Workshop:
Theory, Modelling and Computational Methods for Semiconductor Materials and Nanostructures

University of Manchester, Sackville Street Building
31st January – 1st February 2008

Topics:
Theory, Modelling and Computational Methods for Semiconductor Materials and Nanostructures

Chairs:
- Max Migliorato from the University of Manchester
- Matt Probert from the University of York

Overview
Modelling, theory and the use of sophisticated computational tools have the potential to represent a substantial cost and time saving for R&D. The development of high speed computer architectures is finally allowing the ordinary use of accurate methods for calculating the structural, thermodynamic, vibrational and electronic properties of semiconductors and their heterostructures.

This IOP sponsored workshop, cosponsored by scientific software companies Accelrys and Silvaco, will run for two days, with the objective of bringing together UK and international leading experts in the field of theory of group IV, III-V and II-VI semiconductors together with postdocs and students in their early stages who will benefit from an introduction to a very vast field at this influential point in their careers. Invited, contributed talks and poster presentations will take place, together with two software presentations, tutorials and hands-on sessions to train young and older researchers alike in the use of existing software packages, which will include Castep (DFT) and Silvaco (Device Simulations).

An EPSRC presentation and discussion forum for PIs will also take place.

Topics
- Density Functional Theory Calculations
- Tight Binding, Pseudopotential and Effective Mass Models for Electronic Structure
- Empirical Potential Methods for Calculation of Structural Properties
- Optical and Transport Properties of Quantum Nanostructures including Colloidal and Nanotubes
- Dilute Magnetic Semiconductors
- Laser Devices
- Photonic Structure
- Electronic Devices
Locations map:
School of Electrical and Electronic Engineering,
The University of Manchester,
PO Box 88, Sackville Street Building,
Sackville Street, Manchester, UK, M60 1QD
Sponsors

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Program

9-10.00 coffee and registration

10.00 Opening remarks (Max Migliorato – University of Manchester)

**Ab Initio Modelling (chair: Jean Marc Jancu)**
10.05 Invited: Dzidka Szotek (Daresbury Laboratories)
“Ab-initio Materials Modelling for Novel Electronics”
10.45 Hannu-Pekka Komsa (Tampere University of Technology, Finland)
“Band offset calculation for semiconductor systems with dilute concentration or complex structure”
11.10 Steven D Kenny (Loughborough University)
“Modelling Fullerenes on Si (100)”
11.35 Invited: Stanko Tomic (Daresbury Laboratories)
“Comparative analysis of the electronic structure of III-V’s semiconductors from B3LYP and PBE0 functional”

**Software Presentations (chair: Matt Probert)**
12.15 Jacob Gavertin (Accelrys)
12.40 Ahmed Nejim (Silvaco)
13.05 working Lunch, Networking, Posters

**Activity 1&2: Hands on Session**
13.10-15.10 Materials Studio
13.10-15.10 Silvaco
15.00 Coffee

**Effective Mass Approximation (chair: Stanko Tomic)**
15.20 Invited: Francois Peeters (University of Antwerp)
“Electronic structure calculation of self-assembled quantum dots and molecules”
16.00 Sergey Rybchenko (University of Hull)
“Conduction-band crossover induced by misfit strain in III-V SAQDs”
16.25 David C. Hutchings (University of Glasgow)
“Determination of nonlinear optical coefficients in a semiconductor superlattice using k.p bandstructure methods”

16.50 Break
17.00 Sorcha Healy (Tyndall National Institute, Cork, Ireland)
“A combined theoretical and experimental analysis of gain and loss processes in 1.5 µm quantum dash lasers”

**Computational Methods (chair: David Whittaker)**
17.25 Samir Rihani (University of Cambridge)
“A Finite Element Method Application to Semiconductor Quantum Well Structures: Nonparabolic bound and quasibound states determination”
17.50 Anurag Srivastava (ABV- Indian Institute of Information Technology and Management, Gwalior-10 India)  
“Pressure Induced Structural Transitions in InSb:GaSb mixed semiconductor”

18.15 Break for Social Dinner (8pm)  
Summary: 3 invited, 7 contributed, 2 Presentations

Friday 1st February 2008.  
9-9.20 coffee and registration

Empirical and semi-empirical (chair: Dzidka Szotek)  
9.20 Invited: Gabriel Bester (MPI - Stuttgart)  
“Atomistic Pseudopotential Theory of Excitonic Effects in Nanostructures”  
10.00 Marco Califano (University of Leeds)  
“Auger processes in the absence of the hole: the effect of surface trap states and  
electrochemical charging on the electron intraband decay time in CdSe nanocrystals”  
10.25 Raman Garg (University of Manchester)  
“Strain Dependence of the Piezoelectric Coefficients for Pseudomorphically Grown  
Semiconductors”  
10.50 Thomas Hammerschmidt (University of Oxford)  
“Evidence for Reduction of the Critical Nucleus in QD Stacks”

