07w5057 Physics-Based Mathematical Models of Low-Dimensional Semiconductor Nanostructures: Analysis and Computation

Lok C. Lew Yan Voon (Wright State University, Ohio, USA)
Roderick V.N. Melnik (Wilfrid Laurier University, Ontario, Canada)
Morten Willatzen (University of Southern Denmark, Denmark)

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1 Introduction

In November 2007, some of the world's experts on physics-based mathematical models for nanoscience and nanotechnology met at the Banff Centre, where the Banff International Research Station hosted a workshop on recent developments in the study of the mathematics and physics of nanomaterials and nanostructures. 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 mathematical and computational tools will be needed to advance the science and engineering of nanomaterials and nanostructures [13].

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.

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 mathematical 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 mathematical models in this field, applied widely in the physics and engineering communities, 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. At the same time, precisely these optoelectronic properties are of fundamental importance in a wide range of LDSN applications. Among such effects that may profoundly influence such properties 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. Indeed, from a mathematical point of view the resulting model becomes a challenge due to multiple scale effects we have to deal with in such situations. 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 $k \cdot p$ 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 which are in the heart of current and potential applications of these structures. 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 mathematical 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 coupled to the mathematical models for strain and piezoelectric effects. 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.

Before the workshop, invited attendees were asked to upload their abstracts electronically to stimulate initial discussions (see `http://www.m2netlab.wlu.ca/ldsn-banff/`). Following the conclusion of the event, a selected number of refereed extended papers relating to the workshop presentations were published in the Journal of Physics Conference Series (JPCS). A direct link to the 12 JPCS refereed proceeding contributions can be found on the BIRS homepage for this workshop (or from the above site).

2 State-of-the-art overviews and interdisciplinary efforts in mathematical modelling of low dimensional nanostructures

At the beginning of the workshop, state-of-the-art overviews of the subject from perspectives of experimentalists, physics, applied mathematics and computational science communities were given by key experts in their respective fields. 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 presented their own research in LDSNs. At the last day of the workshop, time was allocated for on-site demonstrations of several model-based software tools such as NextNano by Stefan Birner ($\mathbf{k} \cdot \mathbf{p}$ based models) as well as for the NanoHub project by Gerhard Klimeck (models for bandstructure based on tight-binding methodologies), involving LDSN analysis. Good discussions of strengths and weaknesses using these electronic bandstructure methods in determining basic physical properties of quantum dots and computing characteristics of quantum-dot based devices came out of this session. Indeed, it was one of the main ideas to create this discussion atmosphere so as to identify pros and cons in applying various mathematical and computational methods and to explore how they can possibly supplement each another. There is no doubt that large quantum-dot and quantum-wire based structures are still computationally too demanding when assessing most device applications and physical properties. In particular, investigation of carrier dynamics and light propagation in nanodevices with dynamic coupling to electronic state fillings, Coulomb interactions, electromechanical phenomena requires use of less computationally intensive bandstructure methods.

3 Low dimensional nanostructures as multiscale complex systems

We now discuss some of the main themes in detail. Low dimensional semiconductor nanostructures are multiscale complex systems that require the development of coupled mathematical models for their studies [19]. Parts of these systems (e.g., two bulk materials) are joined together at the atomistic level via interfaces to form a new structure with properties unmatched before. It is an interdisciplinary area where continuum and atomistic, deterministic and stochastic mathematical models go hand in hand. I. Prigogine, a Nobel Laureate in Chemistry, pointed out a while ago that "complexity is no longer limited to biology or human sciences: it is invading the physical sciences as deeply rooted in the laws of nature". Low dimensional nanostructures provide one of the most important examples of coupled complex systems in physical sciences with a fascinating range of current and potential applications.

