Preface

Content

This book explains the thermodynamics and kinetics of most of the important phase transitions in materials science. It is a textbook, so the emphasis is on explanations of phenomena rather than a scholarly assessment of their origins. The goal is explanations that are concise, clear, and reasonably complete. The level and detail are appropriate for upper division undergraduate students and graduate students in materials science and materials physics. The book should also be useful for researchers who are not specialists in these fields. The book is organized for approximately linear coverage in an graduate-level course. The four parts of the book serve different purposes, however, and should be approached differently.

Part I presents topics that all graduate students in materials science must know.[1] After a general overview of phase transitions, the statistical mechanics of atom arrangements on a lattice is developed. The approach uses a minimum amount of information about interatomic interactions, avoiding detailed issues at the level of electrons. Statistical mechanics on an Ising lattice is used to understand alloy phase stability for basic behaviors of chemical unmixing and ordering transitions. This approach illustrates key concepts of equilibrium T-c phase diagrams, and is extended to explain some kinetic processes. Essentials of diffusion, nucleation, and their effects on kinetics are covered in Part I.

Part II addresses the origins of materials thermodynamics and kinetics at the level of atoms and electrons. Electronic and elastic energy are covered, and the different types of entropy, especially configurational and vibrational, are presented in the context of phase transitions. Effects of pressure, combined with temperature, are explained with a few concepts of chemical bonding. The kinetics of atom movements are developed for diffusion in solids, and from the statistical kinetics of the atom-vacancy interchange.

Part III is the largest. It describes many of the important phase transformations in materials, with the concepts used to understand them. Topics include melting, phase transformations by nucleation and growth, spinodal decomposition, freezing and phase fields, continuous ordering, martensitic transformations, phenomena in nanomaterials, phase transitions involving electrons or spins, and quantum phase transitions. These different phase transitions in materials are covered at different breadths and depths based on their richness or importance, although this reflects my own bias. Many topics from metallurgy and ceramic engineering are covered, although the connection between processing and properties is less emphasized, allowing for a more concise presentation than in traditional texts. Part III includes a number of topics from condensed matter physics that were selected in part because they give new insights into materials phenomena.

[1] The author asks graduate students to explain some of the key concepts at a blackboard during their Ph.D. candidacy examinations.

Part IV presents topics that are more modern, but have proved their importance. Low and high temperature treatments of the partition function, the renormalization group, scaling theory, a k-space formulation of elastic energy, nonequilibrium states in crystalline alloys, fluctuations and dissipation, and some complexities of high temperature thermodynamics are presented. The topics in Part IV are explained at a fundamental level, but unlike Parts I through III, for conciseness in Part IV there are some omissions of methods and steps.

The book draws a distinction between phase transformations and phase transitions. Phase transitions are thermodynamic phenomena based on free energy alone, whereas phase transformations include kinetic processes that alter the life cycle of the phase change. Phase transitions originate from discontinuities in free energy functions, so much of the text focuses on formulating free energies for different systems. The book formulates statistical mechanics models for different phase transitions, sometimes using an Ising lattice, which is well suited for such analysis and finds reuse for different phase transitions. Other topics that recur in the text are Landau theory in various forms, the topic of domains, the square gradient energy, the effect of curvature on nucleation, and dynamics with the kinetic master equation. Sometimes the thermodynamics of phase transitions is developed with the partition function, although the classical equation $G = E - TS + PV$ is used widely, and it is assumed that the reader has some familiarity with the terms in this expression. For the kinetics of phase transformations, there is some traditional presentation of diffusion and nucleation, but the kinetic master equation is also used throughout the text.

Many topics in phase transitions and related phenomena are not covered in this text. These include: other mechanisms of atom movements (and their effects on kinetics), polymer flow and dynamics, including reptation, phase transitions in fluid systems including phenomena near the critical temperature, massive transformations. Also beyond the scope of the book are computational methods that are increasingly important for studies of phase transformations in materials, including: Monte Carlo methods, molecular dynamics methods (classical and quantum), and density functional theory with extensions to phenomena at finite temperatures.

The field of phase transitions is huge, and continues to grow. This text is a snapshot of phase transitions in materials in the year 2013, composed from the angle of the author. Impressively, this field continues to offer a rich source of new ideas and results for both fundamental and applied research, and parts of it will look different in a decade or so. I expect, however, that many core topics will remain the same – the free energy of materials will remain the central concept, surrounded by issues of kinetics.

Teaching

I use this text for a graduate-level course taken by Ph.D. students in both materials science and in applied physics at the California Institute of Technology. The 10-week course, which includes approximately 30 hours of classroom lectures, is offered in the third academic quarter as part of a one-year sequence. The first two quarters in this sequence cover thermodynamics and statistical mechanics, so the students are familiar with the use of the partition function to obtain thermodynamic quantities, and have seen basic concepts from quantum statistical mechanics such as the Fermi–Dirac distribution. Familiarity with some concepts from solid-state physics and chemistry is certainly helpful, as is prior exposure to diffusion and transport, but the text develops many of the important concepts as needed.

In the one-quarter graduate-level course at Caltech, I cover all topics in Parts I and II, moving in sequence through these chapters. Time limitations force a selection of topics from Parts III and IV, but I typically cover more of Part III than Part IV. For example, this year I covered Chapters 10, 11, 12, parts of 13, 15, 16, 19, and selections from 20, 22, 24. It may be unrealistic to cover all the content in the book in a 15-week semester with 45 hours of lectures. An instructor can certainly exercise discretion in selecting topics for the second half of her course.

Most of the problems at the end of each chapter have been used for weekly student assignments, and this experience has helped to improve their wording and content. The majority of these problems make use of concepts explained in the text, fill in the explanations of concepts, or extend analyses. Others develop new concepts not described in the chapter, but these problems usually include longer explanations and hints that may be worth reading even without working the problem. None of the problems are intended to be particularly difficult, and some can be answered quickly once the main idea emerges. I usually assign five or six problems every week during the term. An expanding online solutions manual is available to course instructors whose identity can be verified. Please ask me for further information.

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