Crystals, Defects and Microstructures

Materials science has emerged as one of the central pillars of the modern physical sciences and engineering, and is now even beginning to claim a role in the biological sciences. A central tenet in the analysis of materials is the structure–property paradigm, which proposes a direct connection between the geometric structures within a material and its properties.

The increasing power of high-speed computation has had a major impact on theoretical materials science and has permitted the systematic examination of this connection between structure and properties. In this textbook, Rob Phillips examines the various methods that have been used in the study of crystals, defects and microstructures and that have made such computations possible. The author presents many of the key general principles used in the modeling of materials, and punctuates the text with real case studies drawn from recent research. A second key theme is the presentation of recent efforts that have been developed to treat problems involving either multiple spatial or temporal scales simultaneously.

This text is intended for graduate students and researchers in science and engineering with an interest in the theoretical constructs that have been devised to undertake the study of materials.

Crystals, Defects and Microstructures

Modeling Across Scales

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Dedicated to Sonic's accomplices

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Preface

Materials science as a formal discipline has quietly emerged as one of the central pillars of the physical sciences. Whether one interests oneself in the creation of lighter, more durable surfboards, or in the invention of new technologies to free up the traffic jam on the world wide web, in the end, these questions will always imply demands which must be met by new classes of materials.

Though the study of materials is largely rooted in the enlightened empiricism of traditional metallurgy, the advent of high-speed computers and the emergence of robust quantum simulations suggests new engineering strategies in which mechanism-based understanding might be hoped to lead to new materials. As a result of the maturation of theoretical materials science, it has become increasingly possible to identify a corpus of central results which serve as the basis for the analysis of materials. In addition, increasingly complex materials with structures at many different scales have led to the emergence of methods built around the explicit consideration of multiple scales simultaneously. As a result of these advances, this book attempts to take stock of the present capacity for modeling materials, with the word modeling used in the broadest sense.

The book is divided into four basic parts. It opens with an overview of some of the key issues concerning materials that one might hope to succeed in modeling. Special reference is made to the notion of material parameters as characterized by the broad variety of data about materials that may be found in any databook. Though my comments on material response will be rather generic, my efforts to model such response will be restricted almost exclusively to *crystalline* solids. Though I am ashamed to have ignored so many classes of important and interesting materials, in the end, even restricting myself to crystalline materials left me with a project that exceeds my competence. After the introduction to material response, I present something like a modelers toolkit with a review of the key ideas from continuum mechanics, quantum mechanics and statistical mechanics that one might want to bring to the evaluation of a particular problem in the mechanics of materials. My argument here is that these three broad fields of study serve as the cornerstone for the rest of what we will do. The second main section of the book is entitled 'Energetics of Crystalline Solids' and aims to describe the various tools that may be brought to bear on the problem of understanding the properties of perfect crystals. The argument made here is that the understanding we will require later concerning the role of defects in materials will have more impact when measured against the backdrop of the perfect solid. Particular emphasis in chaps. 4–6 is placed on computing the total energies of a given solid and using these energies to deduce the thermal and elastic properties of solids and the structural stability of different materials as revealed by phase diagrams. It should be noted that though I have restricted my attention to crystalline solids, much of what we will say in these chapters can be borrowed without alteration in the context of noncrystalline solids (and even liquids).

Part 3, 'Geometric Structures in Solids: Defects and Microstructures' is organized according to the dimensionality of the various defects that populate materials and considers point defects (chap. 7), line defects (chap. 8) and interfacial defects (chap. 9). The organization of the material along dimensional lines is in the end somewhat artificial, but provides an organizational thread which has been useful to me if not the reader. Once an understanding of these various defects is in hand, I make an attempt at describing the assembly of these defects into a material's microstructure (chap. 10). The final part of the book, 'Facing the Multiscale Challenge of Real Material Behavior', should be seen as the culmination of the efforts set forth in the preceding chapters with the aim being to see just how far the modeler can go in the attempt to concretely consider material behavior. In addition, I have had a go at trying to seek the generic features of those models in which a deliberate attempt has been made to eliminate degrees of freedom. Indeed, my contention is that the enormous current interest in 'multiscale modeling' is born in large part of a self-conscious attempt to construct theories in a way that will lend them computational efficiency. Though there has been an incontrovertible increase in computational power, it has carried with it an attendant perception that almost always our appetite will outstrip our abilities. As a result, modelers throughout the physical sciences have had to seek to reformulate existing theories and to create new ones in a way that is ever mindful of the need to reduce computational burden.