One of the emphases of this workshop was on the development of effective (such as envelope-function) mathematical models for LDSNs, coupled to models of continuum mechanics for strain and electromechanical effects, that mathematically lead to a system of eigenvalue PDE problems. From a physical point of view, electronic bandstructure theory is an important ingredient in the understanding of optical and electronic properties of semiconductors nanostructures. One of the classic tools (since the fifties) for obtaining electronic bandstructures is the envelope-function theory also known as the $\mathbf{k} \cdot \mathbf{p}$ method discussed extensively during the workshop (e.g., [10, 20]). This method has shown its strength in modelling electronic states with remarkable accuracy qualitatively and quantitatively for bulk and quantum-confined structures capturing many of the subtle geometric details as well as microscopic and macroscopic (full nanostructure) symmetry characteristics. The fact that variations in physical fields are larger in smaller quantum-dot structures than in bulk-based semiconductors (due to larger gradients in material-composition in the former as compared to the latter) implies that nonlinear electromechanical coupling effects can play a significantly role not known in bulk applications. In addition, other nonlinear effects, such as nonlinear strain, are becoming increasingly important for such structures [18]. During the workshop, the development of mathematical models for the description of coupled electromechanical effects in low dimensional nanostructures were discussed by Barettin *et al.*, Mahapatra et al, and Lassen et al. Barettin *et al.* presented a method for obtaining accurate strain

distributions in cylindrical quantum dots using Navier's equations, Maxwell's equations, and constitutive electromechanical relations derived from free-energy considerations [1]. Lassen et al [10] demonstrated the impact of using the fully coupled electromechanical equations including piezoelectric effect and spontaneous polarization as compared to the semi-coupled approach. Several insightful examples were provided in this context [10].

The governing constitutive equations in the electromechanical fields in the linear case are:

$$\sigma_{ik} = C_{iklm}\epsilon_{lm} + e_{nik}\partial_n V, \quad D_i = e_{ilm}\epsilon_{lm} - \varepsilon_{in}\partial_n V + P_i^{sp}, \tag{1}$$

where σ, ϵ, V, D, P_i^{sp} are the stress, strain, electric potential, electric displacement, and spontaneous polarization, C, ε, and e are the stiffness, dielectric, and piezoelectric constants, respectively. Combination with Navier's equation and the Poisson equation:

$$\partial_j \sigma_{ij} = 0, \quad \partial_i D_i = 0, \tag{2}$$

in addition to appropriate boundary conditions specify the complete set of model equations. Here the strain is composed of a lattice mismatch part and a part related to spatial derivatives in the displacement vector.

The strength of the model, discussed by Barettin et al, lies in the inclusion of the symmetry and the nanostructure geometry imposing Dirichlet boundary conditions on the mechanical displacement far into the (well) material embedding the quantum dot. They compared four different quantum-dot cases taking into account one or more of the three effects: lattice mismatch between dot and well material, spontaneous polarization, and piezoelectric effects. Their results showed that significant changes in the strain distributions result if any of the three effects are omitted. Hence, since strain modifies qualitatively electronic bandstructures and momentum matrix elements, it is important to always perform a coupled-field investigation when evaluating optoelectronic properties of semiconductor nanostructures, as it was emphasized by Lassen et al [10]. In effect, output results for strain and other physical fields are used as input to envelope-function methods allowing for a computationally fast and accurate determination of optoelectronic properties accounting for electromechanical coupling.

From a mathematical point of view, a system of coupled partial differential equations that needs to be solved in this context (elasticity equations coupled with the Maxwell equation, sometimes referred to as the Navier-Poisson system) leads to non-trivial mathematical difficulties related, in addition to the well-posedness issues [15], to the stability of numerical approximations [16]. The results of the solution of such systems are then used in solving an eigenvalue PDE problem which represents a serious challenge even in the case of single band models, as it was demonstrated in [17] where the issue of correct boundary conditions was addressed. New interesting quantum confinement phenomena, such as existence of critical radius in nanowire superlattices, were studied extensively with such mathematical models [28]. Higher order approximations based on such models both for the strong and weak formulations of the eigenvalue problem were also studied in detail in [11]. However, new challenges appear in attempts to generalize such analyses to the multiband models. Indeed, in the case of 8×8 Hamiltonian, such a system consists of 8 coupled equations where the verification of ellipticity conditions and the issue of spurious solutions lead to another set of non-trivial mathematical difficulties [12].

