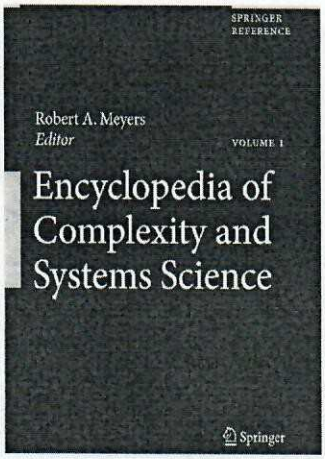

Encyclopedia of Complexity and Systems Science
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Encyclopedia of Complexity and Systems Science

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Melnik, R., Nanoscale Processes, Modeling Coupled and Transport Phenomena in Nanotechnology, Encyclopedia of Complexity and Systems Science (Editor-in-Chief: Meyers, R.A.), pages: 5912-5925, Springer, ISBN: 978-0-387-75888-6, 2009

Multiple Scales and Coupled Effects in Modelling Low Dimensional Semiconductor Nanostructures: Between Atomistic and Continuum Worlds

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Article Outline

Glossary

Low dimensional semiconductor nanostructures Structures that have characteristic dimensions on the order of nanometers (usually between 1 and 100 nm) and such that the motion of electrons in them can be confined spatially. Quantum well heterostructures were the first low dimensional semiconductor nanostructures experimentally developed in the early 1970s. Now, a number of different techniques exist to produce a variety of different low dimensional semiconductor nanostructures, including quantum wells, wires, and dots.

Electronic structure Electrons move from one energy level to another by emission or absorption of a quantum of energy, a photon. They are placed on electronic orbitals and their configuration defines the electronic structure as the arrangement of electrons in an atom, molecule, etc. The knowledge of the electronic structure of a specific material or a structure helps us in predicting its properties.

Electromechanical effects One of the most studied examples of such effects is piezoelectricity, demonstrated for the first time by the brothers Pierre Curie and Jacques Curie in 1880. Now, it is one of the classical examples of coupled phenomena. In the heart of the piezoelectric phenomenon is a coupling mechanism between mechanical and electric fields which is a two-way interaction. In particular, electricity is produced in a piezoelectric body when stress is applied (the direct piezoeffect) and the body is stressed when an electric field is applied (the converse piezoeffect).

Multiple scales In studying complex systems we have to deal with coupled phenomena and processes at a multitude of different spatial and temporal scales. Understanding interactions in the system and its response at multiple scales is a fundamental quest of modern science.

Nanotechnology A multidisciplinary field that develops and extends our present knowledge into the nanoscale. It is the field where two main science and technology approaches, the "bottom-up" approach and the "top-down" approach, go hand in hand emphasizing the importance of systems science view.

Mathematical modeling A universal tool of modern science and technology that uses mathematical language to describe the behavior of systems, processes and phenomena in Nature and man-made.

Definition of the Subject

Low Dimensional Semiconductor Nanostructures (abbreviated, LDSNs) is a class of physical systems with characteristic dimensions on the order of 1–100 nm such that the motion of their charge carriers can be confined from one, two, or even three spatial dimensions. If we start our consideration from a three dimensional (3D) bulk crystal and create a structure where the motion of carriers is confined from only one spatial direction, we will arrive at a simplest example of LDSNs, two dimensional ($2D = 3D - 1D$) nanostructures known as quantum wells. Confining the motion of carriers from two spatial directions would lead us to one dimensional ($1D = 3D - 2D$) nanostructures such as quantum wires or quantum rods. Finally, it is possible to confine the motion of charge carriers in LDSNs from all three spatial dimensions. Such nanostructures are often termed as 0-dimensional ($0D = 3D - 3D$) [redacted] and known in the literature as quantum dots with other terms, such as quantum islands and artificial atoms, also used to describe them.

The history of the subject was closely interwoven first with the works on semiconductor lasers in the early 1970s, but the idea of using heterostructures for emitting purposes can easily be traced back to the early days of electronics and to works of Shockley, Kroemer, Alferov and others [1]. A heterostructure is a semiconductor structure

with heterojunction, that is a junction composed of parts (or layers) of dissimilar semiconductor materials that have different electronic properties such as energy (band) gaps. Such structures have properties unmatched by the underlying bulk semiconductor materials. A structure with periodically alternating layers of several materials is called a superlattice. In semiconductor superlattices the bandwidth can be tuned by changing the width of the barriers wells. Such superlattices attracted attention in early 1960s and the early studies of the effect of a periodic modulation of the potential in one direction on the crystal band structure is due to Keldysh. Later, Esaki and Tsu and others used one dimensional models to study transport effects in semiconductor superlattices. In earlier 1970s, heterostructures were realized in the laboratories.

Since that time, the field of low-dimensional systems and nanostructures has grown substantially and includes now semiconductor heterostructures, quantum wells and superlattices, mesoscopic and two-dimensional electron systems, quantum wires and quantum dots. The field has experienced an unprecedented growth in terms of applications, and in addition to its early focus on semiconductor lasers, it includes now a wealth of applications in optoelectronics, quantum information processing, security and defence, health care and biotechnologies, among many other areas.

