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Physics-Based Mathematical Models for Nanotechnology

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In November 2007, some of the world's best nanoscientists and nanoengineers met at the Banff Centre, where the Banff International Research Station hosted a workshop on recent developments in the mathematical study of the physics of nanomaterials and nanostructures. The Banff International Research Station for Mathematical Innovation and Discovery (BIRS) is a collaborative Canada–US–Mexico venture that provides an environment for creative interaction as well as the exchange of ideas, knowledge, and methods within the Mathematical Sciences, with related disciplines and with industry. The research station is located in a scenic part of Alberta, Canada and is supported by Canada's Natural Science and Engineering Research Council (NSERC), the US National Science Foundation (NSF), Alberta's Advanced Education and Technology, and Mexico's Consejo Nacional de Ciencia y Tecnología (CONACYT). We would like to thank the BIRS and its sponsors for the given opportunity and the BIRS staff for their excellent support during the workshop.

Nanotechnology is the study and application of phenomena at or below the dimensions of 100 nm and has received a lot of public attention following popular accounts such as in the bestselling book by Michael Crichton, Prey. It is an area where fundamental questions of applied mathematics and mathematical physics, design of computational methodologies, physical insight, engineering and experimental techniques are meeting together in a quest for an adequate description of nanomaterials and nanostructures for applications in optoelectronics, medicine, energy-saving, bio- and other key technologies which will profoundly influence our life in the 21st century and beyond. There are already hundreds of applications in daily life such as in cosmetics and the hard drives in MP3 players (the 2007 Nobel prize in physics was recently awarded for the science that allowed the miniaturization of the drives), delivering drugs, high-definition DVD players and stain-resistant clothing, but with thousands more anticipated. The focus of this interdisciplinary workshop was on determining what kind of new theoretical and computational tools will be needed to advance the science and engineering of nanomaterials and nanostructures.

Thanks to the stimulating environment of the BIRS, participants of the workshop had plenty of opportunity to exchange new ideas on one of the main topics of this workshop—physics-based mathematical models for the description of low-dimensional semiconductor nanostructures (LDSNs) that are becoming increasingly important in technological innovations. The main objective of the workshop was to bring together some of the world leading experts in the field from each of the key research communities working on different aspects of LDSNs in order to (a) summarize the state-of-the-art models and computational techniques for

modeling LDSNs, (b) identify critical problems of major importance that require solution and prioritize them, (c) analyze feasibility of existing mathematical and computational methodologies for the solution of some such problems, and (d) use some of the workshop working sessions to explore promising approaches in addressing identified challenges. With the possibility of growing practically any shape and size of heterostructures, it becomes essential to understand the mathematical properties of quantum-confined structures including properties of bulk states, interface states, and surface states as a function of shape, size, and internal strain. This workshop put strong emphasis on discussions of the new mathematics needed in nanotechnology especially in relation to geometry and material-combination optimization of device properties such as electronic, optical, and magnetic properties. The problems that were addressed at this meeting are of immense importance in determining such quantum-mechanical properties and the group of invited participants covered very well all the relevant disciplines in the cross-disciplinary research area: low-dimensional semiconductor nanostructures.

Since the main properties of two-dimensional heterostructures (such as quantum wells) are now quite well understood, there has been a consistently growing interest in the mathematical physics community to further dimensionality reduction of semiconductor structures. Experimental achievements in realizing one-dimensional and quasi-zero-dimensional heterostructures have opened new opportunities for theory and applications of such low-dimensional semiconductor nanostructures. One of the most important implications of this process has been a critical re-examining of assumptions under which traditional quantum mechanical models have been derived in this field. Indeed, the formation of LDSNs, in particular quantum dots, is a competition between the surface energy in the structure and strain energy. However, current models for bandstructure calculations use quite a simplified analysis of strain relaxation effects, although such effects are in the heart of nanostructure formation. By now, it has been understood that traditional models in this field may not be adequate for modeling realistic objects based on LDSNs due to neglecting many effects that may profoundly influence optoelectronic properties of the nanostructures. Among such effects are electromechanical effects, including strain relaxation, piezoelectric effect, spontaneous polarization, and higher order nonlinear effects. Up to date, major efforts have been concentrated on the analysis of idealized, isolated quantum dots, while a typical self-assembled semiconductor quantum dot nanostructure is an array (or a molecule) of many individual quantum dots sitting on the same `substrate' known as the wetting layer. Each such dot contains several hundred thousand atoms. In order to account for quantum effects accurately in a situation like that, attempts can be made to apply ab initio or atomistic methodologies, but then one would face a task of enormous computational complexity in solving a large-scale many-body problem. On the other hand, taking each quantum dot in isolation would lead to a manageable task for modern supercomputers, but accounting for the wetting layer even in the individual quantum dot model would increase the computational complexity of the problem in several times. As a result, the entire problem in its generality would be hardly feasible from a practical, routine-based simulation, point of view. Moreover, in calculating atomic positions the definitions of atomic forces that enter the Hamiltonian in such large scale atomic simulations are approximate by nature and a number of important coupled effects, such as piezoelectric, remain frequently outside the scope of the analysis. To attack the problem in hand, one needs to resort to some clever averaging over atomic scales.

Such averaging can be achieved by empirical tight-binding, pseudopotential, and k.p approximations. These approximations are very important in further development of mathematical models for LDSNs due to the fact they are well suited for incorporating additional effects into the model, including strain, piezoelectric effects, spontaneous polarization, geometric and materials nonlinearities. These effects, despite their importance, have not been studied with vigor they deserve, in particular in the context of mathematical models for bandstructure calculations. There is a growing interest to such models as they should provide a key to better predicting optoelectromechanical properties of LDSNs. With anticipated new discoveries in theoretical and experimental analysis of LDSNs in the coming years, one of the main emphases of the workshop was on the models that would allow incorporating these effects consistently into the state-of-the-art models for LDSNs. From a mathematical point of view, many such models can be reduced to a large eigenvalue PDE problem (e.g., with the Hamiltonian accounting for the Burt-Foreman correction) coupled to strain and piezoelectric potential calculation. In its turn, in its general setting the problem of strain and piezoelectric potential calculation requires the solution of a nonlinear system of partial differential equation. A large experience in solving these two parts of the problem separately, independently of each other, has been already accumulated in the distinct communities of the researchers. This BIRS workshop effectively combined expertise of these research communities, summarized the state-of-the-art for modeling LDSNs and key challenges facing these communities, and explored ways to address those challenges in interdisciplinary team settings.

The workshop brought together researchers working on different aspects of the analysis and modeling of LDSNs which require a concerted efforts of teams of researchers with close interactions between applied and pure mathematicians, physicists (theoreticians and experimentalists), computational scientists, and engineers. These scientific and engineering communities were represented in Banff by the researchers from Japan, Canada, the USA, Russia, France, Denmark, Germany, and the UK (further details can be found at the BIRS website). We had four main plenary talks of one hour duration that gave state-of-the-art overviews of the subject from perspectives of applied mathematics (Professor Russel Caflisch of the University of California at Los Angeles), physics (Professor Antti-Pekka Jauho of the Danish Technical University), and computational science and engineering communities (Professor Gerhard Klimeck of Purdue University), as well as from a point of view of experimentalists (Dr Gail Brown of the Materials Lab/Air Force Research Lab at Wright-Patterson AFB). These talks helped identify the areas where joint efforts needed to be directed to, and they set up the scene for further work during the workshop, including discussions at the workshop open problem sessions. All participants had time to present their research and a specific time was allocated for on-site demonstrations of software and explanations of tools applied in the LDSN analysis.

This special issue provides a flavor of the problems discussed at the workshop. It contains 12 refereed papers. Additional information, including the abstracts of all presented talks, can be found at the BIRS website). Using this opportunity, we would like to thank the referees of this volume for their time and efforts. Without their timely professional comments this volume would not have been made possible.

In conclusion, we note that advances in mathematics, physics and computation of LDSNs, impact such seemingly distant applications as biotechnology and medicine,

quantum information processing and optoelectronics. The research into LDSNs offered exciting new challenges that are intrinsically interdisciplinary in nature and should be addressed by a multidisciplinary team of applied mathematicians, theoretical and experimental physicists, engineers and computational scientists. We hope that we are able to pass this idea to the reader.