My reasons for writing this book are primarily selfish. I have found that the only way I can really learn something is by self-study, and in particular, by seeking understanding at the level of the details – factors of 2 and π included. I consider myself one of the lucky few, namely, those who are able to earn a living as a college professor. Indeed, my privileges are greater yet. Almost daily I count my good fortune for having landed in the Solid Mechanics group at Brown University. One of the challenges in entering such a group has been to grope my way to some modicum of understanding in the area of the mechanics of materials. This book represents one part of that groping and reflects my own sense of some of the key strategies that may be brought to bear on modeling material behavior. As part of the process of bringing myself up to speed for attempting to write this book, I have also undertaken the writing of a number of review articles with which the perceptive reader will undoubtedly see some overlap. This process was intentional in the hope that by working with various coauthors a useful vision of much of the material included here could be built up. Similarly, many of the ideas set forth here have been tested out in courses given at Brown, Caltech, the National University of Singapore and the Institut National Polytechnique de Grenoble.

My intention in writing this book has not been to produce an encyclopedic compendium of all that is known concerning the modeling of materials and their properties. Rather, I have attempted to consider a sufficiently diverse set of problems to reveal the *habit of mind* that can be brought to the study of materials. Indeed, the book is largely anecdotal, with what I perceive to be fundamental ideas punctuated by more speculative 'case studies' that may not stand the test of time. As a result, the book has mixed character, alternating back and forth between text and monograph mode. In his outstanding book *The Gift of Fire*, Richard Mitchell notes the distinction between *knowing* and *knowing about*. The aims of the present work move back and forth between these objectives, with my hope being that after reading those sections having to do with general principles (and working the corresponding problems), the reader will 'know' these ideas. By way of contrast, the case studies are put forth more in the spirit of 'knowing about' with the hope that such studies will familiarize the reader with the implementation of the general ideas as well as the attendant literature, and will embolden him or her to set out to carry through a detailed case study themselves. I should also note that although many a preface emboldens the reader with the claim that various chapters can be read independently, I have written the present work very much as narrative, with the same idea presented in a different light several (or even many) different times, each contrasted with the other. For example, the discussion on Bridging Scales in Microstructural Evolution in chap. 12 presupposes a knowledge of what has gone before in chap. 10. Though it is true that one can read one without the other, it is certain that the message I wish to convey about microstructure and its evolution can only be gleaned by reading them both. For me, the book was written as a single entity and its logic is intertwined accordingly.

In keeping with this general philosophy, the book is populated by a minimum of numerical tables in which specific data are presented. Rather, I have opted for pictorial and graphical representation of numerical results with the aim being the presentation of trends rather than detailed quantitative insights. On the other hand, there are a number of instances in which I present tables of data, but in the more sympathetic form of pictures. The calculations of the group of Skriver come to mind in this regard since they have done the service of providing the energies of a number of defects (vacancies – fig. 7.15, surfaces – fig. 9.5 and step energies – fig. 9.29) for a whole host of different materials, using the same theoretical analysis in each instance raising the possibility of a meaningful assessment of the trends. In addition, at times I have resorted to presenting collages of experimental data since I often feel it is beyond my competence to bring expert judgement to one experiment vs another and thus leave it to the reader to explore several sources and thereby decide for his or herself. My selection of material is also based in part upon a sinking feeling I sometimes get both while attending meetings and while cranking out the next calculation at my desk: it seems that so much of 'research' (mine included) is slated for obsolescence from the moment of its inception. It has always seemed to me that pedagogy is an ideal litmus test of significance. Is a particular piece of work something that I would want to tell my students? The difficulty in answering this question is further exacerbated by the pedagogical uncertainties that attend the increasing reliance on numerical solutions and computer simulation. How exactly are we to communicate what is being learned from computational approaches? I have tried to follow a basic formula in many of the later chapters in the book. An attempt is first made to illustrate the fundamental principles involved in contemplating a given class of material properties. These generic ideas, which are assumed to be largely uncontroversial, are then illustrated in an iterative fashion with a given case study examined from as many different angles as possible. For example, in discussing structural stability of Si, I make a point of showing how these questions can be addressed both from the perspective of empirical potentials and using first-principles quantum mechanical treatments. Similarly, in my treatment of grain growth, I show how the Potts model, phase field models and sharp interface models may all be used to examine the same basic process. My logic in these instances is to encourage a breadth of perspective filtered by a critical eye that sees the shortcomings of all of these approaches. In the end, this book reflects my quest to unearth some of the exciting developments in the modeling of thermomechanical properties which have the power to either instruct or predict or entertain.