Nonlinear strain, polarization and diffused interface effects in low dimensional nanostructures were discussed by D.R. Mahapatra et al who emphasized also the importance of the size effects, as well as nonlinear effects, in the modelling of such structures [18]. Their analysis was based on a self-consistent modeling framework within which they developed a variational formulation of the Poisson-Navier-Schrödinger system.

3.1 Quantum dot arrays and coupling to other fields

In addition to the importance of electromechanical coupling and the development of associated mathematical models accounting for this coupling, as discussed above, a series of discussions were focused on the importance of other physical fields in the study of low dimensional nanostructures, such as magnetic. In addition, several novel concepts were discussed in the context of quantum dot arrays or molecules where a set of several quantum dots are considered as a coupled system.

In particular, quantum dot molecules have been discussed by D.G. Austing et al who observed striking and unexpected magnetic-field induced intra-dot level mixing and quantum superposition phenomena between two, three and four approaching single-particle states in a quantum dot.

3.2 Nonlinear phenomena and mathematical modelling of phase transformations

Coupled nonlinear thermo-mechanical effects were discussed by M. Zhou who focused on the newly identified transformations to novel pseudoelastic behaviors with recoverable strains in nanowires. He pointed out that the transformations also give rise to a coupling between the thermal and mechanical behaviors of the nanowires and offer mechanisms for developing nanocomponents with tunable responses. Problems of structural phase transformations require us to deal with strongly nonlinear effects such as hysteresis and the development of efficient numerical methodologies for such problems represents one of the major challenges in applied mathematics and mathematical modelling [14, 25]. In the context of nanostructures, M. Zhou presented first-principles calculations based on the density functional theory (DFT) and molecular dynamics (MD) simulations that yielded critical conditions for these transformations.

Hysteresis effects without plastic deformation as observed in nanoscale contact experiments were discussed by A. Lew who presented a simple model to explain the observed behavior.

3.3 Mathematics of nanocrystal growth and modelling the synthesis of nanocrystals

Nanocrystal growth is an intrinsically multiscale process. One of the examples includes growth of an epitaxial thin film which involves physics on both atomistic and continuum length scales. Indeed, diffusion of adatoms can be coarse-grained, but nucleation of new islands and breakup for existing islands are best described atomistically. These issues were discussed by R. Caflisch who described mathematical modeling, simulation methods and computational results for epitaxial growth, strain in thin films and pattern formation. His growth simulations used an island dynamics model with a level set simulation method. He pointed out that strain computations can be computationally intensive, so that effective simulation of atomistic strain effects relies on an accelerated method that incorporates algebraic multigrid and an artificial boundary condition. R. Caflisch presented simulations that combine growth and strain showing spontaneous and directed self-assembly of patterns (quantum dots and wires) on thin films.

X.B. Niu et al studied the effect of a spatially varying potential energy surface on the self-organization of nanoscale patterns during epitaxial growth. At the workshop they presented their mathematical model and the developed computational approach based on the level set method.

Modelling the synthesis and thermodynamic properties of nanocrystals remains a challenging task for mathematical modellers, scientists, and engineers. D. Chrzan et al demonstrated new results obtained with the developed model for the nucleation and growth based on both the kinetic Monte Carlo simulations of the growth process, and a complementary approach involving the integration of a set of coupled rate equations [29]. They were able to overcome a number of difficulties and shared with the participants of the workshop their experience with modelling nonlinear effects in the confined nanocrystals, including the large hysteresis in the melting point.

3.4 Developing computational methodologies for modelling properties of nanostructures

A number of important effects at the mesoscopic level were also discussed at the workshop. H. Guo summarized such effects in the context of mesoscopic spin-Hall effect and provided the audience with details of an efficient numerical technique for solving the 2D quantum scattering problem.

A computational framework for studying the effects of dislocations in semiconductor nanostructures on both electrical and optical properties was presented by H.T. Johnson et al.

A novel hierarchical multiscale model, the surface Cauchy-Born (SCB) model, was presented by H. Park et al. He presented a series of results on numerical methodologies for capturing surface stress effects on the mechanical behavior and properties of nanowires. He also demonstrated how to calculate the resonant frequencies, and thus the elastic properties of nanowires.

