

# Lecture Notes in Nanoscale Science and Technology

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# Nonregular Nanosystems

Theory and Applications



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# Preface

A tremendous shift in the emphasis of interests in physics and chemistry of condensed matter towards nanoscale systems has shaken the scientific community in recent years. Experimental research technologies in physical and chemical laboratories all over the world have considerably expanded, with fundamental studies of new classes of materials and phenomena occupying a prominent place. New features of nanomaterials have become a core challenge for theoretical physics, condensed matter physics, computational methods and modelling.

The 1950s–1960s can be considered as the period of emergence of interest in amorphous solids. Since that time, the molecular structure of liquids, amorphous semiconductors, polymer solutions, magnetic phase transitions, electrical and optical properties of liquid metals, the glassy state of matter, disordered alloys, metal vapours and many other systems have provoked scientific and technological inquisitiveness. Brilliant advances in the field of crystalline solids, both in theory and technology, have inspired the desire to obtain the same results in electronics by means of even more efficient technological processes. One example is the effort to replace the relatively long crystal growth process with thin-film deposition or the rapid cooling of melts.

At the same time, the problem of morphological repeatability of the created materials is highly important. Significant interest in disordered materials was justified by the practically proven determinant role of the so-called short-range order with a characteristic size of  $10^{-8}$ – $10^{-9}$  m. Indeed, the electronic structures of amorphous and crystalline solids are very similar. Thus, amorphous silicon, as a basic structure, has become the foundation for the development of optoelectronics and solar cells.

New technological breakthroughs can be associated with research on carbon nanotubes. Scientific and practical interest in these nanostructures was initiated by Sumio Iijima in 1991 (**1991** *Nature* **354**(6348)). However, the key fundamental works of L.V. Radushkevich and V.M. Lukyanovich (**1952** *J Phys Chem* **16**(1) 89, USSR) with clear images of 50 nm diameter tubes should also be mentioned. Furthermore, the works of A. Oberlin, M. Endo and T. Koyama (**1976** *Journal of*

*Crystal Growth* **32**(3) 335) followed in which hollow tubes of rolled up graphite sheets synthesized by a chemical vapour-growth technique were observed.

Significant progress was associated with the discovery of graphene by Kostya Novoselov and Andre Geim (**2004** Novoselov K S, Geim A K et al. *Science* **306** (5696) 666–9, *Nobel Prize in Physics* **2010**). And again, the first theoretical and technological achievements were connected with ‘ideal’, i.e. regular, structures with typical dimensions  $\sim 1$  nm.

Other regular carbon-based structures were also researched, for example, fullerenes (*buckyballs*) which were first generated in 1985 by Harold Kroto, James R Heath, Sean O’Brien, Robert Curl and Richard Smalley (**1985** Kroto H W et al. *Nature* **318** (6042) 162–3) at Rice University.

Similar regular nanosystems were created on a non-carbon basis, e.g. BCN nanotubes (**1994**), boron nitride nanotubes, a polymorph of boron nitride (**1994–1995**), DNA nanotubes (**2004–2005**), gallium nitride nanotubes (**2003**), silicon nanotubes (**2000**), inorganic nanotubes/tungsten(IV) sulphide nanotubes (**1992**), membrane nanotubes (**2008**), titania nanotubes (**2008**), etc.

Two-dimensional materials also received intensive development. Starting with graphene (**2004**), further research turned up graphyne, borophene, germanene, silicene, stanene, phosphorene, molybdenite, single-atom metal layers of palladium and rhodium, etc.

However, it soon became clear that to realize the unique physical and chemical properties of new materials, their functionalization was necessary. It implied, for example, the creation and use of various interfaces, with new nanophenomena corresponding to new non-regular nanostructures. Moreover, nanoeffects with the participation of biological nano-objects open the way for the realization of catalytic reactions and, accordingly, the creation of new nanoscale devices. In this case, we encounter nanophenomena in irregular nanosystems, which is the subject of many sections of this book.

At present, applied and commercial interest encompasses carbon nanotubes, graphene, dendrimers, fullerenes, nanofibers, nanocellulose, nanoclays, nanodiamonds, nanowires and quantum dots (silicon oxide nanoparticles). Interest also focuses on a wide range of nanoparticles, namely, aluminium oxide, antimony tin oxide, bismuth oxide, cerium oxide, cobalt oxide, copper oxide, gold, iron oxide, magnesium oxide, manganese oxide, nanosilver, nickel, titanium dioxide, zirconium oxide and zinc oxide, as well as other nanomaterials including nanoprecipitated calcium carbonate, graphene and carbon quantum dots, hydroxyapatite nanoparticles, palladium/phosphorene,  $C_2N$ , carbon nitride, germanene, graphdiyne, graphane, hexagonal boron nitride, molybdenum disulphide ( $MoS_2$ ), rhenium disulphide ( $ReS_2$ ), diselenide ( $ReSe_2$ ), silicene, stanene/tinene and tungsten diselenide.