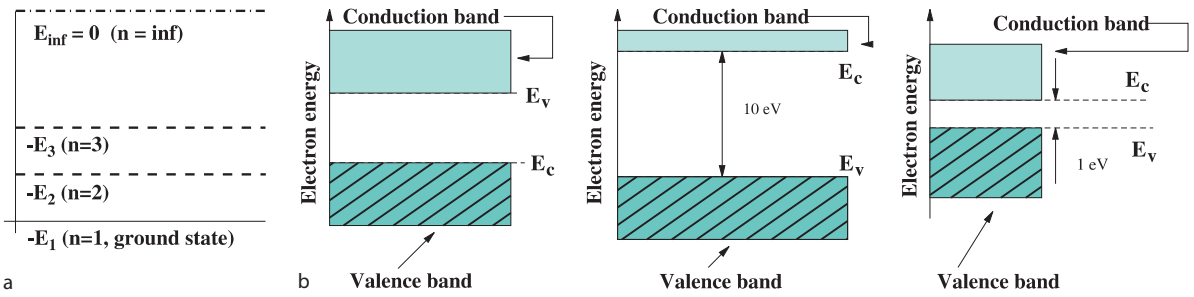
Introduction

Echoing R. Feynman's famous comments on the existence of "plenty of room at the bottom", the discussion about nanoscience and complexity continues in both popular and scientific literature [32,68,84]. In the focus of this discussion is an electron. Electrons have a wave-particle dual nature, occupying regions known as atomic orbitals. Such orbitals form a discrete set of energy levels (see Fig. 1) as they are identified with the quantum states in which electrons, surrounding an atom, may exist. These energy levels (bands) have different widths, depending on the properties of the corresponding orbitals. Mathematically, they are described by a wave function obeying the laws of quantum mechanics, and in particular the Schrödinger equation. In other words, since the electrons of all materials may only have certain allowable energies, we describe each of these allowed energies by the energy levels. From a chemistry point of view, bonding of atoms to form molecules of matter occurs through the interaction of the valence electrons of each atom and in solids atoms are brought together in such a way that the energy levels of individual atoms form bonds of energies.

Electrons tend to occupy energy states with the lowest energy possible and the energy levels corresponding to such states are the valence band's energy levels. The key in differentiating between electric properties of different materials lies with a "forbidden" band (the bandgap), the energy difference that separates the valence band from the more energetic conduction band. More precisely, as seen in Fig. 1, it is the energy difference between the top of the valence band and the bottom of the conduction band. So, from a physics point of view, electrical properties of matter are determined by three main energy bands: valence band, conduction band, and the bandgap. To move into the conduction band, the valence electrons must bridge an energy gap, which determines whether a solid acts as a conductor, a semiconductor, or an insulator (see Fig. 1). Unlike in insulators, in semiconductors enough energy exists in the valence electrons to enable them to cross the energy gap and exist as conduction (free) electrons in the conduction band. It is due to the bandgap that electrons are constrained from jumping easily from the usually more densely populated valence band to the conduction band. Since in a semiconductor bulk, we have continuous energy states, the bandgap is fixed. However, in LDSNs, and in particular in quantum dots, it can be altered to produce a range of energies between the valence and conduction bands, depending on the size, composition, and shape of these structures. Based on the band structures, which can be determined computationally by solving corresponding quantum mechanical models, we can determine optoelectronic properties of LDSNs. These properties are affected by other material properties such as thermal and mechanical, for instance, making the entire problem of determining the properties of LDSNs coupled. This leads to a situation where the systems science approaches become increasingly important in this field.

Low-dimensional semiconductor nanostructures are multiscale complex systems. Parts of these systems (e. g., two bulk materials) are joined together at the atomic level via interfaces to form a new structure with properties unmatched before [6,16]. As pointed out in [70], "complexity is no longer limited to biology or human sciences: it is invading the physical sciences as deeply rooted in the laws of nature".

Today, a number of experimental techniques exist to produce both self-assembled as well as free-standing quantum dots. Typical electronic structures of such systems require calculations with $10^3 - 10^6$ atoms [85]. Already in itself, it is a task of enormous computational complexity. In addition, as applications of nanostructures and nanostructured materials continue to grow rapidly, experimental results clearly point out that there are many additional



Multiple Scales and Coupled Effects in Modelling Low Dimensional Semiconductor Nanostructures: Between Atomistic and Continuum Worlds, Figure 1

a A schematic electron energy level diagram; b A schematic representation of electric properties of solids, depending on the bandgap: (a) conductors, (b) insulators, (c) semiconductors

effects that may influence profoundly optoelectromechanical properties of the nanostructures. Among such effects are strain relaxation, piezoelectric and thermoelectric effects. Indeed, the formation of LDSNs, and in particular quantum dots, is a competition between the surface energy in the structure and strain energy. At the atomistic level, as two different semiconductor materials are joint together, we have a lattice mismatch in the resulting structure that leads to the properties that are substantially different compared to the underlying bulk materials. At the same time, away from the interface between these semiconductor materials, we have to deal with the effects that are pronounced at larger-than-atomistic scales, making the overall problem of determining properties of LDSNs intrinsically multiscale. The solution to this multiscale problem lies with an effective combination of methods based on bottom-up and top-down approaches at the stage of model construction and the application of efficient computational tools at the next stage. We provide further details on these two stages in the next two sections.

Hierarchy of Mathematical Models for LDSNs

The construction of a hierarchy of mathematical models for modeling LDSNs can be started from the quantum Liouville equation. If the nanostructure has n degrees of freedom, its state in the Wigner–Weyl phase space can be described by the Wigner distribution function ρ (the density operator). If we assume that the system's motion is due to a Hamiltonian function $H(\mathbf{q}, \mathbf{p}, t)$ [64], then the evolution of the state of the system can be described by the quantum Liouville equation:

$$i\hbar \frac{\partial \rho}{\partial t} = [H, \rho] = H\rho - \rho H \,, \tag{1}$$

where $\mathbf{q}$ and $\mathbf{p}$ are vectors representing the n coordinate and n momentum operators, respectively. In a number of applications a generalized form of the quantum Liouville equation has proved to be more convenient where we split the Hamiltonian operator

$$H = \sum_{i=1}^{n} \frac{p_i^2}{2m_i} + V(\mathbf{q}, t) \tag{2}$$

into two Hamiltonians describing the nuclear motion for the lower and upper electronic states

$$H_l = T + V_l, \quad H_u = T + V_u \,, \tag{3}$$

where T is the kinetic energy and V_l and V_u are the effective potentials of the neclei in the lower and upper electronic state, respectively. In this case, the generalized quantum Liouville equation can be given as [13]:

$$i\hbar \frac{\partial \rho}{\partial t} = H_u \rho - \rho H_l \,, \tag{4}$$

and it can be shown that this equation has the form of a time-dependent Schrödinger equation for a quantum system with $N = 2n$ degrees of freedom. In what follows we mainly concern with a non-relativistic time-independent version of this equation:

$$\hat{H}\Psi = E\Psi \,, \tag{5}$$

where E is the total energy of (in this general case, many-body) Hamiltonian operator $\hat{H}$ and Ψ is the wave function.