In addition to commenting on what is in this book, it is with a trace of sadness that I also note what is not. With the narrowing of time between a given day of writing and the date of my self-imposed deadline, as well as with the increasingly swollen zip disks and hard copies of my book, it became increasingly clear that I must abandon many of my original intentions and resort to wholesale slashing. It is with particular regret that I eliminated my discussions of thermal conductivity, electromigration, the use of path integral methods to study diffusion and the electronic structure of quantum dots. In the end, I came to the view that I must stop and return to more active daily participation in family, sleep and my own research. I should also note that despite its length, in the end experts will recognize that my book has provided only a caricature of their fields. My aim was to highlight what seemed to me to be either the most general ideas or the most intriguing from each broad area.

A word of explanation concerning references and further reading is in order. Ultimately, I decided to reference the works of others in only two ways. First, the *Further Reading* sections at the end of each chapter make reference only to those books or articles that form a part of my working and thinking vocabulary. Each time reference is made to one of these works, I attempt to provide some editorial comment as to why it has appeared on my list. My taste is idiosyncratic: if given the choice, I will always seek out that author who tells me something other than the party line, who has forged his or her own vision. I hold to this same mean in graduate teaching with the conviction that students are not interested in a watered down regurgitation of what they can read in the textbook – a unique perspective is what interests me.

In addition to the suggestions for further reading, I have also compiled a single bibliography at the end of the book. This list serves an entirely different purpose and there is only a single way to get on it. These books and articles are those from which I have borrowed figures, followed derivations or turned the analysis into a 'case study'. One of my abiding aims has been to try to figure out which part of the work on modeling has earned some level of permanence. Certain models (for example the quantum corral discussed in chap. 2) are pedagogically satisfying and at the same time permit immediate comparison with experiment. This is the ideal situation and, wherever possible, I have attempted to include them. In addition, I have also sought those steps forward that illustrate a certain approach that, in my opinion, should be imitated.

As is evident from the preceding paragraphs, my bibliographic acumen is severely limited. The reference list is not encyclopedic and reflects my taste for browsing the index in a few favorite journals such as *Physical Review B* and *Physical Review Letters*, *Journal of Mechanics and Physics of Solids*, *Metallurgical Transactions A*, *Philosophical Magazine* and *Acta Metallurgica*. I am a particular fan of the 'Overview' sections in *Acta Metallurgica* and the articles written by award recipients in *Metallurgical Transactions*. Further, my choice of references is biased in favor of friends and acquaintances, due largely to the fact that in these instances I have had the benefit of private discussions in order to learn what *really* happened. This is especially true in those cases where I sought a picture to illustrate a concept such as, for example, a polycrystalline microstructure. In these cases, it was most convenient to tap acquaintances, resulting in an over representation of work carried out at Brown. Hence, while my choice of references should be seen as something of an endorsement for those that are here, it should not be seen as a rejection of those that are not.

Another feature of the book deserving of comment is the problem sets that are to be found at the end of each chapter. Many of these problems have already had a tour of duty in the various courses that I have taught at Brown and Caltech. On the other hand, there is a reasonable fraction of these problems that have not seen the light of day before now and thus risk having bugs of various types. The problems come in all types ranging from the fleshing out of material covered in the chapters themselves to the construction of full-fledged computational solutions to problems that are otherwise not tractable.

A few stylistic comments are also in order. For the most part, I have written the book in the first person plural, making constant reference to 'we' this and 'we' that. My reason for selecting this language is an honest reflection of my presumed relation with the reader – I imagine us both, you the reader and me, side by side and examining each question as it arises, almost always in a questioning tone: can we do better? I have reserved the more personal and subjective 'I' for those places where it is really my opinion that is being espoused as, for example, in the sections on *Further Reading*. In addition, the book is written in an informal (and at times light) style with various asides and observations. I fear that I will probably be charged with both flippancy and arrogance, but wish to note at the outset that my hope was to produce a book that was to some extent fun to read. But even more importantly, I have tried to have fun in its writing. Three hours a morning for four years is a lot of hours to sit by oneself and I confess that on many occasions I could not resist certain turns of phrase or observations that amused *me*.

Rob Phillips
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2000

Acknowledgements

As a voracious reader myself, I am a veteran of many a preface and its attendant list of acknowledgements. What I realize now that it is my turn to make such a list is that for one such as me, who owes so much to so many, acknowledgements are deeply felt and yet are probably irrelevant to the anonymous reader. As said above, I wrote this book largely for myself in the hope that I would learn something in the act of so doing. This learning can be divided along two main lines, one emanating from the isolated groping I did at my desk, and the other from the pleasant meaningful interactions I have had with the people it is the business of this section to acknowledge. These paragraphs are for me and my family, my friends and my teachers. To all of you who have taught, tolerated, scolded, encouraged, discouraged, challenged and befriended me, let me state it simply: thank you for enriching my life.

I now see the dangers inherent in making a list of names, but have decided to risk it on the grounds that I wish to express my indebtedness to some people publicly. I am grateful to William Martin and Andrew Galambos who literally opened up a new world of scientific thinking to my teenage mind, and life has never been the same. I am also grateful to Solomon Deressa, Chuck Campbell and Anders Carlsson, all of whom gave me a chance when I probably didn't deserve one, and from whom, I have learned much. It is a pleasure to acknowledge my various friends at Brown from whom I have taken the vast majority of the courses offered in our Solid Mechanics curriculum (B. Freund – Stress Waves, Thin Films; R. Clifton – Advanced Continuum Mechanics; K.-S. Kim – Foundations of Continuum Mechanics; A. Bower – Plasticity; F. Shih – Finite Element Method; C. Briant – Mechanical Properties of Materials; and Mig Ortiz who taught Dislocations in Solids and much else through private consultation). Indeed, the inimitable Professor Ortiz has been the kind of friend and collaborator that one is lucky to find even once. My good fortune at Brown has also been built around the chance to learn from a series of outstanding graduate students and postdocs. Ellad Tadmor, Ron Miller, Vijay Shenoy, David Rodney and Harley Johnson all were a key part of my first five years at Brown and I can only hope they learned a fraction as much from me as I did from them. More recently, I have benefited enormously from my interactions with Nitin Bhate, Dan Pawaskar, Kedar Hardikar and David Olmsted.

As I said above, much of the fun in writing this book came from the interactions I had with others. I must single out Kaushik Bhattacharya, Rick James, Art Voter, Mig Ortiz, Chris Wolverton, Vivek Shenoy and Mark Asta, all of whom need special acknowledgement for running a veritable intellectual babysitting operation. I have also benefited from expert advice on a number of different chapters from Janet Blume, Jane Kondev, Craig Black, Saryn Goldberg, Deepa Bhate, Anders Carlsson, K.-J. Cho, John Jameson, Tim Kaxiras, Stephen Foiles, Fabrizio Cleri, Mark Asta, Chris Wolverton, Art Voter, Luciano Colombo, Ladislas Kubin, Lyle Roelofs, Lloyd Whitman, Clyde Briant, Ben Freund, Dan Pawaskar, Karsten Jacobsen, Perry Leo, Kaushik Bhattacharya, Rick James, Simon Gill, Kevin Hane, T. Abinandanan, Peter Gumbsch, Long-Qing Chen, Georges Saada, Peter Voorhees, Alan Ardell, Emily Carter, Alan Needleman, Sam Andrews, Didier de Fontaine, Jakob Schiotz, Craig Carter, Jim Warren, Humphrey Maris, Zhigang Suo, Alan Cocks, Gilles Canova, Fred Kocks, Jim Sethna, Walt Drugan, Mike Marder, Bob Kohn, and Bill Nix and Mike Ashby indirectly as a result of a series of bootlegged course notes from excellent courses they have given. My book has also been read cover to cover by a number of hearty souls (Ron Miller, David Rodney, David Olmsted, Rob Rudd, Nitin Bhate, Walt Drugan and Bill Curtin) who made immensely useful suggestions that took my manuscript from an infantile performance to something that might be considered presentable. Of course, any errors that remain are strictly my own responsibility and indeed, at several junctures throughout the text, my arguments are suspect. It is also my great pleasure to thank Maryam Saleh who literally sketched, traced, drew and redrew over 300 figures, and Lorayn Palumbo who took care of everything from making sure I didn't forget to teach my class to taking care of all manner of miscellaneous tasks. I am happy to extend my warmest thanks also to Amy Phillips who submitted literally hundreds of requests for permission to reprint figures. I would also like to thank Florence Padgett from Cambridge University Press who has supported me through the various stages of frustration that attended the writing of this book and, similarly, Simon Capelin. I would also like to acknowledge the outstanding editorial efforts of Maureen Storey who suggested all manner of improvements. The opportunity to write this book was supported generously through my wonderful NSF Career Award.

