighted.