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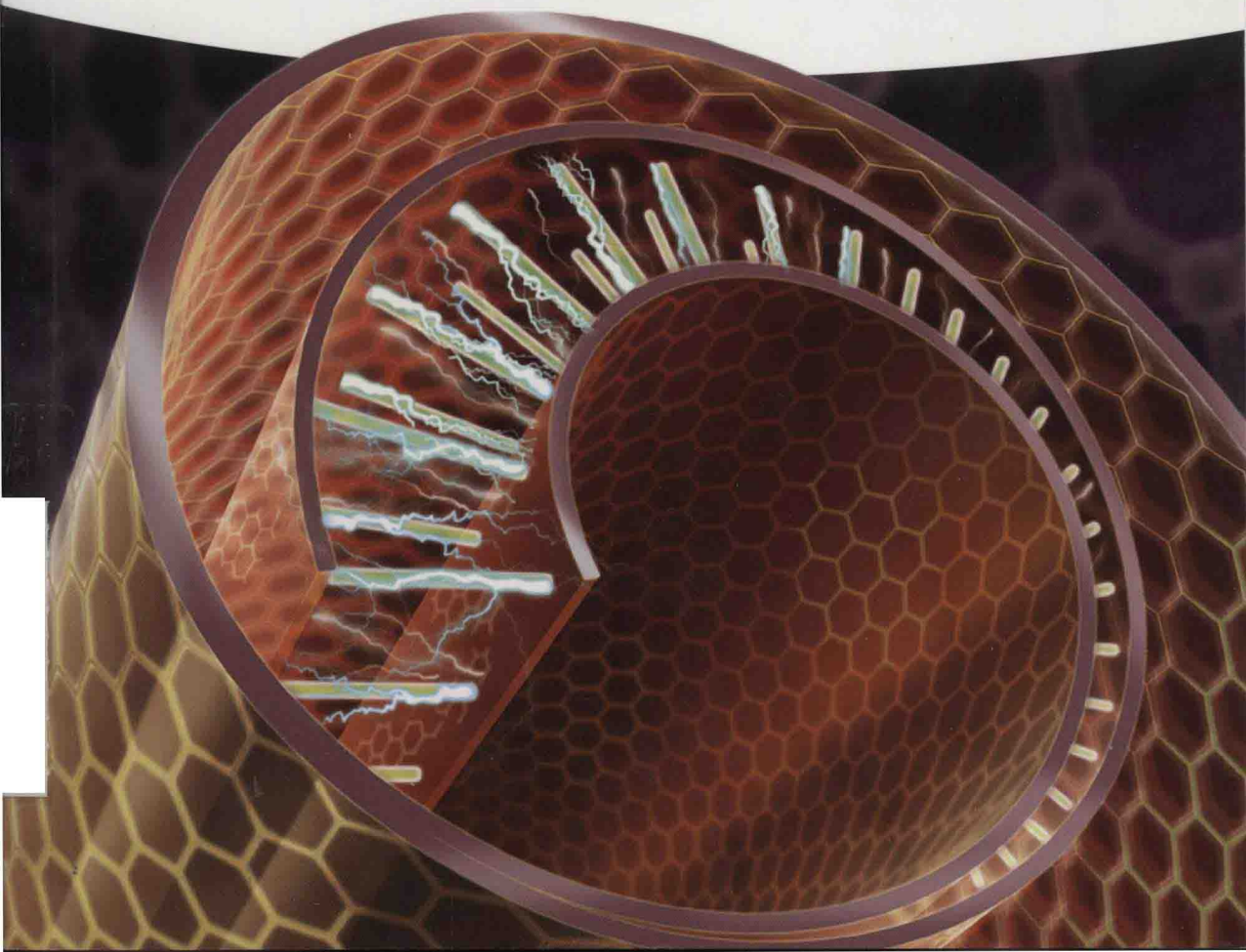
In Silico Materials Design

Modern Atomistic Simulation Methods for Engineers



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Preface

In many academic and industrial R&D projects, physicists, chemists and engineers are working together. In particular, the development of advanced functionalized materials requires an interdisciplinary approach. In the last decades, the size of common devices and used material structures has become smaller and smaller. This has led to the emergence of the so-called nanotechnology, that is, a technology that uses material systems with an extent of less than several hundred nanometers. The enormous technical advances in this field are subject to two mutually amplifying effects. On the one hand, modern experimental techniques have been developed that allow the observation, manipulation, and manufacturing of materials at an atomic length scale with an industrially relevant production rate. On the other hand, the enhancements in the computer technology have led to a tremendous growth of the scientific field of computational material sciences. Nowadays, modern simulation methods are indispensable for the design of new and functionalized nanomaterials. They are essential to understand the chemical and physical processes beyond many macroscopic effects.

However, the basic concepts of modern atomistic simulation methods are not very well established in common engineering courses. Furthermore, the existing literature either deals with very specific problems or is at a very deep physical or mathematical level of theory. Therefore, the intention of this book is to give a comprehensive introduction to atomic scale simulation methods at a basic level of theory and to present some recent examples of applications of these methods in industrial R&D projects. Thereby, the reader will be provided with many practical advices for the execution of proper simulation runs and the correct interpretations of the obtained results.

For those readers who are not familiar with basic modern mathematical and physical concepts, Part I will give a rough introduction to Newtonian and quantum mechanics, thermodynamics, and symmetry-related properties. Furthermore, necessary mathematical concepts will be introduced and the reader will be provided with the denotation and terminology that will be used later on. Readers with a fundamental physical and mathematical knowledge may skip this part and look up certain aspects later, if it is necessary.