4 Mathematical models for low dimensional nanostructures in biological sciences and medicine

As mentioned above, the quickly progressing technology of low-dimensional semiconductor nanostructures requires and depends on reliable predictive theoretical methods for systematically improving, designing and understanding the electronic and optical properties of such structures. The problem complexity becomes even more pronounced if the nanostructures are combined with biomaterials to form bio-sensors. In this case, new mathematical difficulties are quick to appear. At the same time, commercial applications of nanodevices, like pH, protein, virus or DNA sensors (bio-chips) are gaining in importance in recent years. Therefore, the development of mathematical models and computational tools for their solution are becoming increasingly pressing.

In the paper and presentation by Birner *et al*. [2], realistic models of an electrolyte solution, its interaction with a semiconductor device surface, and of the semiconductor device itself were discussed in the framework of a bio-sensor device based on a silicon-on-insulator structure. Detailed simulations of protein sensors based on silicon allow demonstrations of the applicability of the model approach. The Schrödinger equation and Maxwell's equations (with the Poisson-Boltzmann equation describing ion charge distributions spatially) are coupled and solved for the electrolyte and semiconductor regions. A standard approach was used to calculate the energy levels and wavefunctions based on the one-band envelope function approximation. As aqueous electrolytes for use in bio-sensors are usually buffer solutions they resist changes in H_3O^+ and OH^- ion concentrations (and consequently the pH) upon addition of small amounts of acid or base, or upon dilution. The concentrations of the ions that are contained in the buffer depend on the pH and the dissociation constant. These were calculated using the well-known Henderson-Hasselbalch equation. In addition, the dissociation value depends on temperature and on ionic strength in a self-consistent way. When using a phosphate buffer, the concentrations of the buffer ions at a particular pH are governed by three different dissociation constant values making it extremely difficult to derive concentrations analytically. In order to circumvent this problem, Birner *et al.* followed a Schrödinger-Poisson coupled numerical scheme in an iterative way. This was one out of several examples presented at the workshop where good qualitatitive agreement were found with a multiphysics model employed a fairly simple bandstructure model. It is expected that the use of multiband electronic bandstructure models would lead to improved results and better agreement with experiments.

According to Birner *et al.*, it is necessary to solve the Schrödinger equation in regions where the quantum mechanical density is negligible or zero such as in insulators. Also wavefunction penetration into the barrier materials (e.g. at Si-SiO_2 interfaces) is fully taken into account by including a small region of the barrier material into the Schrödinger equation. Model results were compared with available experimental data and it is found that the Poisson-Boltzmann equation is able to reproduce experimental data in contrast to the widely used Debye-Hückel approximation which faces severe limitations.

One of the applications of the nanoHUB framework presented by G. Klimeck and his collaborators was on biologically active field-effect transistors, or BioFETs. They have been analyzed as potentially fast, reliable, and low-cost biosensors for a wide range of applications as they are direct, label-free, ultrasensitive, and (near) real-time operation. The development of multiscale mathematical models for planar sensor structures and for nanowire sensors requires the drift-diffusion type equations coupled with the mean-field Poisson equation and a Boltzmann model for the ions. The multiscale models are essential in this field due to the large difference in the characteristic length scales of the biosensors: the charge distribution in the biofunctionalized surface layer varies on the Angstrom length scale, the diameters of the nanowires are several nanometers, and the sensor lengths measure several micrometers. It is also important to note that the multiscale models for the electrostatic potential can be coupled to any charge transport model of the transducer. Among others, one of the mathematical challenges that need to be overcome here is the treatment of the boundary layer which cannot be modelled by including its total charge. The authors overcome these difficulties, and on several interesting examples demonstrated the importance of the dipole moment of the biofunctionalized surface layer in addition to its surface charge [7].

Non-conventional nanostructures were reviewed by Y. Zhang who focused on computational challenges for mathematical modelling of such nanostructures properties. Examples included inorganic-organic hybrid nanostructures, core-shell nanowires and others.