11.15 Coffee

Tight Binding Method (chair Gabriel Bester)  
11.40 Invited: Jean-Marc Jancu (LPN-CNRS Paris)  
“Atomistic simulations in materials science: from bulk properties to nanostructures”  
12.20 Andrew Lindsay (Tyndall National Institute, Cork, Ireland)  
“Role of N cluster states in the band structure of GaNxA s1-x and related alloys”  
12.45 working Lunch, Networking and Posters

Activity 3: presentation for Principal Investigators and discussion forum  
13.15 Matthew Ball (EPSRC - Materials Panel)  
"The EPSRC Materials Programme: The Year Ahead"  
Followed by a discussion

Photonic and Electronic Devices (chair: Francois Peeters)  
14.20 Tim Schmielau (Sheffield Hallam University)  
“Implementation of a Quantum Cascade Laser Simulator based on Nonequilibrium  
Green Functions”  
14.45 John R Barker (University of Glasgow)  
“3D Non-Equilibrium (Keldysh) Green Function modelling of 4 nm channel silicon  
nanowire devices with wrap-round gates”  
15.10 Invited: David Whittaker (University of Sheffield)  
15.50 Concluding remarks from the workshop chairs

16.00 End  
Summary: 3 invited, 6 contributed, 1 Presentation
Poster Session (Thursday 13.05-15.20 and Friday 12.45-14.20)

1. “Pseudopotential calculations of interband and intraband optical transitions in InAs nanocrystal quantum dots”, Puangmali, T; Califano, M.; and Harrison, P. (University of Leeds)
4. “Physical Modelling of δ-doped GaAs/AlGaAs HEMT”, Muhammad Mohiuddin, S. Arshad, A. Bouloukou, A. Sobih and M. Missous (University of Manchester)
5. “Theoretical analysis of 1.55 µm emitting GaInNAs quantum dots”, Stanko Tomić, (STFC Daresbury laboratory)
6. “Theoretical modelling of manipulation of covalently bound molecules using atomic force microscopy”, N. Martsinovich and L. Kantorovich (King's College London)
7. “Applicability of k·p Method for Modelling of Type-II InAs/GaSb Superlattices”, B. H. Hong, S. I. Rybchenko, I. E. Itskevich, and S. K. Haywood (University of Hull)
8. “Interacting electrons in semiconducting carbon nanotube quantum dots: a 2-band effective mass approach” Mervyn Roy and P. A. Maksym (University of Leicester)
9. “Two-dimensional physical modelling of InP-Based Single Heterojunction Bipolar Transistors (SHBTs)” T. Tauqeer, J. Sexton and M. Missous (University of Manchester)
10. “Plane wave methodology for electronic structure of single quantum dot” Stanko Tomić and Nenad Vukmirovic, (STFC Daresbury laboratory) & (University of Leeds)
11. “Investigations of the Kink effect in InAlAs/InGaAs pHEMTs”, Shahzad Arshad, M. Mohiuddin, A. Bouloukou and M. Missous (University of Manchester)
13. “Empirical Bond Order Potential for calculating the elastic properties of epitaxial InGaSbAs layers”, Vesel Haxha and Max Migliorato, (University of Manchester)
14. “Ab initio calculations of electron energy loss near edge structure of ternary alloys: AlGaN”, David Holec and Colin Humphreys (University of Cambridge)
15. “Multi-Band k·p Calculations for Valence Band Structure of Strained Type-II InSb/InAs Quantum Dots”, G. H. Yeap, S. I. Rybchenko, R. Gupta, I. E. Itskevich, and S. K. Haywood, (University of Hull)
Abstracts of Thursday's Talks
Invited

Ab-initio Materials Modelling for Novel Electronics

Z. Szotek, Daresbury Laboratory, Daresbury, Warrington, WA4 4AD, UK

The formulation and some challenging applications of the self-interaction corrected local spin density (SIC-LSD) approximation are overviewed. The focus is on correlated d and f electron materials of possible interest for spintronics. In particular, the Mn-doped semiconductors GaN, GaP, GaAs, and Mn- and Co-doped ZnO are discussed. In addition, the electronic properties and exchange splittings of rare earths doped GaN and GaAs are presented. Finally, spinel ferrites, such as MnFe$_2$O$_4$ and NiFe$_2$O$_4$, of possible use as spin filters, and LiNiO$_2$ of interest for rechargeable batteries, are also reviewed.

Band offset calculation for semiconductor systems with dilute concentration or complex structure

Hannu-Pekka Komsa, Eero Arola and Tapio T. Rantala, Department of Physics, Tampere University of Technology, Finland

Band offsets are the key parameters in semiconductor heterostructure device design. Although not exceedingly demanding to obtain experimentally, a reliable method to predict the band offsets, and also, other material parameters computationally would be appreciated.

We present an approach based on first-principles DFT calculations of the heterostructure interface and respective bulk compounds. The electrostatic potential in the core regions of atoms is used to estimate the interface dipole and to align the band structures obtained from the independent bulk calculations. By using the ion core potentials we are able to accurately estimate changes of the potential, and thus, the band structure through the heterostructure. Here, we use, but are not restricted to, the planewave DFT code VASP for practical computations.

We first test our method on AlAs/GaAs superlattice system, for which the experimental band offset is well known. As the tests prove to be successful, we apply the method on GaAsN/GaAs and InGaAsN/GaAs interfaces. Computationally these interfaces are challenging due to low concentration of nitrogen and the interplay between indium and nitrogen. However, these material systems have gained a lot of interest in recent years due to their unusual properties.

We have focused on three different goals: extraction of accurate band offset values for dilute alloys, study of the interfaces of dilute alloys and study of the effect of indium and nitrogen interplay on the band offset. The method has proven to be reliable and should be readily applicable to other systems. Even strained materials or non-commutative band offsets can be expected to be extracted reliably.
Modelling Fullerenes on Si (100)

Paul C Frangou, David J King, Steven D Kenny and Ed Sanville, Department of Mathematical Sciences, Loughborough University, United Kingdom

Fullerenes on Si (100) are of great interest both from a fundamental science point of view and due to their potential for the creation of devices. They are one of a number of systems to have been proposed as a possible building block for a solid-state quantum computer. A number of experimental studies have studied fullerenes on Si surfaces, mainly focusing on the position of the fullerenes on the surface and the nanomanipulation of the fullerenes. Nanomanipulation in these systems has proven to be very successful in that it has shown to be reproducible and can be carried out at room temperature.

We will describe ab-initio work using the PLATO\(^1\) code on the simulation of both the C\(_{60}\) and the C\(_{82}\) fullerenes on a Si (100) surface. In this work we have studied the stability of these molecules on the surface to help elucidate the experimental results for this system. We will show that the smaller and higher symmetry C\(_{60}\) molecules appear to bind more strongly to the surface. We will also show that the orientation of the C\(_{82}\) molecule can have a large influence on its binding energy. Analysis of these systems has been performed through the use of the ideas in Bader’s atoms in molecules and utilising a new grid based algorithm\(^2\).

We will also present a study of the interaction between two C\(_{60}\) molecules on a Si surface. The interaction between multiple fullerenes on a surface is essential if we are to create devices from these systems. This work will show that when placed a short distance apart two C\(_{60}\) molecules can interact very strongly causing significant changes to the bonding within the fullerene cage.

Invited

Comparative analysis of the electronic structure of III-V’s semiconductors from B3LYP and PBE0 functional

Stanko Tomić¹, Barbara Montanari, and Nicholas M Harrison¹,²,
¹Computational Science and Engineering Department, STFC Daresbury laboratory, Cheshire WA4 4AD, United Kingdom, Department of Chemistry, ²Imperial College, London SW7 2AZ, UK

In order to study the electronic and optical properties of III-V zinc-blend and wurtzite semiconductor materials an approach providing a reliable estimate of band gaps while retaining an accurate and efficient method for computing the ground state energy surfaces is required. The hybrid exchange approximations to density functional theory (DFT) approach, such as the B3LYP and PBE0, were originally developed to improve the description of the ground state energetics of small molecules. Subsequently, they have been demonstrated to be significantly more reliable than the best gradient corrected (GGA) functionals for computing atomisation enthalpies, geometries and vibrational frequencies. The B3LYP and PBE0 have the following form:

$$E_X = E_X^{LSDA} + 0.2(E_X^{Fock} - E_X^{LSDA}) + 0.72 \Delta E_X^{GGA},$$

and

$$E_{XC} = E_{XC}^{PBE} + 0.25(E_X^{Fock} - E_X^{PBE})$$

respectively, where the LSDA, GGA, and PBE energies are taken from widely used functionals and $E_X^{Fock}$ is the non local Fock exchange energy. These functionals can be implemented readily and very efficiently within a Gaussian basis set as used in the CRYSTAL code¹. The main numerical approximation is the selection of the local Gaussian basis set.

