Chapter 1

Introductory Chapter: Molecular Dynamics: Basic Tool of Nanotechnology Simulations for "Production 4.0" Revolution

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Additional information is available at the end of the chapter

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1. Introduction

One of the main tasks of the modern industrial revolution "Production 4.0" is the translation of all processes preceding the actual receipt of a new product in a digital representation. Forecasts for the development of this stage of production point to the ever-increasing value of computer modeling, the urgency of which will constantly increase. It is expected that computer modeling will be invested more financial and intellectual resources. This is especially relevant for one of the main tasks of the industrial revolution "Production 4," called "designing materials with controlled properties," which is the basis for the development of effective biotechnologies and nanotechnologies. A full and exact solution to this complex problem is impossible without considering the properties and processes of the formation of materials with controlled properties at the atomic and nanoscale of mathematical description and modeling.

However, specific feature of the physical processes in nanoscale systems is that the key phenomena determining the behavior of a nanoscale system in real time at the macroscale take place at small space and time scales [1, 2]. Many experimental and theoretical studies have shown that the properties of a nanoscale system depend not only on the properties of its constituent elements but also on the regularities of the spatial arrangement of the nanoelements in nanosystem and the parameters of the nanoelements interaction.

In this perspective, the molecular dynamics, which allows to describe the formation, evolution, and properties of the above-mentioned nanosystems in a sufficiently complete and precise manner, should become one of the methods for calculating and modeling modern

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engineers and technologists. This is explained by the fact that molecular dynamics, being a powerful tool of scientific research, is increasingly becoming a full-fledged stage in obtaining new materials, creating a new technological process and designing a new product at the nanoscale level. This process was observed in the 1960–1980s of the last century with respect to the finite element method and led to the fact that this method is now being applied well and confidently by modern engineers and technologists in the creation of new materials and machines. We can expect that the process of industrial revolution "Production 4.0" method of molecular dynamics will be adopted as an instrument of engineers and technologists.

However, this will only be the beginning of a deeper penetration of modeling into digital production. It should be noted that, at present, in modern scientific research methods of modeling, the molecular dynamics is usually the key element of a more complex and comprehensive multilevel mathematical modeling comprising multiple spatial and temporal scales [3–5]. The main stages of such a multi-level modeling of nanosystems are quantum modeling, molecular dynamics, mesomechanics and continuum mechanics.

The calculation of the configurations of a molecular formation, which are the constituents of a nanoparticle, is based on the quantum mechanics ("ab initio") methods of modeling. These methods give the most complete and precise presentation of nano-objects and take into account quantum effects, but they are very intensive computationally. At present, the use of the quantum mechanics methods for the calculation of nanoscale systems is limited to 1000–2000 atoms composing a nanoscale system.

The modeling of the coalescence of molecules into nanoelements can be performed by the molecular dynamics method. The method allows to consider systems containing up to 10 million atoms and more than that, but it does not take into account quantum phenomena.

The calculation of the movement of nanoelements and their coalescence is the task for mesodynamics. The characteristic feature of mesodynamics is the simultaneous use of the methods of molecular and classical dynamics.

It should also be noted that a number of phenomena, in particular, the phenomena taking place at the final stages of the nanoscale system formation, can be considered within the framework of continuum mechanics.

Each of the above methods has its own advantages and limitations. The use of any of the above methods of modeling or their combination for specific nanotechnology problems depends on the calculation accuracy required.

One can point to a number of problems of such modeling listed below:

- multiscale nature and connectedness of problems,
- large number of variables,
- variation of scales both over space and in time,
- characteristic times of processes at different scales differ by orders of magnitude,
- variation of the problem variables at different scales of modeling,

- matching of boundary conditions at the transition from one modeling scale to another when the problem variables are changed,
- stochastic behavior of nanoscale systems.

Molecular dynamics allows us to proceed correctly from the study of atomic and molecular processes by methods of quantum mechanics to the study of processes at the macrolevel by the methods of continuous medium mechanics. The main problem here is the matching of the boundary conditions of the modeling problems at each space-time scale.

Thus, we can distinguish two main functions of molecular dynamics:

- the method of modeling the processes of nanosystem formation and theoretical analysis of their properties
- the bridge connecting the various stages of multilevel modeling of nanosystems.

Based on the foregoing, the purpose of this book is to describe a number of problems in the modeling of nanosystems and a detailed exposition of the application of molecular dynamics methods to problems from various fields of technology: material science, the formation of composite molecular complexes, transport of nanosystems, etc. The book summarizes the research results of the authors in the field of modeling of various nanosystems: soft supramolecular nanostructures, nano-sized beams of single-crystal Cu, metallic nanosized crystals, drug delivery systems, and systems stabilized by hydrogen bonds.

The study of the materials of this book can be the beginning of the reader's study of the whole complex of modeling based on the concept of molecular dynamics modeling.

In addition, it should be noted that the research materials dynamics methods presented in the book can be the basis for the development of artificial intelligence methods in relation to the problem "designing materials with controlled properties."

To get more complete information about the methods of molecular dynamics and its significance in the overall complex multilevel task of modeling nanosystems and nanomaterials, the novice reader can get additional information from the list of literature. In this list of papers and books, the works [6–23] to modeling by methods of quantum mechanics, works [24–31] to molecular dynamics, and works [32, 33] to mesodynamics are devoted.

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