Nikolas Provatas and Ken Elder

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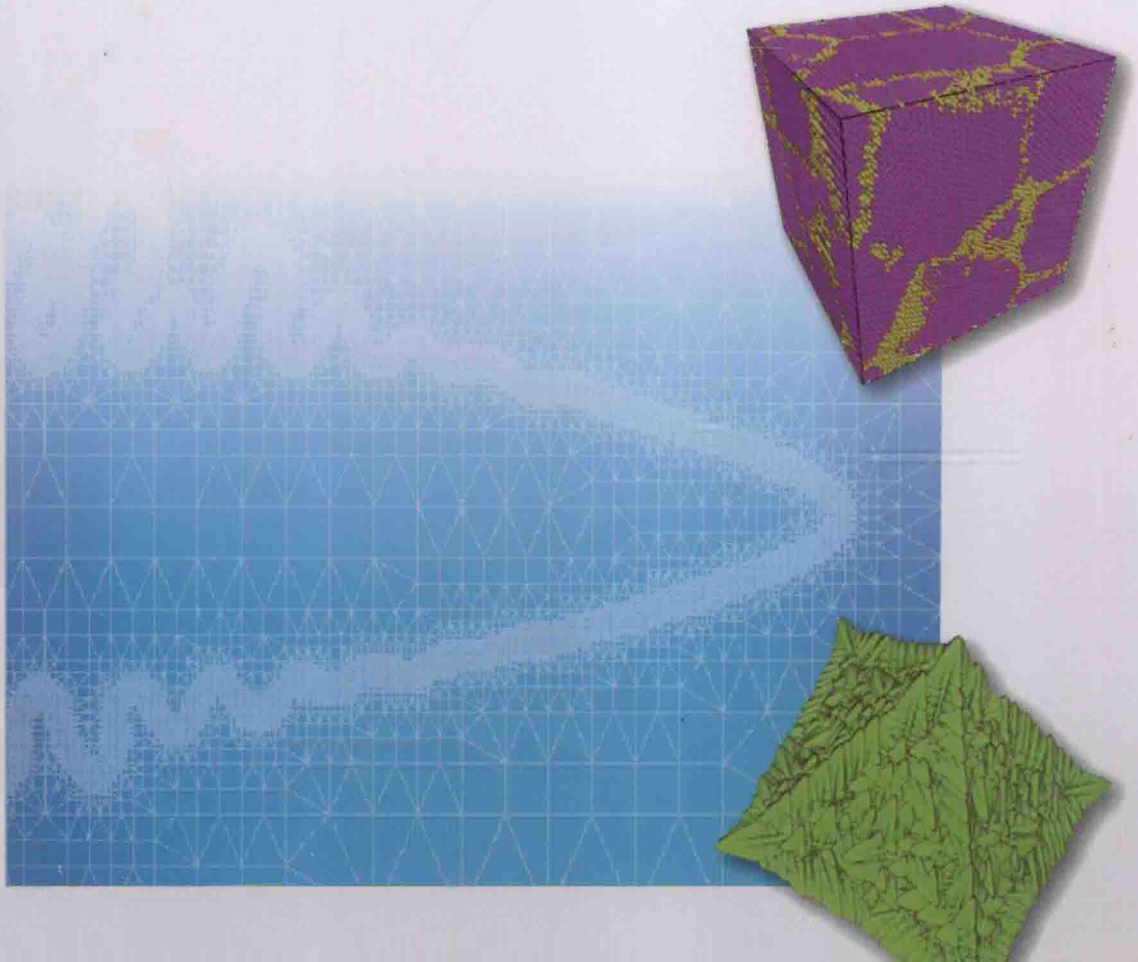
Phase-Field Methods in Materials Science and Engineering



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Preface

The idea for this book grew out of a series of workshops that took place at the McMaster University from 2002 to 2005 in which a couple of dozen researchers and students (called the Canadian Network for Computational Materials Science or CNCMS) were invited to discuss their research and their visions for the future of computational materials science. One serious concern that surfaced from the discussions and the proceedings regarded the gaping hole that existed in the standard pedagogical literature for teaching students – and professors – about computational and theoretical methods in phase field modeling. Indeed, unlike many other fields of applied physics and theoretical materials science, there is a dearth of easy-to-read books on phase field modeling that would allow students to come up to speed with the details of this topic in a short period of time. After sitting on the fence for a while, we decided to add our contribution by writing an introductory text about phase field modeling.

The aim of this book is to provide a graduate-level introduction of phase field modeling for students of materials science who wish to delve deeper into the underlying physics of the theory. The book begins with the basic principles of condensed matter physics to motivate and develop the phase field method. This methodology is then used to model various classes of nonequilibrium phase transformations that serve as paradigms of microstructure development in materials science phenomena. The workings of the various phase field models studied are presented in sufficient detail for students to be able to follow the reasoning and reproduce all calculations. The book also includes some basic numerical algorithms – accompanied by corresponding Fortran codes that come on a CD with this book – that students can use as templates with which to practice and develop their own phase field codes. A basic undergraduate-level knowledge of statistical thermodynamics and phase transformations is assumed throughout this book. Most long-winded mathematical derivations and numerical details that can serve as references but would otherwise detract from the flow of the main theme of the text are relegated to appendices.