For elements like Al, N and P, we use all electron triple valence 6-311G* basis sets; while for heavier elements: Ga, In, As, and Sb, we used pVDZ-PP relativistic effective core potentials and double valence basis sets. To avoid quasi linear dependence in the condensed phases all basis sets are truncated to have a most diffuse exponent of 0.12 a.u.,². Residual problems being removed by projecting out Bloch functions associated with eigenvalues of the overlap matrix that are below certain predefined threshold (~1-10 × 10⁻⁴ Ha) which affects the total energy by no more than a few mHa compared to full basis set calculation. This results in an approach that avoids the computational cost and numerical instability that result from using diffuse molecular basis sets in solids. In reciprocal space the Brillouin zone integration was performed using 29 symmetry irreducible points in k-space for zinc-blend structures and 50 k-points for wurtzite structure. Band gaps were obtained simply as Kohn-Sham eigenvalue differences at the Γ point for direct gap semiconductors and as a minimal energy difference between Γ₁₅ point and X₁ point or minimum along Δ direction in the case of the indirect gap materials (GaP, AlP, AlAs, AlSb). It has been shown that, at the experimental lattice constant, the B3LYP approximation predicts energy gaps in excellent agreement with those observed for the most of III-V semiconductor binaries,³. The predicted constants are, however, in better agreement with those observed when the PBE0 approximation is used: the B3LYP approximation systematically overestimates values of the lattice constant by 1-2%.

³ S. Tomić, B. Montanari, and N.M. Harrison, Physica E (in press)
Invited

Electronic structure calculation of self-assembled quantum dots and molecules

François Peeters and Vladan Mlinar, Departement Fysica, Universiteit Antwerpen, Groenenborgerlaan 171, B-2020 Antwerpen, Belgium

A full three-dimensional model for the calculation of the electronic structure of semiconductor quantum dots (QD) and molecules (QDM) grown on high index surfaces and/or in the presence of an external magnetic field was realized. The strain distribution of the self-assembled dots is calculated using continuum elasticity theory. The single particle states are extracted from a nonsymmetrized eight-band $k\cdot p$-theory. We fully take into account the effects of different substrate orientation by rotation of the coordinate system in such a way that one coordinate coincides with the growth direction. The tilted magnetic field, that can be in an arbitrary direction with respect to the quantum structure, is included through the Zeeman and the orbital effect by employing a gauge invariant scheme based on Wilson’s formulation of lattice gauge theory.

The role of piezoelectricity is pointed out for InAs/GaAs QD’s grown on [11k], k=1,2,3,…9 and for QDMs containing eight InAs/GaAs QDs grown on [11k], k=1,2,3 surfaces.

The variation of the transition energies of the QD and the QDM are obtained as a function of: 1) the substrate orientation, 2) the interdot distances in the molecule, and 3) the strength and orientation of the magnetic field.
Conduction-band crossover induced by misfit strain in III-V SAQDs

S. I. Rybchenko, R. Gupta, K. T. Lai, I. E. Itskevich, and S. K. Haywood, Department of Engineering, University of Hull, Hull HU6 7RX, United Kingdom

Self-assembled quantum dots (SAQDs) offer many opportunities both in fundamental and applied research. While possessing properties of the “artificial atom”, the SAQDs are fully compatible with traditional semiconductor technology and provide a prospective material for active media in optoelectronic devices. To cover a wider optical wavelength range, SAQD heterostructures using novel material combinations are continually being developed. A specific feature of SAQDs is large lattice-mismatch strain which is inherent to growth by the Stranski-Krastanov method. Significance of the effect of strain on the electronic band structure in SAQDs has been realised a decade ago. In particular, it has been shown that due to large lattice misfit (≥ 2 %), strain-induced shift and/or splitting of the band edges is comparable to the optical band gaps in the dot and/or matrix materials. However, modelling of the electronic band structure in III-V SAQDs has been largely limited to the fundamental band gap at the Γ-point of the Brillouin zone, as it appears in the unstrained materials. On the contrary, effect of the misfit strain on the gaps between the conduction bands of different symmetry has not been analysed specifically. Such an analysis is particularly important because the strain can have a dramatic effect on the conduction band, inducing a crossover of the Γ-, L- and/or X-valleys. In this case, the ground electron level in the SAQD heterostructure would be of different symmetry to that in the unstrained dot material, which would have a critical effect on the optical properties. We have examined the possibility of such conduction-band crossover in III-V self-assembled quantum dots. The strain problem was solved within the anisotropic continuum elasticity approximation using the Finite Elements Method. Size-quantized electronic levels were determined using the standard kp approximation. The analysis of band profiles in terms of standard deformation-potential theory shows that Γ-X crossover is realistic in the dot, while both Γ-X and Γ-L crossovers are possible in the matrix at the interface. We discuss sensitivity of the crossover parameters to the dot shape and size, as well as to the approximations used in modelling. In the particular case of realistic InSb/GaSb (001) SAQD heterostructures, we demonstrate occurrence of the Γ-L crossover effect for the ground electron state, with the ground-state optical transition becoming indirect in the k-space. The results of these calculations are in excellent agreement with recent photoluminescence data. The results obtained indicate that conduction band crossover induced by lattice mismatch is realistic for III-V SAQD heterostructures. Due to the critical effect this has on the optical properties, it needs to be taken into account in fundamental analysis and band-profile engineering.

1 D. Bimberg, M. Grudman, and N. N. Ledentsov, Quantum Dot Heterostructures (Wiley, Chichester, 1999);
Determination of nonlinear optical coefficients in a semiconductor superlattice using \textit{k.p} bandstructure methods

David C. Hutchings, Department of Electronics and Electrical Engineering, University of Glasgow, United Kingdom

Direct-gap semiconductors are leading candidates as nonlinear optical media for waveguide devices. Specifically, the ultrafast Kerr nonlinear refraction at 1.55\,\mu m in Al$_{0.18}$Ga$_{0.82}$As is around 1000 times that in silica. Similarly, the second-order nonlinear optical coefficient in GaAs is around an order of magnitude larger than conventional ferroelectric crystals. The growth, lithography and etching technologies for conventional III-V semiconductors are at a mature level and there is the potential prospect of monolithic integration with semiconductor diode laser pump sources. A key requirement is the ability to pattern the nonlinear coefficients across the device, for example in the implementation of quasi-phase-matching for efficient frequency conversion. One such technique is based on semiconductor superlattices combined with the technology of quantum well intermixing\textsuperscript{1}. Therefore it is imperative to develop a predictive capability for the nonlinear optical coefficients in both as-grown and intermixed semiconductor superlattice media.

Calculations of the nonlinear optical coefficients are based on \textit{A.p} perturbative expansions\textsuperscript{2}. This requires knowledge of both the momentum matrix elements and the energy differences between sets of electronic states. To this end a compatible \textit{k.p} bandstructure solver for superlattices has been developed. It uses a \textit{\Gamma}-point expansion of the singlet \textit{s}-states corresponding to the lowest conduction band and the \textit{p}-states both from the topmost valence band triplet (heavy-hole, light-hole and split-off) and the next conduction band triplet. Incorporating the higher conduction bands is essential to include anisotropy in the bandstructure algorithm, necessary to obtain non-zero second-order coefficients, and account for the substantial anisotropy in the third-order coefficients. A Fourier series expansion is taken for the incorporation of the superlattice structure, typically truncated around the seventh order. The effect of intermixing is the suppression of the higher-order Fourier terms. The figure shows an example calculation of the modification of the second-order coefficient under intermixing\textsuperscript{3}.

Figure. The calculated modification of the second-order susceptibility upon intermixing for a GaAs/AlAs superlattice in type-I (left) and type-II (right) phase-matching configurations for second harmonic generation. The vertical dashed lines indicate the half-bandgap.


We have used the 8-band \(k, p\) method to investigate the potential of InAs/InGaAsP/InP quantum dash-in-a-well devices for use in the 1.5 \(\mu\)m telecommunications window. We show that these quantum dashes have a unique band structure, with holes much more strongly confined than electrons. Figure 1 shows the band offsets and lowest confined state energies for an InAs quantum dash in a well (DWell) structure, calculated using an 8-band \(k, p\) envelope function Hamiltonian. Given the low electron mass and small conduction band offset, we calculate that there are no confined electron states in a single InAs dash in the given DWell structure (Fig. 1). By contrast the heavy holes see a deep confining potential in the quantum dash, and so the hole states are well confined in the dash, with a large splitting between heavy- and light-holes due to the dash strain. This stronger confinement of holes than electrons leads to improved gain characteristics in an ideal quantum dash. The outer well acts to confine the electron states, helping to maintain a strong overlap between the confined electron and hole wavefunctions, thereby giving low transparency carrier density and high differential gain in an ideal DWell structure. Photovoltage measurements confirm the strong hole splitting (Fig. 2). Analysis of the facet and spontaneous emission however show the presence of temperature dependent non-radiative current paths process and the onset of a temperature dependent optical loss, indicating the likely presence of similar loss mechanisms in 1.5 \(\mu\)m quantum dash and quantum well lasers.

