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Paper Title	Page
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<u>Molecular Dynamics Simulations of Atoms Diffusion in Solid</u> Authors: Yu Lu Zhou, Xiao Ma Tao, Qing Hou, Yi Fang Ouyang Abstract: Molecular dynamics (MD) simulations, which treat atoms as point particles and trace their individual trajectories, are always employed to investigate the transport ...more	51

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Paper Titles

- Preface >
- Kinetic Simulations of Diffusion-Controlled Phase Transformations in Cu-Based Alloys** < p.1
- Phenomenological Investigations on Diffusion Kinetics in Multicomponent Metallic Melts > p.23
- Molecular Dynamics Simulations of Atoms Diffusion in Solid > p.51
- Reviews on Modeling of Diffusion-Induced Mass Transportation in Functionally Graded Cemented Carbides > p.65
- The Diffusion and Solid-Liquid Phase Transformation in Directional Solidification of Alloy: A Quantitative Phase Field Characterization and Real-Time Observation > p.97
- Tilted Dendritic Growth Dynamics and Dendrite to Degenerate Seaweed Transition in Directional Solidification: Insights from Phase-Field Simulations > p.128
- Ginzburg-Landau Modeling for Martensitic Transformation Coupled with Composition Redistribution > p.154

Home » Diffusion Foundations » Diffusion Foundations Vol. 15 » Kinetic Simulations of Diffusion-Controlled Phase...

Kinetic Simulations of Diffusion-Controlled Phase Transformations in Cu-Based Alloys

Abstract:

In this chapter, we present computational kinetics of diffusion-controlled phase transformations in Cu-based alloys, which becomes possible only most recently due to the establishment of the first atomic mobility database (MOBCU) for copper alloys. This database consists of 29 elements including most common ones for industrial copper alloys. It contains descriptions for both the liquid and Fcc_A1 phases. The database was developed through a hybrid CALPHAD approach based on experiments, first-principles calculations, and empirical rules. We demonstrate that by coupling the created mobility database with the existing compatible thermodynamic database (TCCU), all kinds of diffusivities in both solid and liquid solution phases in Cu-based alloys can be readily calculated. Furthermore, we have applied the combination of MOBCU and TCCU to simulate diffusion-controlled phenomena, such as solidification, nucleation, growth, and coarsening of precipitates by using the kinetic modules (DICTRA and TC-PRISMA) in the Thermo-Calc software package. Many examples of simulations for different alloys are shown and compared with experimental observations. The remarkable agreements between calculation and experimental results suggest that the atomic mobilities for Cu-based alloys have been satisfactorily described. This newly developed mobility database is expected to be continuously improved and extended in future and will provide fundamental kinetic data for computer-aided design of copper base alloys.

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