A more conventional way to construct a model hierarchy, in particular at the device simulation level, would be to start from the classical Liouville equation for the evolution of the position-velocity probability density $f(x, v, t)$ and to derive a hierarchy of mathematical models based on the relaxation time approximations, leading to the Boltzmann, hydrodynamic type models and, in the simplest

case, to the classical drift-diffusion models [55]. To account for quantum effects in such models several different avenues have been proposed in the literature and examples of such quantum-corrected models include the smooth quantum hydrodynamic approximation and the quantum drift-diffusion model [72]. The resulting models offer a substantial speed up compared to the Schrödinger models. These models start from continuum (e. g., fluid dynamics like) representations and attempt to account for the discrete nature of the problem by incorporating a contribution of quantum effects. This modelling technique is usually associated with the top-down approach. Alternatively, we can start from the Schrödinger type models and move on to incorporate additional important effects that are pronounced at larger-than-atomistic scales. This technique allows us to move from discrete to continuum representations and it is usually associated with the bottom-up approach [56]. As the characteristic dimensions of devices continues to shrink and the number of charge carriers in many applications can be small, highlighting the importance of quantum effects, models based on the mixed-state Schrödinger equation coupled to Poisson's equation for the electrostatic potential have been playing an increasingly important role. However, in the context of LDSNs, such models should be extended to account for strain and the piezoelectric effect responsible for the interaction between electric and mechanical fields, as well as for other coupled effects that may influence the overall properties of the structure.

Atomistic simulation methodologies to solving problem (5) include ab initio methods, molecular dynamics and Monte-Carlo. They have a substantial, and often prohibitive for practical applications, computational cost. Inevitably, they are based on a set of assumptions and approximations. One has to approximate the many-body Hamiltonian and the first frequently used simplification lies with the Born–Oppenheimer approximation leading to decoupling between nuclear and electronic coordinates. This decoupling procedure results in the Schrödinger equation for electrons. In deciding which methodology to apply we should balance between the accuracy of the problem solution and the computational efficiency. For example, quantum dots may contain different amount of charge, from one electrons to thousands [30,38]. If the number of electrons in the structure is small and dynamic properties are not of the major concerns, atomistic methodologies can be preferential. In most realistic cases, however, several other factors should be taken into account. Indeed, if a LDSN is part of a device or a larger structure, the resulting system usually contains a number of atoms far beyond the efficient reach of atomistic methodologies. As a result, the development of other-than-atomistic techniques has become increasingly important. Moreover, even if we are able to complete calculations of the characteristics of the structure with an atomistic methodology, understanding of the interactions between atomistic and larger-than-atomistic scales is often of utmost importance. It has been acknowledged in the literature (e. g., [27,28]) that the key conceptual difficulty in materials science in general, and in computational materials science in particular, is to learn how to deal efficiently with a large range of length and time scales. This is also important for nanostructure studies where accounting for additional phenomena may often bring unexpected results. For instance, for LDSNs nonequilibrium phenomena resulting from fluctuating material interfaces may become of great importance [31].

Even if the time-dependency is neglected in the first approximation in the modelling of LDSNs, as we did by considering model (5), we still have to face a challenge of multiple scales that is different from many other areas of computational materials science. Indeed, for a long period of time, while modelling semiconductor devices (including transport phenomena) by using tools and methods of computational solid state electronics, researchers were able successfully applied classical models where the quantum theory was used for calculating necessary parameters dependent on the microscopic atomistic properties of the structures. As the spatial regions in new devices are becoming comparable with the De Broigle wave length of charged particles, the emphasis on quantum effects is ever increasing. This should come at no surprise because it is exactly the applications of such quantum effects that lead to further advances in nanoelectronics. In the heart of what we call 'quantum devices' is a quantum phenomenon or phenomena where the application of quantum mechanics is essential for predicting properties of such devices. What is often missing in these arguments is the fact that, given passive and contact regions of such devices, in most practical situations they have some "macroscopic" dimensions in a sense that we have to deal with micron or sub-micron regions of the device. In such cases, models that go beyond conventional drift-diffusion approximations and can be applied at sub-micron scales are quite useful [53,54,55]. With an increasing importance of quantum effects microscopic and macroscopic properties of devices we study in nanotechnological applications are interconnected, they are coupled [56,58]. The study of such properties leads to multiple scale problems in computational materials science that represent non-trivial difficulties for both theory and simulation [56,61]. Relating the quantum mechanical description of the processes and

phenomena that are taking place at the atomic level to the behavior of matter at the meso- or macroscopic levels is a key task in studying properties of the materials, the task that has been attempted by many scientists ever since the dawn of quantum mechanics (e. g., [26] and references therein).

Numerical Methodologies

The band structure calculation is a generic problem occurring in many fields of science and engineering. This problem is not limited to solid state physics applications as we need to face similar problems when we are dealing with wave phenomena in other fields, including acoustics, electromagnetism, and other areas [57]. In addressing this problem in the context LDSNs, the systems science approach becomes most natural. One of the reasons for that has already been emphasized in the previous section – in studying LDSNs we have to deal with intrinsically coupled systems. Another important reason lies with the fact that there is an intrinsic loss of information[1] when we construct a model for the electronic structure calculations. At the level of measurements the problem of the loss of information is well known and widely discussed in the literature (e. g. [8]). In such cases, it is essential to use prior knowledge from other methods and from other scales if the original problem was coarse-grained. Since semiconductor nanostructures are used as parts of electronic and optoelectronic devices, in their modelling a detailed microscopic scale should be combined with larger scales where such effects as strain relaxation and piezoelectric effects are pronounced. A complete description of the system in such cases can be given with a high computational efficiency within the framework of the $k \cdot p$ theory. It is true that with an increasing computational power (and indeed, we are moving steadily towards a petaflop computer [74]), several more refined methodologies, including empirical and density functional tight-binding and pseudopotential, become more approachable for the modeling of LDSNs [17]. Nevertheless, it should be realized that the problem remains its multiscale nature as long as the nanostructure under consideration is intended to be embedded as a functional element in a device, a chip, or eventually in a larger scale structure intended for the human use. In such cases, the influence of microscopic and macroscopic domains in the structure should be understood as a two-way interaction. As a result of such interactions, more refined atomistic methodologies mentioned above should be viewed only as a part of the problem solution. We need to integrate effects and phenomena that are pronounced at larger-than-atomistic scales into our mathematical models in such a way that the analysis of the entire system would still be possible within a computationally acceptable time.