Figure 1: Calculated conduction and heavy hole band edges for DWell. Unstrained band edges are given by dashed lines and electron ground state and heavy hole ground state are given by thin lines with circles at end points.

Figure 2. Photovoltage spectrum for DWell laser sample. TE (upper plot) spectrum shows clearly the onset of the first HH transition. TM spectrum (lower plot) shows the LH band and the 1.1\(\mu\)m transition, which can be attributed to the barrier.
A Finite Element Method Application to Semiconductor Quantum Well Structures: Nonparabolic bound and quasibound states determination

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²TeraView LTd. St John's Innovation Park, Cambridge CB4 0WS, United Kingdom

A finite element model (FEM) is implemented for solving the effective mass Schrödinger equation in an arbitrary layered semiconductor nanostructures with an arbitrary applied potential. The model also includes nonparabolicity effects, which become more important once the energy levels are comparable to the band gap of the material used. Nonparabolicity was included using an energy dependent effective mass where the resulting nonlinear eigenvalue problem was solved using an iterative approach. Our results were in excellent agreement with a more rigorous eight-band second order k.p calculation.

As well as giving a detailed description of the implementation of the finite element method we have also explored the application of different boundary conditions for the extraction of bound and quasibound states of the system. Example structures have been studied to demonstrate the accuracy of the calculation using the FEM.
Pressure Induced Structural Transitions in InSb:GaSb mixed semiconductor

Anurag Srivastava and Pankaj Srivastava, Computational Science Group, ABV-Indian Institute of Information Technology and Management, Gwalior-10 India
R. K. Singh, Department of Physics, Ch. Devi Lal University, Sirsa-25 India

The present paper is about the study of pressure induced structural phase transitions in InSb:GaSb mixed compound semiconductor, from its original ZnS type phase to the most stable high-pressure NaCl type phase. The computation has been performed using the three body potential (TBP) approach that takes care of long range and short range type interactions. The long range part of the approach consists of Coulomb and three body interactions whereas the short range part includes the van der Waals (dipole-dipole and dipole-quadrupole interactions) and repulsive terms of Hafemeister Flygare type (effective up to the next nearest neighbour). The findings with present TBP approach are well matched to the observed results for the end point members of this mixed system by the other workers. Under the application of pressure the role of short range interactions dominates in form of van der Waals contribution and is an important conclusion to the present study.
Abstracts of Friday’s Talks
Invited

Atomistic Pseudopotential Theory of Excitonic Effects in Nanostructures

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The confinement in all three space dimensions given in nanostructures leads to several new phenomena of fundamental interest that can be handled by different levels of theory. For nanostructures of small size, the atomistic nature and ensuing symmetry is most relevant and the system should be viewed as a large assembly of atoms. The adequate description then is atomistic in nature, such as in tight binding or pseudopotential approaches. For larger structures, the atomistic nature tends to become less important while particle-particle correlations become more relevant. In this size regime descriptions such as effective mass in the single band or in the multiband approach (k.p) followed by configuration interaction are the prevailing methods. I will present a theoretical framework, based on empirical pseudopotentials and configuration interaction calculations that enables us to address the intermediate length scale where both, the atomistic nature and correlations need to be retained. I will illustrate the method by showing recent applications in the realm of quantum dot physics where properties such as fine-structure\(^1\), piezoelectricity\(^2\) or Coulomb blockade\(^3\) have been investigated.

\(^3\) Ediger, Bester, et al., Nature Physics 3, 774 - 779 (01 Nov 2007)
Auger processes in the absence of the hole: the effect of surface trap states and electrochemical charging on the electron intraband decay time in CdSe nanocrystals

Marco Califano, Institute of Microwaves and Photonics, School of Electronic and Electrical Engineering, University of Leeds, Leeds LS2 9JT, United Kingdom

The absence of a phonon bottleneck in the electron relaxation from an excited p-like to the s-like state in chemically synthesised semiconductor nanocrystals is generally ascribed to an Auger-like process whereby the electron excess energy is transferred to the photogenerated hole which is excited to deep valence levels. However the fast relaxation of electrons observed in the absence of a hole or in the presence of a hole trapped in a surface state have raised serious questions about the suitability of this model.