As will be evident to any reader of my book, I have tried to present as many of my conclusions as possible in pictorial form. The task of amassing the various figures that form the backbone of this work was lightened enormously by the generous help of many friends, namely, Sharvan Kumar, Mike Mills, Peter Voorhees, Dan Fridline, Allan Bower, Alan Schwartzman, Harley Johnson, Karsten Jacobsen, Jakob Schiøtz, Rolf Heid, Rajiv Kalia, Sanjay Kodiyalam, Rick James, Kedar Hardikar, Dan Pawaskar, Charles McMahon, Vasily Bulatov, David Vanderbilt, Ralf Mueller, Lindsey Munro, Luciano Colombo, Tomas de la Rubia, George Gilmer, Christophe Coupeau, Marc Legros, Kevin Hemker, Sean Ling, Ian Robertson, Torben Rasmussen, Nasr Ghoniem, Klaus Schwarz, Marc Fivel, Bill Gerberich, David Rodney, Vivek Shenoy, Hans Skriver, Lloyd Whitman, Furio Ercolessi, Martin Bazant, Dieter Wolf, David Seidman, Craig Carter, Eric Chason, Stuart Wright, Brent Adams, Bob Hyland, Subra Suresh, Clyde Briant, Alan Ardell, Mitch Luskin, Liz Holm, Simon Gill, T. Abinandanan, Long Chen, Michael Ortiz (da Mig), Eberhard Bodenschatz, Art Voter, Chris Roland, Chris Wolverton, Charles-Andre Gandin, Michel Rappaz, Nik Provatas, John Hamilton, Farid Abraham, Harry Bhadesia and David Clarke. Thank you all again.

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Notes on Units, Scales and Conventions

In the chapters to follow, one of our aims is to try to recast many of our results in numerical form, giving an impression of the many interesting scales (length, time, energy, stress, etc.) that arise in discussing solids. A prerequisite to such discussions is to make sure that a correspondence has been constructed between the units favored here and those encountered in the everyday experience of the reader.

Geometric and Structural Notions. One of the most significant single ideas that will appear in what follows is the important role played by geometric structures at a number of different scales within materials. Indeed, the coupling between structure and properties is an element of central orthodoxy in materials science. In characterizing the structures within materials, it is clearly overly pedantic to hold to any single set of units for characterizing such structures, and we will comfortably interchange between a few different units of measure. The smallest scales that we will touch upon are those tied to the existence of atoms and their arrangements to form crystalline solids. Two fundamental units of length are most popular in this setting, namely, the ångstrom (1 Å $=$ 10^{-10} m) and the Bohr radius ($a_0 \approx 0.529\,177 \times 10^{-10}$ m). The ångstrom should be seen as a member in the series of scales which are all simple factors of 10 away from the meter itself. On the other hand, the Bohr radius arises as a natural unit of length in assessing atomic-scale processes since it is built up as a combination of the fundamental constants characterizing these processes, namely, $a_0 = \hbar^2/m_e e^2$, where $\hbar$ is Planck's constant, m_e is the mass of the electron and e is the charge on an electron.