It should be specified at the outset that this book *is not* intended to be an exhaustive survey of all the work conducted throughout the years with phase field modeling.

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There are plenty of reviews that cover this angle and many of these works are cited in this book. Instead, we focus on what we feel is missing from much of the literature: a fast track to understanding some of the "dirty" details of deriving and analyzing various phase field models, and their numerical implementation. That is precisely what we have observed new students wishing to study phase field modeling are starving for as they get started in their research. As such, this book is intended to be a kind of "phase field modeling for dummies," and so while the number of topics is limited, as many of the details as possible are provided for those topics that are covered.

The broad organization of the material in following chapters is as follows. The first half of the book begins by establishing the basic phase field phenomenology, from its basic origins in mean field theory of phase transformations to its basic form now in common use as the base of most modern phase field models in computational materials science and engineering. Phase field theory is applied to several examples, with a special emphasis placed on the paradigms of solidification and solid-state transformations. An appendix is also dedicated to the important issue of mapping the phase field model onto specific sharp interface limits. The last two chapters of this book deal with the development of more complex class of phase field models coined "phase field crystal" models. These are an extension of the original phase field formalism that makes it possible to incorporate elastic and plastic effects along side the usual kinetics that governs phase transformations. We will see that these models constitute a hybrid between traditional phase field theory and atomistic dynamics. After motivating the derivation of phase field crystal models from classical density functional theory, these models are then applied to various types of phase transformation phenomena that inherently involve elastic and plastic effects. It is noted that some sections of the book are marked as "Optional." These are sections that can be skipped at first reading without losing the main flow of the text and without detracting from the minimum path of topics comprising the basic principles of phase field theory.

Writing this book involved the valued help of many people. We would like to thank all the graduate students in the Department of Materials Science and Engineering at the McMaster University who took MATLS 791 in the Fall of 2009. Their help and advice in editing and proofing the first edition of this book is greatly appreciated. I (NP) would like to thank my wife Photini and sons Spiro and Aristotle for their love and patience during the writing of this book; doing science for a living is fun but their love is what living is actually about. I also suppose thanks are in order to Starbucks Coffee for providing me – at the cost of lots of overpriced bitter coffee – many hours of escape from the mundane administrative environment of a modern university in order that I could work on this book in peace and talk politics with other patrons. I would also like to thank the Technical Research Centre of Finland (VTT) and the Helsinki University of Technology for hosting me during my sabbatical leave in 2009 and for flipping the bill for some of my travels to Helsinki where I also worked on this manuscript and other cool stuff.

As with anything in print, this book very likely contains typos and oversights. We would be delighted to hear from readers about any such errors or omissions. Please do not hesitate to contact us at provata@mcmaster.ca or elder@oakland.edu.

I (KE) would like to thank my wife Nancy, daughter Kate and parents Fay and Stan for the tremendous support they have given me over many years and throughout the writing of this text. In addition I would like to thank Tapio Ala-Nissila and the Helsinki University of Technology (now Aalto University) for providing me the opportunity to give several short courses on phase field and phase field crystal modelling. Some of the material developed for those courses has found its way into the text.

Nikolas Provatas
Ken Elder

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Introduction

1.1
The Role of Microstructure Materials Science

The properties of most engineered materials have a connection with their underlying microstructure. For example, the crystal structure and impurity content of silicon will determine its band structure and its subsequent quality of performance in modern electronics. Most large-scale civil engineering applications demand high-strength steels containing a mix of refined crystal grains and a dispersion of hard and soft phases throughout their microstructure. For aerospace and automotive applications, where weight to strength ratios are a paramount issue, lighter alloys are strengthened by precipitating second-phase particles within the original grain structure. The combination of grain boundaries, precipitated particles, and the combination of soft and hard regions allow metals to be very hard and still have room for ductile deformation. It is notable that the lengthening of span bridges in the world can be directly linked to the development of pearlitic steels. In general, the technological advance of societies has often been linked to their ability to exploit and engineer new materials and their properties.

In most of the above examples, as well as a plethora of untold others, microstructures are developed during the process of solidification, solid-state precipitation, and thermomechanical processing. All these processes are governed by the fundamental physics of free boundary dynamics and nonequilibrium phase transformation kinetics. For example, in solidification and recrystallization – both of which serve as a paradigm of a first-order transformation – nucleation of crystal grains is followed by a competitive growth of these grains under the drive to reduce the overall free energy – bulk and surface – of the system, limited, however, in their kinetics by the diffusion of heat and mass. Thermodynamic driving forces can vary. For example, solidification is driven by bulk free energy minimization, surface energy and anisotropy. On the other hand, strain-induced transformation must also incorporate elastic effects. These can have profound effects on the morphologies and distribution of, for example, second-phase precipitates during heat treatment of an alloy.

