

Preface

Diffusion is an omnipresent but important phenomenon in a wide variety of disciplines and applications in physical, chemical, biological, geologic, materials science and engineering processes. While diffusion-controlled phase transformations involve in a variety of materials processes, ranging from solidification to different solid-state transformations. Modeling of diffusion and diffusion-controlled phase transformations in alloys has been of long-standing fundamental interests because advance modeling can help to improve the understanding of complex materials processes. Moreover, as the recent boost in Integrated Computational Materials Engineering (ICME) and Materials Genome Initiative (MGI) projects, additional emphasis on the necessity and urgency of the quantitative modeling of diffusion and diffusion-controlled phase transformations in alloys has been laying, which can provide useful information for accelerating the novel alloys design. Consequently, the purpose of this book, entitled "Modeling of Diffusion and Diffusion-Controlled Phase Transformations in Alloys" is to provide a collection of the commonly used computational approaches for modeling diffusion and diffusion-controlled phase transformations, as well as their current status, recent developments, future trends and applications in different alloys.

In Chapter 1, Y. Tang, Q. Chen and A. Engström present thorough computational kinetics of diffusion-controlled phase transformations in Cu alloys in the framework of Calculation of PHase Diagram (CALPHAD) approach based on their established thermodynamic and atomic mobility databases for Cu alloys. In Chapter 2, W. Chen *et al.* propose a phenomenological approach for predicting the composition- and temperature-dependent diffusivities in multicomponent metallic melts, and demonstrate its applications in alloys during different processes. In Chapter 3, Y. Zhu *et al.* conduct a mini review of molecular dynamic simulations of atoms diffusion in solid, and give an example of diffusion of helium in tungsten. In Chapter 4, K. Cheng *et al.* demonstrate quantitative numerical modeling of diffusion-induced mass transportation in functionally graded cemented carbides using different techniques, including one-dimensional sharp-interface models and two-dimensional diffuse-interface phase-field model. In Chapters 5 and 6, two groups of researchers summarize their own work on phase-field simulations of phase transformation and microstructure evolution in Al-Cu alloys during direction solidifications. While in Chapter 7, G. Xu and Y. Cui show their recent progress on Ginzburg-Landau modeling for martensitic transformation coupled with composition redistribution. The Fe-C binary system is chosen for demonstration.

Considering the wide scope of the presented topics, this book should be interesting to the scientists active in the fields of physics, materials science and engineering processes. It is also anticipated that representatives of industrial R&D centers will also be found among the readers.

Lijun Zhang
State Key Laboratory of Powder Metallurgy
Central South University
Changsha, Hunan 410083
PR China