The semiempirical pseudopotential calculations reported in this work show that electron-electron scattering in chemically reduced or electrochemically charged (i.e., hole-less) CdSe nanocrystals leads to short p electron lifetimes comparable to those calculated in the presence of a photogenerated hole delocalised in the dot core. Furthermore, I show that efficient energy transfer can also be achieved between a delocalised electron and a surface-trapped hole leading to p electron lifetimes in the (sub-) picosecond range for shallow traps and of hundreds of picoseconds for deep trap states, in quantitative agreement with the observed trend of increasing lifetimes in the presence of increasingly softer ligands.

The results presented here therefore show that, although alternative models for electron relaxation in CdSe nanocrystals may be consistent with the observed lifetimes, Auger cooling cannot be ruled out based on the present experimental evidence.

The fast sub-picosecond electron relaxation times calculated in the presence of a hole localised in a shallow surface trap raise the intriguing question of whether in earlier measurements in TOPO-capped nanocrystals ¹ the hole was indeed delocalised within the dot core, as it was believed at the time, or whether it could have been in a trap state.

Strain Dependence of the Piezoelectric Coefficients for Pseudomorphically Grown Semiconductors

Raman Garg and Max Migliorato, School Electronic and Electrical Engineering, University of Manchester, United Kingdom
G.P.Srivastava, School of Physics, University of Exeter.
T.Hammerschmidt, Department of Materials, University of Oxford

In epitaxially grown semiconductors, the piezoelectric effect can be observed via the off-diagonal strain tensors that exist in quantum wells, grown on (111) substrates, quantum wires and quantum dots. Piezoelectric effects in such nanostructures have attracted a substantial amount of interest in recent years and were identified as the source of experimentally observable anisotropies. Earlier work has considered only first-order piezoelectric effects and employed either the experimental piezoelectric coefficients of the bulk semiconductors or linear interpolation of the two compounds. Bester et al\textsuperscript{1} has pointed out that neglecting the second order effects leads to substantial errors in the calculation of piezoelectric fields. In our previous work\textsuperscript{2} we established an alternative reliable approach to calculating first and second order piezoelectric coefficients based on the semi-empirical formalism of Harrison\textsuperscript{3} and parameters obtained from the Density Functional Theory. Our model is based on expressing the direct and dipole contributions to the polarisation in terms of microscopic quantities that can be calculated within a DFT-LDA and DFPT (Density Functional Perturbation Theory) schemes. Our approach can be easily extended to any III-V semiconductor in the zinc-blende crystal structure.

We find that strain considerably modifies the value of the piezoelectric coefficients, which has important consequences for self assembled nanostructures such as quantum dots where shear as well as tetragonal distortions are present. For 7\% compressive strain in the layer and 7\% tensile strain in the growth direction (which is the case for InAs pseudomorphically grown on GaAs substrate), our model predicts a sign reversal of the piezoelectric coefficients $e_{14}$, $e_{25}$ and $e_{36}$ from negative to positive. This also explains several discrepancies between the theoretical and experimental observations made on nanostructures such as III-V quantum dots.

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\textsuperscript{2} M.A Migliorato, D Powell and A.G Cullis, Phys Rev B 74, 245332 (2006)
Evidence for Reduction of the Critical Nucleus in QD Stacks

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Growth of quantum dot (QD) stacks is a possible route to influence the lateral arrangement of self-assembled semiconductor QDs. In stacks of InAs QDs in GaAs substrates, the QDs in a new layer form preferably right above those in the previous layer. It is surprising, how the weak interactions of surface atoms with the buried QD trigger this ‘correlated’ growth. In this work we offer a quantitative explanation based on the influence of elastic interactions on the critical nucleus for QD formation.

In particular, we apply a recently developed Abell-Tersoff potential to realistic QD nanostructures and combine these results with classical nucleation theory. We will show that the scaling-law coefficients for the QD formation energy obtained with this approach are in good agreement with the results of a previously employed hybrid approach based on finite-element and density-functional theory calculations.