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The ability to model and predict materials' properties and microstructures has greatly benefited from the recent "explosion" of new theoretical and numerical tools. Modern parallel computing now allows billions of atoms to be simulated for times on the scale of nanoseconds. On higher scales, various continuum and sharp interface methods have made it possible to quantitatively model free surface kinetics responsible for microstructure formation. Each of these methodologies, however, comes with its advantages and deficiencies.

1.2
Free Boundary Problems and Microstructure Evolution

Solidification has typically served as a paradigm for many classes of nonequilibrium phase transformations that govern the formation of complex microstructure during materials processing. The most commonly recognized solidification microstructure is the tree-like *dendrite* pattern (which comes from the Greek word for tree, "dendron"). The most popular example of a dendrite is a snowflake, which is a single crystal of ice, solidified from water that falls through the sky. Figure 1.1 shows an image of a branch of a snowflake in an organic material known as succinonitrile (SCN) solidifying from its melt. This material is a favorite with researchers because it solidifies at room temperature and is transparent, affording us a good look at the solidification process. It is also often referred to as a "metal analogue" as it solidifies into a cubic crystal structure. Surprisingly, the properties learned from this organic material essentially remain unchanged qualitatively in metals and their alloys. Patterns like the one in Figure 1.1 are not limited to solidification. They are also found in solid-state transformations. Figure 1.2 shows dendrite patterns that emerge when one solid phase emerges from and grows within another. Microstructure modeling involves understanding the physics governing such microstructure formation.

Figure 1.1 A snowflake of succinonitrile, an organic compound that solidified at room temperature. The image shows the characteristic "dendritic" tree-like pattern of the crystal, typical of crystal formation in nearly all anisotropic solids. It is a ubiquitous shape that depends on the physics of reaction–diffusion and the properties of the surface energy between the solid and the liquid. Vincent Proton, McMaster University, 2008.

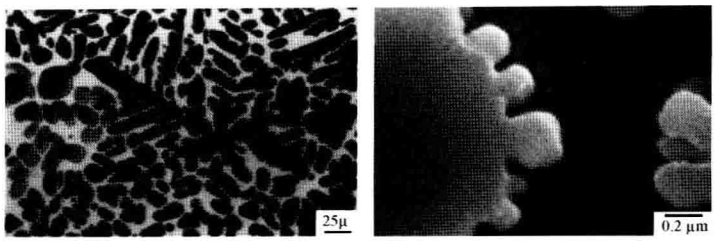

Figure 1.2 *Left*: Solid-state dendrites in an alloy of copper (Cu) and zinc (Zn). *Right*: Dendrite in a nickel-based superalloy, a material commonly used in aerospace because of its very high strength. Reprinted from Refs [1] (left) and [2] (right).

Solidification is at the heart of all metal casting technologies. Figure 1.3 shows a typical layout for casting slabs of steel used in many industries. The basic idea is that a liquid metal alloy enters a region like the one between the rollers in the figure. There the liquid is sprayed with water, which establishes a cooling mechanism that extracts heat from the casting at some rate ($\dot{Q}$). The liquid solidifies from the outer surface inward. The rate at which heat is extracted – that is, the cooling rate – is key to establishing the morphology and scale of the solidification microstructure, as seen in the inset of Figure 1.3. Typical dendrite microstructures in many steel alloys resemble those shown in Figure 1.4. In this situation, the competitive growth and interaction of

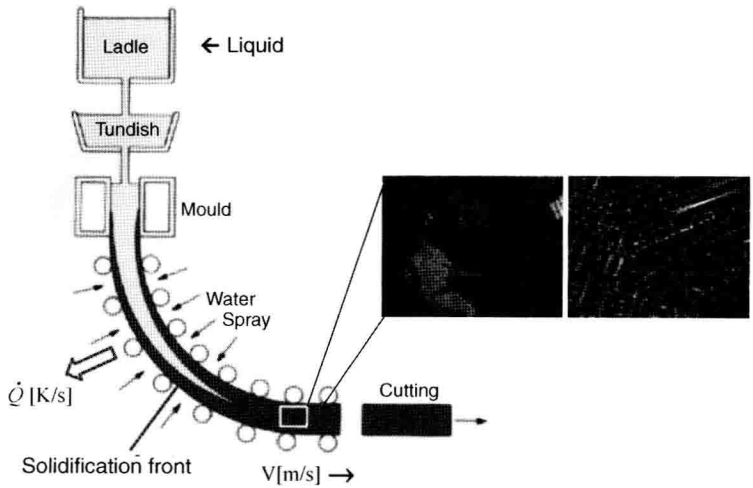

Figure 1.3 Typical industrial layout for thin slab casting. Liquid is entered from top, is cooled by splashing water, and is directed – as it solidifies – at some speed (V) to the right. Most steels will then be cut and thermomechanically treated to improve their strength properties. In spite of the postsolidification treatment that the metal may receive, the so-called "as-cast" structure (inset) that is established initially is always, to some extent, present in the final product.