5 Quantum information, photonics, and telecommunication applications

During the last decade, In(Ga)As/GaAs quantum dots (QDs) have received considerable attention due to the predicted improvements in device performance that can be achieved because of their reduced dimensionality and novel behavior enabling development of new technologies such as single photon sources and qubits for quantum information applications. The operating wavelength of GaAs-based optoelectronic devices can be tuned within the important telecom wavelength range (1300-1550 nm) by appropriate material and geometry control of quantum-dot wetting-layer structures. A variety of experimental techniques are known including alternate layer epitaxy, use of low InAs growth rates or by capping the QDs with a thin layer of InGaAs before subsequent GaAs growth or encapsulating the QDs within an InGaAs quantum well (dots-in-a-well or DWELL systems). Clarke *et al.* [4] presented investigations of growth and optical properties of InAs/GaAs quantum dot (QD) bilayers examining the influence of strain. Optical emission-wavelength tuning between 1400 nm and 1515 nm is demonstrated experimentally. The conference included mainly theoretical presentations and methods albeit, ultimately, it is the interplay between theory and experimental methods that most effectively leads to technological improvements and understanding of the important physics involved. One of the issues that certainly needs better understanding is the possibility to control to a higher degree the composition grading and formation of nanostructure shapes and sizes. At present, the use of self assembly such as for, e.g., InGaAs-based quantum-dot structures is a critical point. Theoretical models of growth under temperature, gas inlet control dynamically exist but they are still far from being able to describe qualitatively and, in particular, quantitatively the formation of realistic quantum-dot based nanostructures under laboratory conditions. One of the major conclusions of the workshop is the importance of obtaining in future better theoretical guidance to experimentalists on the growth process and dynamics as well as for theoreticians verification of theoretical models against experimental results. The answer to these questions can open up possibilities for producing new quantum-dot structures and ultimately improved device applications. Secondly, theoretical modelling of the influence of statistical fluctuations, non-ideal nanostructure surface shape- and composition grading effects, which are always present in today's grown structures, was identified at the workshop as an important issue to tackle and address.

Modelling of optical gain as an important task in the applications of quantum dot lasers was discussed by S.L. Chuang.

Slow down of light in a highly dispersive media has gained enormous attention since reportings in the late ninetees on light propagating at 17 m/s through a vapor of ultra cold Na atoms [5]. A large research effort has been put into extending these results to semiconductor nanostructures at room temperature for applications in, e.g., telecommunication. Quantum dot-based devices are promising candidates for applications exploiting quantum coherence phenomena due to their atom-like properties and large dephasing times. For instance, an all optical buffer based on slow light in quantum dots has been proposed. Houmark *et al.* [6] investigated the impact of many-particle interactions on group-velocity slowdown through Electromagnetically Induced Transparency (EIT). At the workshop, a so-called ladder scheme in the active quantum-dot energy levels (effective using an appropriate pump-probe excitation configuration) in the steady-state was demonstrated vs. earlier attempts based on transient schemes. Moreover, the model accounts for Coulomb interaction effects leading to an increase in maximum slow-down as compared to the non-interacting case. The susceptibility was found by computing the microscopic polarizations of the material using density-matrix equations. Emphasis was put on the differences between an atomic model or one that includes many-particle interactions in the Hartree-Fock approximation. Their results also showed that the necessary pump power at which maximum slow down is obtained for EIT remains unchanged. Discussions at the workshop revealed that the use of more realistic electronic bandstructures (envelope-function, empirical, or ab-initio atomistic calculations) and resulting more accurate dipole moments for EIT is expected to be of significant importance for quantitative conclusions on slow down and pump-power requirements. Future investigations along this line and verification against measurements are thus essential.

Advances in quantum dots theory and applications for nanophotonics and quantum information devices were reviewed by Y. Arakawa. Further discussions were centered on quantum dots as promising elements to control single photons and entangled photon pairs.

6 Dynamic and transport phenomena in low dimensional nanostructures and devices

The development of mathematical models for nanodevice simulation brings a number of serious challenges at theoretical and numerical levels, in particular for the time-dependent models [22]. During the workshop, they were discussed by D. Vasileska et al who emphasized the dominant role of quantum effects in addressing the issue of quantum transport. Among the most commonly used in nanostructure calculations schemes are the Wigner-function approach, the Pauli master equation, and the non-equilibrium Green's functions (NEGF) known also as the Keldysh formalism. The authors showed that the key to the successful application of the NEGF formalism to the 3D quantum transport problem in semiconductor nanostructures is the numerical efficiency of the contact block reduction (CBR) method [9].

A number of new phenomena theoretically predicted with mathematical models were also discussed at the workshop. One of them is spontaneous excitation of coherent nano-particle dipole oscillations through interaction with a quantum-dot two-level system subject to population inversion [21]. Several important observations were made: dipole momentum of nano-particle leads to coherent dipole radiation, optical cavity is not necessary, the size of the dipole laser can be smaller than the optical wavelength (it is effectively a dipole nano-laser). It was demonstrated that the proposed mathematical model allows us to analyze threshold conditions and optical bistability in dipole nano-lasers.

7 Atomistic and molecular dynamics approaches for low dimensional nanostructures

The importance of the development of predictive modelling tools was emphasized in the presentation by H. Huang who argued that at this stage it is already feasible to model atomistic processes of pico-/nano-seconds using classical molecular dynamics and density functional theory methods. However, the structure evolution processes on the order of minutes remains a challenge once the nanorods or nanowires have variable crystalline orientations. The atomistic methodologies for the structure evolution processes, based on a lattice kinetic Monte Carlo method, were in the focus of this discussion. It was demonstrated that coupling of density functional theory ab initio, classical molecular dynamics, and kinetic Monte Carlo simulations can enable us to achieve a predictive design of nanorods synthesis [8].

A novel multiscale nonequilibrium dynamics (MS-NEMD) model was presented by S. Li who demonstrated that the developed model is capable of simulating coupled thermo-mechanical coupling at small scales, such as nanoscale heat conduction and phonon scattering by defects, e.g. dislocations.

The effect of bandstructure in the atomistic treatment of electronic transport was discussed by N. Neophytou et al who focused on such important effects as non-parabolicities and anisotropies in the electronic structure, strong coupling of bands, degenerate valley splittings due to enhanced quantum interactions, strain, material and potential variations on the nanoscale.

M. Korkusinski et al presented new results on atomistic calculations of electronic and optical properties of semiconductor nanostructures. They found the optimal atomic positions by minimizing the total elastic energy of the system using the Valence Force Field model in the first-nearest-neighbor approximation. Once the equilibrium structure of the sample is established, they proceeded to calculating the single-particle states of the electron and hole confined in the nanostructure using tight-binding approaches.

Atomistic simulation of nanosize electronic devices was discussed by L.-W. Wang who presented a method which uses atomistic pseudopotentials to calculate the electronic structures and electrical properties of the million atom devices. He explained that he uses a linear combination of bulk band (LCBB) method to solve the electron eigenstates of the system, and special formalism to occupy the eigenstates in an nonequilibrium system. He discussed the importance of quantum mechanical effects in the developed modelling framework.

8 Stochastic mathematical models and control

Another important issue discussed at the workshop was the development of state-of-the-art stochastic models for dynamic problems describing the behavior of low dimensional nanostructures. It is well known that some of the most peculiar features of quantum theory such as the existence of quantum superpositions and of entangled states are typically destroyed by uncontrolled and ultimately inevitable interactions with a surrounding, often incoherent environment [3]. Nevertheless, as it was pointed out during the workshop by Kyriakidis et al most of the recent theoretical analysis done in the area of low-dimensional dynamical quantum systems has been either for open Markovian systems, where the past memory of the system is neglected, or for closed unitary systems, where the dynamics are reversible [24]. He further argued that much of the research done until recently has focused on steady state phenomena where a Markovian approach can be expected to provide reasonable results. However, the transient behavior of the system carries a tremendous amount of information in the form of coherence and relaxation dynamics (examples include, but not limited to ultrafast laser pulse excitations that provide insight into the heterostructure dynamics on a femtosecond timescale). Therefore, the development of a mathematical theory which accounts for quantum dynamical behavior on the same time scale would be of great benefit not only to experiment, but also to basic understanding.