[1] The definition of information can be found in [37].

Let us consider this issue in more details. It has already been emphasized that in designing new devices, it is paramount to know the properties of the materials they are made of. One of the most important steps in this direction is to find the solution to the electronic and ionic structure problem, achievable only by using efficient computational tools. As we know, under appropriate assumptions the ionic degrees of freedom can be separated from those of the electrons and then the problem of electronic structure calculations can be approached from a number of different directions which rely on a set of underlying assumptions. For example, the problem (5) can be re-formulated by using the variational principle:

$$\delta E[\Psi] = 0\,, \tag{6}$$

so that if we look for its solutions in the subspace of the products of single particle orbitals we will arrive at the well-known Hartree method. Alternatively, if we seek the solutions to the problem in the subspace of Slater determinants (that is antisymmetrized products of single-particle orbitals), the Hartree–Fock (HF) approximation is obtained. A single Slater determinant of single-electron wave function corresponds to the spin-orbitals. In the latter case, the problem is reduced to n one-body problems which should be solved self-consistently.

An essentially different concept is used in density functional theory (DFT) approaches where instead of the wave function as in the HF method, we use the spin density (the density of electrons). In practice, by using additional assumptions such as the local density approximation or the generalized gradient approximation we can proceed with the solution of the problem. The problem is usually reduced in this case to the Kohn–Sham (KS) equations requiring a self-consistent solution. From a numerical point of view, this can be done in several different ways, e. g. by using the plane-wave cutoff approximation or real-space methodologies [33]. In both cases, the main idea is that the occupied states of the electrons generate a charge density that corresponds to the same potentially used to derive KS equations.

In the context of LDSNs, depending on the specific application at hand, nanostructure modelling can be approached based on several different techniques. The top-down approach provides us a tool to construct a hierarchy of mathematical models of various complexity for semiconductor device modelling [55]. As the size of semiconductor devices become smaller, quantum effects, non-homogeneity and defects, along with surface effects, become

increasingly important. As a result, an increasing attention is paid to a hierarchy of mathematical models for nanostructures that can be constructed based on the bottom-up approach, starting from the first-principle methods. In a number of cases, this allows us to develop multiscale techniques based on subsequent averaging procedures (e. g., [79]). In modeling LDSNs, it is important to retain the computational efficiency while coupling the scales. Several approaches have been suggested in the literature to address the problem of scale coupling in the context of modelling nanostrucrures. Classifying multiscale methods, some authors even put the coupling methodologies into a separate group, identifying them with the "direct" coupling methodologies [76]. Note, however, that a coupling procedure is required regardless whether we follow the top-down or bottom-up approach, without formally combing them. A review of several methodologies for the atomistic to continuum coupling can be found in [14]. Other multiscale approaches are based on various forms of averaging and coarse grained techniques [18,80]. In the context of nanostuctures with interfaces such techniques have been recently discussed in [40]. Among recently proposed techniques in this direction, we also note [45], where based on the variational multiscale methodology, the authors developed an extension of the two-scale bridging technique to quantum mechanical/continuum coupling. They provided interesting examples, including the coupling procedure between a virtual atom cluster (VAC) model for the continuum modelling with tight binding calculations. In its essence, however, their approach is the top-down approach discussed above. A concurrent multiscale approach that allows one to integrate different scales "seamlessly" was proposed in [46] for metals. Finally, we note that several multiscale techniques based on the renormalization group approach have also recently been discussed [28,31]. The latter approach may prove to be potential useful for nanostructures if the renormalization is applied to atomistic models. The underlying idea in the development of all these new methodologies is to achieve "not only higher accuracy, but also more efficient, cost-effective and if possible simpler computational methods in electronic structure calculations" [5,49].

Many applications of LDSN, and in particular quantum dots, make the simulations based on atomistic methodologies (ab initio, molecular dynamics or Monte Carlo) impractical. While dealing with an isolated nanostructure we have to deal with at least two scales, the atomic scale at the interfaces and the mesoscopic scale of the structure itself, any such a structure embedded into a working device would require dealing with much more scales. It is this multiscale nature of the problem that makes atomistic approaches very problematic to apply in an efficient manner in applications ranging from basic nanoelectromechanical systems (NEMS) [76] to the development of quantum dot-protein bioconjugate nanoassemblies used for imaging in systems biology [50], or in LDSN applications for RNAi technologies [12]. The field of biological and biomedical applications of LDSNs will continue to grow in the context of the development of new biosensing methodologies [2,36]. By conjugating certain proteins to quantum dots a new class of bioluminescent probes can be created [20]. The models describing these processes and systems are intrinsically multiscale. But even in relatively simple physics applications, the complexity of the problem will increase substantially if we take into account the wetting layer on which the quantum dot is grown. Furthermore, such a systems approach in considering the quantum-dot/wetting layer as a coupled structure will lead to the necessity of the formulation of correct boundary conditions and dealing with an additional disparity in spatial scales between the dot and the wetting layer. This issue of multiple scales and the formulation of correct boundary conditions in this case has been dealt with only recently [58].

In moving to more complicated cases, such as those, for example, discussed above in the context of biological and biomedical applications, an averaging over atomic scales is required. It can be carried out by a number of techniques available, and in particular by the empirical tight-binding, the pseudopotential methodology, or by using the $k \cdot p$ approximation. As we need to address the problem in a systemic way and to include a range of additional effects that are pronounced at larger-than-atomistic scales, we note that the $k \cdot p$ theory represents the electronic structure in a continuum-like manner and as such is well suited for incorporating additional effects into the model, including strain relaxation and piezoelectric effects. Within this framework, we can apply a range of powerful numerical discretization procedures well established in mechanics of solids, including finite element methods (FEM). The entire problem can be solved numerically in a computationally efficient manner. It is worthwhile to note further that many methodologies described above, including the KS approach, use a representation of the wave function in a way similar to FEM:

$$\Psi(\mathbf{r}) = \sum_{i=1}^{n} \alpha_i \psi_i(\mathbf{r}) \tag{7}$$

with $\{\psi_i\}$ being a set of the basis functions and $\{\alpha_i\}$ being the set of the coefficients to solve for. For example, models

based on linear combination of atomic orbitals (LCAO) use the representation (7) as does the tight binding model.

Interface boundary conditions in nanostructure modelling deserve special attention. As mentioned, accounting for the correct boundary conditions is often a non-trivial task [58]. Furthermore, when coupling different scales in atomistic and continuum theories, one needs a procedure that should connect these two levels of modelling, atomistic and continuum. Different approaches to construct such procedures have been discussed in the literature. For example, in the context of nanoidentification problems, the authors of [35] surveyed existing so-called "handshake" approaches to coupling the localized fine-grain (e. g., atomistic) domains with their coarse-grain counterparts, where in the latter case the continuum-based modelling is acceptable. Based on the Fourier analysis of the lattice structure, they focused their attention on a particular case of this procedure that allowed them to derive multiscale boundary conditions for the specific problem they analyzed. In the remainder of this section, we show how simple averaging procedures at the fundamental atomistic level allows us to couple quantum mechanical and continuum models for LDSN bandstructure studies in an efficient computational manner. As we have seen, many interesting applications of LDSNs are connected with their optical properties. The main tool for the analysis of the optical properties of these structures is based on atomistic models of the Schrödinger–Poisson (SP) type. However, this model alone is usually not sufficient. Indeed, we recall that the formation of these structures in an industrial setting is based on a competition between the surface energy in the structure and strain energy, making mechanical effects paramount in determining and optimizing the properties of these structures. In addition, coupled effects, such as piezoelectric, could also be important, as it is the case for wurtzite materials (materials with hexagonal crystal lattice). The piezoeffect, responsible for the two-way coupling between mechanical and electric fields, is a coupled electromechanical phenomena that is convenient to describe with continuum models [51]. Moreover, as we have recently discussed in [56], nonlinear effects may also become important. As a result, in studying optoelectromechanical properties of low-dimensional semiconductor nanostructures it is essential to combine atomistic and continuum models.

Let us highlight how it can be done. We start from incorporating the lattice mismatch in the models for bandstructure calculations by defining the strain associated with that as a mismatch between two material layers. This is followed by the consideration of the Schrödinger–Poisson model where we account for the piezoelectric effect by coupling the SP model with the model for piezoelectricity. The latter procedure is carried out naturally within the $k \cdot p$ approximation of the electronic structure. This implies an averaging procedure over the atomistic scales, but as a trade-off, it allows us a straightforward coupling of the atomistic part of the model (Schrödinger–Poisson) with its continuum counterpart (elasticity with piezoeffect). The complete model is then implemented in a finite element (or finite difference) code. Recent results on the influence of electromechanical effects, including piezoelectric and strain contributions, on optoelectronic properties of the structures can be found in [56] where both linear and nonlinear strain components were considered.

The $k \cdot p$ approximation is based on the first-principle envelope function theory [10,25,39] and offers a computationally attractive tool for simulating LDSNs and the opportunity to incorporate additional effects within its framework. As all techniques arising from the effective mass theory approximations, where an appropriate fitting the model with experimental parameters is required, in the applications of $k \cdot p$ we may have to deal with the problem of spurious solutions, but several methodologies exist now to overcome this difficulty [40]. In the context of modelling LDSNs, the $k \cdot p$ framework provides a way for consistently incorporating some of the key larger-scale effects that influence the band structure computed with the SP model. Before proceeding to the description of the main implementation steps of this framework, recall that the accuracy of the $k \cdot p$ approximation is dependent on the set of basis functions that span the functional space where we seek the envelope function. A practical balance between the physics of the problem and its computational complexity for LDSNs do not usually lead to the choice of "n" in (7) higher than 8, which is the case, for example, for wurtzite semiconductors. This leads to models based on the 8×8 Hamiltonian. From a physical point of view, the model is based on 6 valence subbands and 2 conduction subbands, accounting for spin up and down situations and has the form of (5) requiring the solution of the following PDE eigenvalue problem with respect to eigenpair (Ψ, E):

$$\begin{aligned} H\Psi &= E\Psi\,, \\ \Psi &= (\psi_S^{\uparrow}, \psi_X^{\uparrow}, \psi_Y^{\uparrow}, \psi_Z^{\uparrow}, \psi_S^{\downarrow}, \psi_X^{\downarrow}, \psi_Y^{\downarrow}, \psi_Z^{\downarrow})^T\,, \end{aligned} \tag{8}$$

where $\psi_X^{\uparrow} \equiv (|X> \,|\uparrow)$ denotes the wave function component that corresponds to the X Bloch function of the valence band with the spin function of the missing electron "up", the subindex "S" denotes the wave function component of the conduction band, etc, and E is the electron/hole energy, as before.

Of course, the form of the Hamiltonian in (..) depends on a particular problem at hand, but a generic representation of the Hamiltonian in the $k \cdot p$ theory can be given as

$$H \equiv H^{(\alpha,\beta)}(\vec{r}) = -\frac{\hbar^2}{2m_0}\nabla_i \mathcal{H}_{ij}^{(\alpha,\beta)}(\vec{r})\nabla_j \,, \qquad (9)$$

where $\mathcal{H}$ is defined by the standard Kohn–Luttinger Hamiltonian or by its refined version based on the Burt–Foreman correction, accounting for the properties of degenerate valence states in an electric field. It represents the kinetic energy plus a nonuniform potential field and other effects contributing to the total potential energy of the system. The superindices (α, β) denote a basis for the wave function of the charge carrier.

Next, we have to incorporate into the model (8), (9) strain relaxation effects in LDSNs. In a sense, accounting for strain effects in this model provides a link between a microscopic (quasi-atomistic after averaging) description of the system with the effects that are pronounced at a larger-than-atomistic scale level as a result of interacting atoms. Indeed, in the case of self-assembled quantum dots, for example, during their growth from the crystal substrate wetting layer, atomic displacements *collectively* induce strain in our finite structure. This fact leads to a modification of the bandstructures obtainable for idealized situations without accounting for strain effects.

Fundamental works in the area by Pikus and Bir, Rashba and Sheka, as well as many others (e. g., [9]) has lead to what is now termed as the Rashba–Sheka–Pikus (RSP) Hamiltonian. Recently, such a Hamiltonian has been applied for the modelling of LDSNs, in particular those made of wurtzite materials (e. g., [23]). The question remains, however, on how to resolve adequately physical effects at edges, corners, and interfaces, including strain nonhomogeneities. Although such effects are quite important in many cases, and in particular for a wide range of quantum dot applications, conventional models for bandstructure calculations are based on the original representation of strain for the bulk materials [9] where strain can be treated on the basis of infinitesimal theory with the linear Cauchy relationships between strain and displacements. Unfortunately, geometric irregularities can make such approximate models insufficiently accurate.

Another type of nonlinearity that is worthwhile mentioning in the context of modeling LDSNs is related to material nonlinearities. For example, can we still use linear stress-strain relationships in the modelling of LDSN? Since for LDSNs, strain remains orders of magnitudes smaller than their elastic limits, the linear relationship is acceptable, at least in a first approximation. Nevertheless, material nonlinear effects may still be important. Firstly, semiconductors are piezoelectrics and higher order effects may become important at the level of device simulation. Secondly, elastic and dielectric coefficients, being functions of the structure geometry, are nonlinear, but the elasticity in this field is treated by the valence-force-field approaches.

Another very important point is related to the definition of the total potential energy when modelling LDSNs, in particular those made of wurtzite materials. For quite some time, it has been emphasized that both deformational energy and piezoelectric field functionals should be included consistently in the formulation of problems where coupled electromechanical phenomena are pronounced [51,59,66,83]. However, most results obtained so far in the context of bandstructure calculations are pertinent to minimization of elastic energy only [23]. It is true that in some cases, such an approach could be sufficient, in particular for zinc-blende materials (materilas with cubic crystal lattice) and where the piezoelectric effect is relatively small, but it does produce inaccurate results in other cases, in particular for wurtzite-based LDSNs. Furthermore, if geometric irregularities are accounted for with nonlinear strain-displacement relationship [62], the resulting coupled models based on the equation of elasticity and the Maxwell equation in dielectric approximation [51,59] become nonlinear. Even in the linear approximation, the coupling between the field of deformation and the piezoelectric field is of fundamental importance [34,83].

One of the main advantages of the $k \cdot p$ theory lies in its simplicity, but this comes at a cost of being required to fit experimental parameters into the model and generally the number of such parameters increases with the requirement of higher accuracy. For example, the model (8), (9) we described above for wurtzite-based LDSNs would contain 10 parameters. In order to reduce this number, it is important to seek any prior knowledge about the problem such as a specific geometrical shape of LDSN under consideration. Indeed, in the case of cylindrical geometry, the above model can be reduced to a simpler one. As it has been demonstrated in [41], this can be done by applying the Sercel–Vahala (SV) approach to the Rashba–Sheka–Pikus strain Hamiltonian (9) with details for WZ CE3 materials given, e. g., in [23]. As usual, Hamiltonian entries in this case will remain PDE operators, but their representations will be simplified [41]. While the originally discussed model still need to be applied for most quantum dot structures, its simplified version is convenient to use for modelling rods, cylindrical nanowires, as well as many superlattices.

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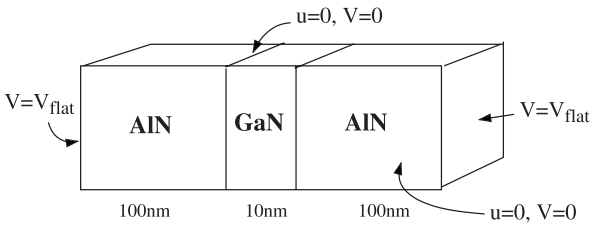


Multiple Scales and Coupled Effects in Modelling Low Dimensional Semiconductor Nanostructures: Between Atomistic and Continuum Worlds, Figure 2
A schematic representation of the geometry of the three-layer AlN/GaN WZ nanostructure

Now, we will highlight the main steps of incorporating coupled physical effects in modelling LDSNs, on the example of strain relaxation and piezoeffect. Firstly, we reduce the Maxwell equation to its dielectric approximation

$$\nabla(\epsilon\nabla\varphi) = -\rho + \nabla\cdot(P^s + P^p) \tag{10}$$

and solve it *simultaneously* with equilibrium equations by using, e. g., the finite element methodology:

$$\frac{\sigma_{xx}}{\partial x} + \frac{\partial\sigma_{xy}}{\partial y} + \frac{\partial\sigma_{xz}}{\partial z} = 0\,, \tag{11}$$

$$\frac{\sigma_{xy}}{\partial x} + \frac{\partial\sigma_{yy}}{\partial y} + \frac{\partial\sigma_{yz}}{\partial z} = 0\,, \tag{12}$$

$$\frac{\sigma_{xz}}{\partial x} + \frac{\partial\sigma_{yz}}{\partial y} + \frac{\partial\sigma_{zz}}{\partial z} = 0\,. \tag{13}$$

These equations are coupled by constitutive stress-strain relationships which differ depending on crystal configuration of the lattice [51,56,59]. In (10) P^s and P^p are spontaneous and strain-induced polarization, respectively.

Secondly, the outputs from this model allow us to define the Hamiltonian of system (9) on the same computational grid.

Thirdly, by solving the remaining eight coupled elliptic PDEs (8), we find both eigenfunctions and energies corresponding to all subbands under consideration.

This procedure can be extended to account for the carrier density and charge, in which case an additional coupling loop is necessary between the Schrödinger and Poisson parts of the model [56].

This procedure can be used for modelling most LDSN, including dots, rods, wires, and superlattices. As a representative example in Fig. 3 we show electronic states in the conduction band in a structure depicted in Fig. 2. Different confinement patterns under coupled and uncoupled situations have important practical implications.