Part II gives a brief introduction to important aspects of state-of-the-art atomic scale simulation techniques. In particular, the basics of classical and reactive

force field methods, the density functional and Hartree–Fock theory, as well as multiscale approaches will be discussed. Possible fields of application will be depicted, and limitations of the methods are illustrated. Furthermore, several more advanced methods, which are able to overcome some of these limitations, will be shortly mentioned. The intention of this part is to enable the reader to decide which simulation method (with which limitations) would be optimal to investigate a certain problem of interest.

The last part illustrates possible application scenarios of atomic scale simulation techniques for industrially relevant problems. It is divided into three chapters that consider three different industrial fields: microelectronics, chemical processes, and nanotechnology. Real industrial problems and the corresponding contributions of atomic scale simulations will be presented to the reader. Thereby, the set up, the execution, and the analysis of the results will be discussed in detail, and many practical hints for potential users of atomic scale simulations are provided.

Chemnitz
April 2015

Roman Leitsmann

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Part I
Basic Physical and Mathematical Principles

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1
Introduction

The scope of this part is to provide the reader with basic physical and mathematical principles that are necessary to understand the discussions in the following chapters. Furthermore, a notation is introduced, which will be utilized throughout the remaining book. No special previous knowledge is required from the readership. Nevertheless, a basic scientific knowledge is advantageous. Part I makes no claim to provide a complete overview. Many things can be discussed only very briefly. For a more detailed description of special topics and background information, the readers are provided with suitable references.

Those readers who are already familiar with the physical and mathematical concepts can skip this part and look up certain points later if necessary.

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2
Newtonian Mechanics and Thermodynamics

Classical or Newtonian mechanics describes the motion of objects, from small particles to astronomical objects. Newtonian mechanics provides extremely accurate results as long as the domain of study is restricted to macroscopic objects and velocities far below the speed of light. When the objects being dealt with become sufficiently small, it becomes necessary to include quantum mechanical effects (see Chapter 4). In the case of velocities close to the speed of light, classical mechanics has to be extended by special or general relativity.

The following section introduces the basic concepts of classical Newtonian mechanics and its application to atomistic objects. At the end of this section, a critical discussion about the restrictions of this approach is given.

2.1
Equation of Motion

Quite often, objects are treated as point particles, that is, objects with negligible size. The motion of a point particle is characterized by a small number of parameters: its position, its mass, and its momentum.

> **Note:** In reality, all objects have a nonzero size. However, often, they can be treated as point particles, because effects related to the finite size are either not of interest or have to be described by more sophisticated theories such as quantum mechanics.

The position of a point particle $\mathbf{r}$ can be defined with respect to an arbitrary fixed reference point $\mathbf{R}_0$ in space.[1] In general, the point particle does not need not be stationary relative to $\mathbf{R}_0$, so $\mathbf{r}$ is a function of the time t

$$\mathbf{r} = \mathbf{r}(t). \tag{2.1}$$

1) Classical mechanics usually assumes an Euclidean geometry [1] accompanied by a certain three-dimensional coordinate system. For simplicity, we use in this book a simple Cartesian coordinate system.

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Without loss of generality, the reference point can always be assumed to be at the origin of the used coordinate system, that is,

$$\mathbf{R}_0 = (0, 0, 0). \tag{2.2}$$

Note: The position of the point particle and all similar quantities are three-dimensional vectors. They must be dealt with using vector analysis. They will be denoted by

$$\mathbf{r}(t) = (x(t), y(t), z(t)),$$

where x, y, and z are the Cartesian coordinates of the point particle.

The velocity $\mathbf{v}$, or the rate of change of position with time, is defined as the derivative of the position with respect to the time

$$\mathbf{v} = \frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t} \equiv \dot{\mathbf{r}}. \tag{2.3}$$

The acceleration, or rate of change of velocity, is the derivative of the velocity with respect to time (the second derivative of the position with respect to time)

$$\mathbf{a} = \frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} \equiv \dot{\mathbf{v}} = \ddot{\mathbf{r}}. \tag{2.4}$$

The acceleration can arise from a change with time of the magnitude of the velocity or of the direction of the velocity or both.

Note: If only the magnitude $\mathrm{v} = |\mathbf{v}|$ of the velocity decreases, this is sometimes referred to as deceleration, but generally, any change in the velocity with time, including deceleration, is simply referred to as acceleration.

As we all know from our everyday life, an acceleration of an object requires the action of a force on it. Sir Isaac Newton was the first who mathematically described this relationship, which is known today as *Newton's second law*[2)]

$$\mathbf{F} = \frac{\mathrm{d}\mathbf{p}}{\mathrm{d}t} = \frac{\mathrm{d}(m\mathbf{v})}{\mathrm{d}t} = m\mathbf{a}. \tag{2.5}$$

The quantity $\mathbf{p} = m\mathbf{v}$ introduced in this equation is called (canonical) momentum. The force acting on a particle is thus equal to the rate of change of the momentum of the particle with time.

As long as the forces acting on a particle are known, Newton's second law is sufficient to completely describe the motion of the particle. Hence, written in a slightly different form, it is also called *equation of motion*

$$\dot{\mathbf{p}} = m\mathbf{a} = \sum_i \mathbf{F}_i, \tag{2.6}$$

2) The last identity is only true in cases where the mass m of the particle is constant.