Earlier in the report, we have already mentioned the Keldysh formalism of non-equilibrium Greens functions (NEGF) and formalisms based on NEGF, which have been very successful in the analysis of many phenomena in mesoscopic systems, including transport through quantum dots. However, as it was argued by Kyriakidis et al, NEGF is inherently a closed-system formalism where the system has Hamiltonian dynamics, and thus does not account for irreversibility arising from interactions with an unseen, unknown, or otherwise intractable environment. Promising attempts have been made to extend NEGF to open quantum system by treating, for example, the environment as a correction to the systems self-energy, or by calculating two-time correlation functions, effectively separating the time scales into transient and steady-state regimes. Kyriakidis et al investigated the dynamics of bound particles in multilevel current-carrying quantum dots where they looked specifically in the regime of resonant tunnelling transport. Through a non-Markovian formalism under the Born approximation, they analyzed the real-time evolution of the confined particles including transport-induced decoherence and relaxation. In the case of a coherent superposition between states with different particle number, they found that a Fock-space coherence may be preserved even in the presence of tunneling into and out of the dot [24].

During the workshop it was emphasized that to create quantum devices that perform useful functions, we must be able to understand their behaviour, and have effective means to controllably manipulate it [23]. Analysis of system dynamics and the design of effective control strategies require the availability of sufficiently accurate mathematical models of the device as we discussed earlier in the report. New mathematical challenges appear in the task of intrinsic control system identification for quantum devices. The problem of experimental determination of subspace confinement becomes of primary importance in this case. It was argued during the workshop that a fundamental prerequisite for constructing a Hilbert space model for characterizing subspace confinement is knowledge of the underlying Hilbert space. This is a nontrivial problem as most systems have many degrees of freedom, and thus a potentially huge Hilbert space, but effective characterization of the system often depends on finding a low dimensional Hilbert space model that captures the essential features of the system. Schirmer et al proposed simple general strategies for full Hamiltonian identification and decoherence characterization of a controlled two-level system [23].

9 Physics-based mathematical models and experiments

The development of physics-based mathematical models in this field is closely connected with the state-of-the-art experimental results. In Fig. 1 we schematically presented three main areas that influence significantly the development of mathematical models for nanostructures and nanostructure-based devices. The participants of the workshop identified, in each of these three areas, the significant experimental achievements in recent years. We summarize them below:

- Growth/Nanomechanics (emerging nanoscale experiments; 3D atom precision probe method for positions and compositions; mechanical, thermal, optical and other measurements);

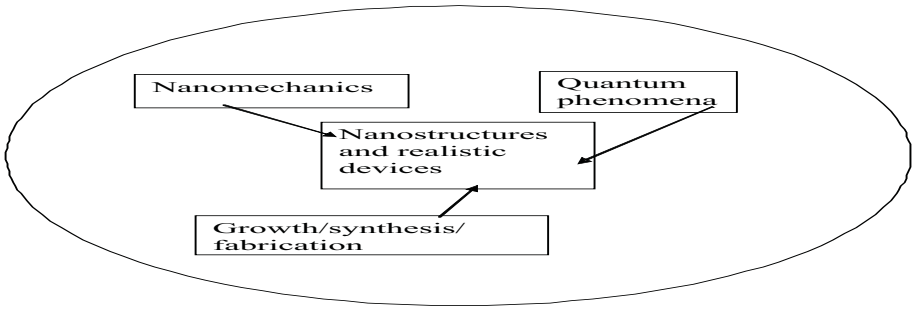

Figure 1: Main components to be accounted for in the development of physics-based mathematical models for low dimensional nanostructures.

- Nanodevices and Simulation (multicell junction and core-shell solar cells; entangled photon states; DNA sensitive FETs);
- Nanophysics and Quantum Phenomena (single-photon emission; single-electron spin detection; quantum spin-Hall effect).