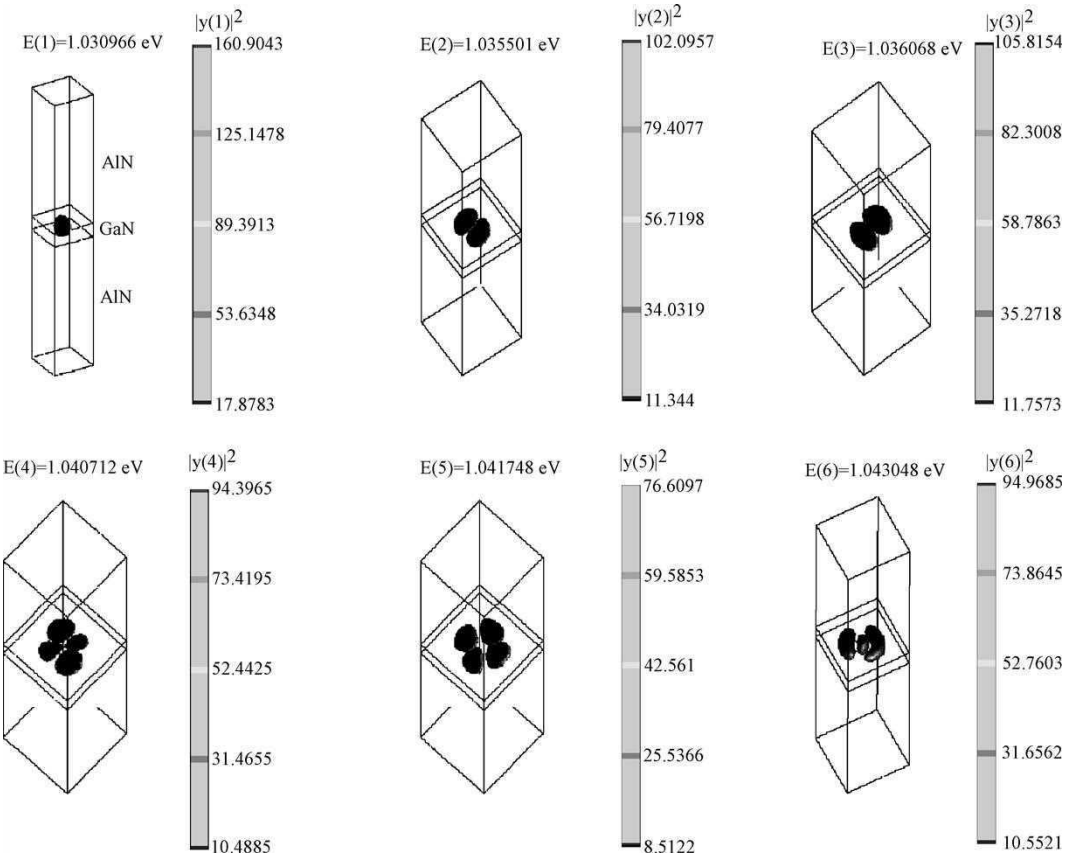
Indeed, LDSNs are designed with an ultimate goal to be used in functional devices where we would like to preserve their properties. For example, in designing new optoelectronic devices, we want to preserve properties of LDSNs such as quantum dots. When such LDSNs are studied theoretically, atomistic (zero-dimensional) density of states in quantum dots allow us to predict some of the characteristics of such structures, e. g. optical gain. If models used for such predictions are uncoupled, a theoretically predicted optical gain can be reduced in practice which may in some cases reduce or even prohibit lasing from the ground state. The reason for that lies with the fact that strain and piezoelectric effects may lead to the elongated ground state carrier function, and hence to a smaller overlap between the electron and hole wave functions, resulting in very different properties as compared to the uncoupled case.

Incorporating New Effects

In the previous section, we discussed two important effects that can substantially influence electronic bandstructure calculations, strain relaxation and piezoeffects. It has been known for quite some time that we have to deal with an inter-dependence between confinement, strain and piezoelectric effects, but quantitative results with the coupling effects accounted for in predicting nanostructure properties have started appearing relatively recently (e. g., [23,56,66] and references therein). The effects of strain and piezo-charge on the properties of LDSNs have been analyzed within the framework of the envelope function approximation as well as within other approaches discussed in the previous section. As we have already emphasized, a systematic approach is required in incorporating such effects into the existing models. In this section, we briefly review other important coupled effects that ultimately should be incorporated in the bandstructure calculation procedures.

Coupled Phenomena due to Mechanical and Electric Fields Interactions

The piezoeffect is one of the most important examples of electromechanical coupling where mechanical and electric fields interact with each other in a two-way interaction manner. The models for coupled dynamic piezoelectricity were put on a rigorous mathematical basis relatively recently [51], and now it is a combination of the piezoelectric effect with semiconductor properties that has attracted attention of the engineers with expectations of a wide range of applications in coupled electronics, sensing and the development of environmentally friendly technologies [82]. Even a new word was coined to reflect these expectations: *nanopiezotronics*. Most of Group III–V com-



Multiple Scales and Coupled Effects in Modelling Low Dimensional Semiconductor Nanostructures: Between Atomistic and Continuum Worlds, Figure 3
States of conduction band electron confinement (thanks to Roy Mahapatra for producing a figure for this example)

pounds used for LDSNs, such as GaAs, have a cubic (zinc-blende) crystal structure and these materials are much better studied. However, it is known also that wide band gap materials such as GaN-based alloys lead to very different properties compared to their zinc-blende counterparts. Usually, they have a hexagonal (wurtzite) crystal structure and a much stronger piezoelectric effect compared to the cubic structures [3]. Anisotropic properties of the material make all the difference, resulting in different properties. The electromechanical coupling is not always linear, and nonlinear electromechanical effects such as electrostriction have recently attracted the attention of researchers working on the properties of LDSNs and materials [7,29,34,63]. The phenomenon of electromechanical coupling is also in the heart of new types of systems known as quantum electromechanical or nano-electromechanical systems (NEMS). In studying such systems quantum effects also become important, and the other level of coupling comes in this case from quantum mechanics where light is coupled to the matter. The first such coupled model was a model describing the photoelectric effect. A more complex type of coupling is observed in quantum electro-mechanical systems where mechanical motion is quantized with many interesting potential applications reported in the literature (e. g., [78] and references therein).

Coupled Effects due to Spatio-temporal Interactions in LDSNs

Although acting on very small scales, temporal effects (see p. 518 in [61]) can be important in a number of applications. These also include many types of NEMS such as quantum shuttle systems, quantum information processing and control. Furthermore, some effects in LDSNs such as Franz–Keldysh oscillations, observed originally in superlattices, require a more careful examination of spatio-temporal interactions in LDSNs. Other spatio-temporal phenomena that have recently been receiving increasing

attention are related to phase transformations [60] as they have been analyzed in LDSNs [42]. Such phenomena will become even more important for LDSN-based nanocomposites [65] due to the fact that many of their properties which promise new advances in nanotechnological applications are related to interface effects and phenomena.

Coupled Phenomena due to Thermal and Electric Fields Interactions

Another important group of coupled phenomena important in LDSNs is related to thermoelectricity. Indeed, thermoelectric effects can be substantially enhanced in LDSNs compared to their bulk counterparts [43]. The analysis of such effects is important in the context of the integration of these structures into optoelectronic devices [44]. Furthermore, it is believed that thermoelectric coupling phenomena can facilitate the next generation of electronics and optoelectronics [47].

Coupled Phenomena due to Thermal, Mechanical, and Electric Fields Interactions

It is not difficult to deduce from the above discussion that a combined effect of thermal, mechanical, and electrical fields should be considered. Models of coupled thermoelectroelasticity are known [52] and await their integration into the models for electronic bandstructure calculations. There is another important reason for incorporating coupled effects due to the thermal field at the nanoscale. Indeed, at the nanoscale junctions of LDSNs, the importance of such effects as local electron heating may also become important to account for [15]. In such cases hydrodynamic types of models are needed in a way similar to what was developed in the past for sub-micron devices [53,54,55]. Such models allow us to deal with non-equilibrium and nonlocal phenomena in an efficient computational manner. Recently, in order to deal with the nonequilibrium quantum many-body problem, the time dependent local deformation approximation theory was proposed allowing to recover both Kohn–Sham and the hydrodynamic formulations [77].

Coupling due to the Magnetic Field

While it is customary for the modelling of LDSNs to apply the Maxwell equation in its dielectric approximation, there are cases where such an approximation may not be sufficient and the full electromagnetic model could be required. With the magnetic field is accounted for, there are additional nonlinear effects that in many cases would need to be incorporated into the model. For example, it is known that the quantum dot nuclear spin polarization may depend nonlinearly on applied magnetic fields [48].

Many-Body Coupled Effects

Among such effects are excitonic effects whose importance has been emphasized by a number of authors (e. g., [23] and references therein). Furthermore, in addition to electron-hole Coulomb effects responsible for excitonic transitions, electron-electron Coulomb interactions and the associated Coulomb blockade phenomena, as well as other many-particle effects, may also be important in a number of applications of LDSNs. For example, in the context of quantum dot applications, Coulomb blockade phenomena reflect the finite capacitance of the dot and is effectively an energetic discrimination against two electrons of opposite spin being on the same dot.

More on Nonlinear Coupling

It is generally true that to better understand the electronic properties of materials with strong correlations between the electrons, nonlinear properties become important. One of the examples is provided by the Kondo effect which is particularly pronounced for the low temperature transport in LDSNs [71]. In addition to nonlinear coupled effects already discussed, in the context of excitonic effects it is important to remember that Rabi oscillations of excitons [75] can show a nonlinear signature in LDSNs such as quantum dot array systems. These oscillations have interesting implications in quantum information processing applications since in the case of a single quantum dot they correspond to the one-qubit rotation (e. g., [75] and references therein). Furthermore, the optical response from LDSNs is typically nonlinear [69].

Spin Coupling

Spin is the only internal degree of freedom of an electron, and it is natural to attempt to employ the spin-orbit coupling for creating electronic and optoelectronic devices with new functionalities. One of the possibilities includes the injection of nonequilibrium spins with further manipulations of spin polarization at given locations [73]. While coupled systems is a rule rather than an exception in quantum mechanics, spin-orbit coupled systems have a special place among them as they gave birth to the entire new branch of condensed matter physics, spintronics, where we deal with devices whose functionality depends on the manipulation and control of the spin rather than the charge of electrons.

Applications and Concluding Remarks

As we have seen, LDSNs have led to a number of conceptually new ideas in many applications. Most of these ideas are related, in one way or another, to coupled phenomena being exploited and being put to work in practical applications. By now, strong coupling of light and matter at the single-photon level has led to many important advances [4]. LDSN photonics is an important player in optical information processing [67] and quantum-dot-based photonic crystal lasers represent a reality of today [19]. We are able to create sophisticated nanowires and provide a conceptual framework for nanomachines. In addition to the orbital, we can exploit the spin degree of freedom of the electron and analyze its applicability in spin-based quantum computing, e. g. with the spins of electrons confined to quantum dots [11]. Spin-quantum-NEMS is another example of such an exploitation [22]. We can use LDSNs in energy saving technologies, e. g. in solar panels, as well as in acousto-electronics, photonics, and spintronics with many exciting new developments in these fields happening over the recent years. As the range of applications of LDSNs continue to grow the complex systems science approach in modelling these structures becomes increasingly important. As we have highlighted in the previous sections, in developing new models for LDSNs a systematic combination of bottom-up and top-down techniques is necessary. Based on such a combination a hierarchy of mathematical models of various complexity can be constructed with coupled effects being incorporated in a systematic manner.

Developing this idea, we have discussed two main approaches to nanostructure modelling and highlighted the main procedures for the coupling between quantum mechanical and continuum models. Our approach to multiscale modelling of nanostructures is based on an initial averaging of the quantum mechanical models over the atomic scales and their subsequent coupling to the continuum models. This approach is sufficiently flexible to incorporate other coupled effects discussed in the previous section. We have emphasized that in assisting the design and optimization of new LDSN-based systems by developing the models for LDSNs , it is essential to account for the coupled effects that may lead to well pronounced modifications of properties of the systems being designed. The modelling framework described here is applicable to both low-density isolated LDSNs as well as dense LDSN arrays. The latter is important, given the fact that many systems we have to deal with can be viewed as complex networks. This also includes quantum networks based on LDSNs with application to quantum information processing [21] and the usage of LDSNs in biological network applications [36]. The area of applications of LDSNs in biology and biomedicine will continue to grow rapidly. Quantum dot-based bioconjugate nanoasembly promises to revolutionize the world we live in. A bridge between biology and nanoscience is being created and such complex systems as DNA-NEMS provides just one, albeit very important, example of this trend. Systems biology and systems science approaches in analyzing such coupled systems are becoming more important than ever and it opens new opportunities for a wider applications of these approaches in this exciting interdisciplinary area.

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