We will also occasionally resort to the use of nanometers (1 nm $= 10^{-9}$ m) as an alternative unit of length when characterizing atomic-scale processes. When characterizing structures at the microstructural level, we will try to hold to a single unit of length, the micron (1 μm $= 10^{-6}$ m). Note that a human hair has dimensions on the order of 50 μm. The use of both nanometers and microns will be seen as characteristic of the dimensions of many structural features such as precipitates and inclusions as well as the grains making up polycrystals. In our ambition of providing meaningful geometric classifications of solids, it will also be necessary to make reference to units of area and volume, both of which will be reported either using ångstroms or meters as the base unit, resulting in either Å^2 or m^2 for areas and Å^3 or m^3 for volumes.

Time Scales and Temporal Processes. One of our recurring themes in the pages to follow will be the role of disparate scales in characterizing processes and structures within materials. In addition to the diversity of spatial scales, there are a host of processes in solids which are themselves characterized by widely different time scales. As a result, we will be forced to adopt a series of different measures of the passage of time. One of the elemental processes in solids that will occupy much of our attention is that of the vibrations of solids. As will become evident in later chapters, atomic vibrations are characterized by frequencies on the order of 10^{13}–10^{14} Hz, which corresponds to a time scale on the order of one-tenth of a picosecond. As a result, we will make use of both 1.0 fs $= 10^{-15}$ s and 1.0 ps $= 10^{-12}$ s in describing atomic motions.

Force and Energy. Just as with the characterization of the various geometric structures that populate solids we will stick to a few standard units of measure: we will adopt a strategy of characterizing the various measures of force, stress and energy in terms of a few basic units. The two units of force that will occupy centerstage in the pages that follow are the standard MKS unit, the newton, and the less familiar choice of eV/Å (eV is a unit of energy) which is much more representative of the types of forces that arise in characterizing atomic-scale motions. When translated into units of stress, we will find it advantageous again to adopt two distinct sets of units, namely, the MKS unit of stress, the pascal (1 Pa $=$ 1 N/m^2) and the atomic-scale analog, eV/Å^3. In addition, we will find it convenient to interchange between units of energy reported in both joules and electron volts (eV). In particular, we recall that the conversion between these two sets of units is given by 1.0 eV $\approx 1.602 \times 10^{-19}$ J. On the other hand, from time to time we will also invoke the rydberg as a unit of energy. This unit of energy arises naturally in characterizing the energy levels of atoms and can be expressed in terms of fundamental constants as Ry $= me^4/2\hbar^2$. Note that the conversion between Ry and eV is, 1 Ry $=$ 13.6058 eV. In our analysis of activated processes, we will repeatedly find it advantageous to reckon our energies in dimensionless form, where the energy scale is determined by $k_B T$, here $k_B \approx 1.38 \times 10^{-23}$ J/K is Boltzmann's constant. We note that a useful rule of thumb is that for room temperature, $k_B T \approx 1/40$ eV. For the remainder of the book, we will suppress the subscript on k_B.

Material Parameters. The key means whereby material specificity enters continuum theories is via phenomenological material parameters. For example, in describing the elastic properties of solids, linear elastic models of material response posit a linear relation between stress and strain. The coefficient of proportionality is the elastic modulus tensor. Similarly, in the context of dissipative processes such as mass and thermal transport, there are coefficients that relate fluxes to their associated driving forces. From the standpoint of the sets of units to be used to describe the various material parameters that characterize solids, our aim is to make use of one of two sets of units, either the traditional MKS units or those in which the eV is the unit of energy and the ångstrom is the unit of length.

Conventions. During the course of this work we will resort to several key conventions repeatedly. One important example is that of the summation convention which instructs us to sum on all repeated indices. For example, the dot product of two vectors may be written

$$\mathbf{a} \cdot \mathbf{b} = a_1 b_1 + a_2 b_2 + a_3 b_3 = a_i b_i. \quad (1)$$

A second key notational convention that will be invoked repeatedly is the definition of the dyadic product given by $(\mathbf{a} \otimes \mathbf{b})\mathbf{v} = \mathbf{a}(\mathbf{b} \cdot \mathbf{v})$. Another key convention that will be used repeatedly is the notation that $\{a_i\}$ refers to the set $a_1, a_2, \ldots, a_N$. When carrying out integrations, volumes will typically be denoted by Ω while the boundary of such a volume will be denoted as $\partial\Omega$.