Current state-of-the-art modeling achievements were also identified in the same three areas:

- Growth/Nanomechanics (methodologies based on kinetic Monte Carlo (kMC), accelerated MD, longer time scale simulations, multiscale, multiphysics models, atomistic/continuum, density-functional theory (DFT), level set, and others);
- Nanodevices and Simulation (50+ million atoms + Valence Force Field; time-dependent DFT; quantum MC);
- Nanophysics and Quantum Phenomena (DFT relaxation + tight-binding electronic structure; ab initio and temporal behavior; non-equilibrium Green's function, NEGF).

Finally, the feasibility of mathematical and computation methodologies in two of the areas were brought up:

- Growth/Nanomechanics (currently it is possible to simulate 1000 atoms with DFT, while realistic problems often require 1 000 000 for QD and quantum wires; kMC for cluster distribution; MD for diffusion; continuum approach for surface morphology; DFT for sticking coefficients);
- Nanodevices and Simulation (multiphysics modeling of nanostructures; multiscale techniques from atomistic level to the device level; NEGF techniques for transport).

10 Open problems, points of controversy, new directions, and outcomes

The complexity of present-day laboratory nanostructure growth imposes a strong need for better interaction between theoretical physicists, applied mathematicians, and experimentalists to improve technological development in the field and to advance physics-based mathematical models that would assist this development. Today, only very limited knowledge is available on the influence of growth parameters on the details of nanostructure shape and size, composition determining the important physical properties and ultimately device applications. Finally, an important aspect of this workshop was to remove barriers in communication between theoreticians using different mathematical models and methodologies for the analysis of growth, electronic bandstructures, and device characteristics. This is important for obtaining a better understanding of individual methods and how they can be combined effectively in studying complicated nanostructure phenomena. As we pointed out in the previous sections, current state-of-the-art methodologies cannot be efficiently used to design nanoscale structures and their properties. During this workshop, the study groups were formed to identify some of the key open problems in this rapidly developing interdisciplinary field. Each study group had experts in all three main areas represented at this workshop: experimental physics, theoretical physics, applied mathematics and computational science. The summary of study groups work on the identification of open problems is summarized below:

- Growth/Nanomechanics (reliable surface structure prediction beyond periodicity; reliable growth process control and simulation, including 3D nucleation, defect control; uniformity and quantity of a few nm materials);
- Nanodevices and Simulation (control of carrier injection, and photons and phonons; realistic and reliable device modeling; coherence/decoherence);
- Nanophysics and Quantum Phenomena (reduction for decoherence; quantum system identification; measurement in quantum physics; strongly correlated quantum systems; quantum transport phenomena in complex systems).

There were a number of productive discussions during the workshop that highlighted some points of controversy. For example, given that a range of coupled multiscale effects must be accounted for in the development of mathematical models for LDSNs, how to quantify the quality of approximations and limitations in applicability of main methodologies for bandstructure modelling such as $\mathbf{k} \cdot \mathbf{p}$ envelope function approximations, tight-binding, ab initio methodologies? The workshop generated a substantial interest to these nontrivial issues. It became also apparent that the practitioners who are using one of the above methodologies were not fully aware in the utility and degree of advancement of the other methods.

One of the doctoral students (D. Barettin), working on continuum models, was invited to spend six months visiting one of the plenary speakers working on atomistic models (G. Klimeck). The interest of the participants, who traditionally were working on continuum models, to atomistic first principle analyses has increased as a result of the BIRS workshop which led to several subsequent presentations and publications (e.g., [26, 27]).
The outcomes of this workshop included:

- Networks created across disciplinary borders;
- Recognition of physics and mathematics driven nanoscale modeling and addressing some of the most challenging multiscale problems in mathematical modelling of complex systems;
- Consensus-building towards real-time modelling and simulation for design and control of nanostructures and devices.

The above consensus is being built via the development of physics-based deterministic and stochastic mathematical models for studying low dimensional nanostructures along with the development of coupled atomistic-continuum methodologies for the applications of such models, ranging from growth modelling to the quantum mechanical analysis of electronic properties.

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