Within the format of the present book, the authors consider it necessary to discuss the social and technological challenges of nanotechnology. Although advances in the fields of nanoscience and nanotechnology have resulted in thousands of consumer products that have already migrated from laboratory benches onto store shelves and e-commerce websites, the general public often lacks

awareness and understanding of the basic properties, and sometimes even the existence, of nanotechnologies and their implications for the consumption of nanoproducts. Areas of research at the intersection of nanotechnology and biotechnology, including food, healthcare and environmental issues, elicit complex debates within society today. Moreover, current developments in scientific and technological research raise a number of ethical questions and the potential for fragmenting of responsibility. Therefore, one of the chapters of the book (Chap. 11) is devoted to nanomaterial consumers, managers, education practitioners, students–researchers, manufacturers, work health and safety practitioners and other interested people who need to understand the benefits and hazards of engineered nanomaterials.

It is clear that to discuss all of the problems and results of scientific research in physics and chemistry of irregular systems within one book is practically impossible. However, the concept of non-regularity can be fundamental for a deeper understanding of the key properties of nanoscale systems. Structural imperfections of nanomaterials, and the non-stationary nature of many nanoprocesses, determine the functionality of potential nanoscale devices.

There is hope that many specific materials and observed phenomena will allow us to grasp the general theoretical and mathematical principles of a unified theory.

Some reliable and attractive theoretical results, for example, related to models of perfect nanostructures such as carbon nanotubes, graphene, fullerenes, etc., do not solve the problems of the general theory of non-regular nanosystems associated with their diverse interfaces and the specific tasks of their functionalization.

Apparently, the theory of non-regular nanosystems should be considered as part of the general theory of disordered systems, which itself has not yet developed as a unified theory and contains a multitude of phenomenological constructions.

This book focuses on specific verified results obtained by instruments of theoretical physics, computer simulations and the analysis of experiments. However, some results should be considered tentative. The ways of creating new unique nanodevices are very complex and consist of numerous stages. A new nanophenomenon does not always give way to a new nanodevice.

Our goal also extends to showing the connection of phenomena in non-regular nanosystems with the basic characteristics of various theoretical model systems. In this context, we discuss the limitations of theoretical models as well. In some cases, excessive idealizations that simplify the mathematical description can lead to inexplicable artefacts and imaginary false coincidences with experiments. References to the specific results of numerous studies do not claim to be complete, because the data of experiments are too numerous, sometimes contradictory, and since the conditions of the experimental protocols are not always comparable and require special attention and analysis.

The present book is not a textbook. However, the reader will find consistently outlined subjects of the educational value, which have been methodologically verified by the experience of presenting university lectures at different levels and making reports at international conferences.

It may be impossible in the theory of non-regular disordered systems to find such a powerful principle as the Bloch theorem in regular condensed materials.

Descriptions of the type of scaling theory, percolation theory or similarity theory are not free from essential empirical parameters and can hardly fulfil the role of a universal theoretical tool in the case of non-regular systems. One can only rely on the search for adequate topological transformations of regular morphological systems into non-regular ones. Obviously, this is not a trivial task.

The materials for the book are selected based on many years of scientific work of the authors and their numerous topical researches. For a comfortable comprehension of the content, the insights into the standard university course in theoretical physics will be enough for the reader. Some sections of the book are conceptual in nature and address specialists covering a wide profile in the fields of nanotechnology and nanoelectronics. However, many theoretical and experimental research results lie in the plane of mixed scientific trends. Unfortunately, the bibliography of any book can never reflect all of the relevant literature to date. The bibliography is huge and the rate of its growth is ruthless in relation to the author of any book on such a dynamic topic. We apologize in advance to any colleague whose publication we did not cite.

The conceptual approaches to the content of this book have evolved over the past few years. This is a generalization of a long-term research experience of the authors and their continual scientific cooperation with colleagues coming from the *Institute of Solid State Physics, University of Latvia* (Riga, Latvia), *Avionics Institute of Riga Technical University* (Riga, Latvia), *Faculty of Physics, Vilnius University* (Vilnius, Lithuania) and *Laboratori Nazionali di Frascati INFN* (Frascati-Rome, Italy). Obviously, participation in numerous international conferences, workshops and seminars enriched knowledge and experience; allowed putting the necessary accents in the direction of nanotechnology development; and simply gave pleasure in sharing ideas with colleagues. At the same time, this book is undoubtedly the authors' views on the problems under consideration.

The authors are also indebted to the technical editor of the book, *Natalia Burlutskaya*, and express their warm gratitude for her assistance in many practical problems that had to be resolved in a timely manner and which made it possible to bring this publication to print.

On behalf of the authors Yuri Shunin

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