For the formation of a new layer of QDs on a capping layer above a layer of buried QDs, we study systematically the formation energy as a function of lateral distance of buried and free-standing QD. We find it to be minimal if the freestanding QD is placed exactly vertically above the buried QD, in line with the growth correlation observed in most experiments of stacked QD growth. The elastic interactions observed in our calculations lower the energy barrier for QD nucleation significantly as compared to nucleation in a single QD layer. The reduced size of the critical nucleus increases the nucleation rate by several orders of magnitude.
Invited

Atomistic simulations in materials science: from bulk properties to nanostructures

Jean-Marc Jancu, LPN-CNRS Marcoussis France

Availability of very powerful computer and improvement in atomistic methods have vastly improved our ability to model the physical properties of multi-million atom systems. Small details of the band structure such as spin splitting as well as global properties are reproduced in a quantitative way. The scientific perspectives opened by this digital revolution are obvious because almost all fields in nanosciences and nanoengineering fall within the field of application of atomistic simulations. This is particularly the case for the observation (e.g. understanding STM images of individual atoms), the prediction of new functionalities in matter at the nanometer scale, or for the study of optical properties of self-assembled quantum dots. A particularly striking example is the theoretical discovery of the intrinsic birefringence in ultra-short period superlattices which was successively observed at LPN¹. In this seminar, I illustrate how the recent developments of tight-binding² can be used to accurately compute the electronic states in semiconductor nanostructures having potential applications in spin-electronics, nano-electronics, and non-linear optics.

Role of N cluster states in the band structure of GaN_xAs_1-x and related alloys

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The band-anticrossing (BAC) model describes the rapid reduction of energy gap with composition in GaN_xAs_1-x in terms of an anti-crossing interaction between the host matrix conduction band edge and a single band of N resonant defect states, with the general increase of electron effective mass also explained through this interaction. Although the BAC model explains qualitatively the behaviour of dilute nitride alloys, it fails to provide an accurate quantitative description of many experimental results, including the observed variation with N composition x of the electron effective mass and gyromagnetic ratio in GaN_xAs_1-x. Detailed theoretical and experimental studies show a wide range of N states above and close to the conduction band edge in the dilute nitride alloy GaN_xAs_1-x, due to the formation of N-N pairs, where a gallium atom has two neighbouring N atoms, and due to the formation of other, larger, N clusters. We show that the tight-binding based Linear Combination of Isolated N States model (LCINS model), which treats explicitly the interactions between the host conduction band edge and this distribution of N states, explains quantitatively the observed non-monotonic variation both of effective mass and of gyromagnetic ratio with composition. Recent luminescence measurements have shown that two nitrogen pair states emitting at 1.488 eV and 1.508 eV contribute mainly, but to a different extent, to determining the steep increase in the electron mass observed in GaN_xAs_1-x for x~0.1%. Ultra-large LCINS supercell calculations assign the lower energy level to isolated N pairs and the upper states to N pairs perturbed by a nearby N atom, in disagreement with previous attributions but consistent with the electron mass data. We show that this unexpected ordering of levels occurs due to N atoms on certain neighbouring As sites reducing the overall strain energy associated with the N-N pair.

Implementation of a Quantum Cascade Laser Simulator Based on Nonequilibrium Green Functions

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We present our approach to implement a simulation code for quantum cascade lasers (QCLs) using nonequilibrium Green functions (NGFs), which leads to more efficient and less restrictive algorithms than earlier approaches.

Electron transport through QCLs under operation conditions is determined by the interplay between coherent transport and scattering. Nonequilibrium Green functions are ideally suited to describe both mechanisms on the same footing. The nonequilibrium steady state GFs are given by Dyson's equation $G(\Sigma) = G_0 + G_0 \Sigma G$ with periodic boundary conditions and an applied electric field. No a-priori assumptions (like that of local thermal equilibrium) about distribution functions are necessary other than the coupling to a bath of thermal phonons. All approximations are condensed into the choice of an appropriate self-energy functional $\Sigma(G)$. We use self-energies that fully depend on frequency, in-plane momentum and position in growth direction. The effects of some simplifying approximations typically used in previous simulation schemes\cite{1,2,3} are also discussed (like fixing the momentum arguments of the self-energy at typical values) and compared with our less restrictive approach. (cf. fig. 1) The steady-state nonequilibrium solution to the self-consistent problem is then found by iterating $G \rightarrow \Sigma(G) \rightarrow G(\Sigma)$, starting from suitable initial values.

Figure 1: Spectral function (thick lines) and self-energies (thin lines) of electrons calculated self-consistently using the full momentum dependence (solid lines) or momenta fixed at typical values (dashed). The spectral function determines a quasi-particle with its maximum giving rise to renormalized quasi particle energies and its broadening related to the dephasing that ultimately determines spectral broadening in optical transitions.

3D Non-Equilibrium (Keldysh) Green Function modelling of 4 nm channel silicon nanowire devices with wrap-round gates

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As silicon technology continues to mature it is gaining a new lease of life from the encouraging fabrication of prototype integratable MOSFET devices with advanced architectures that could permit Moore’s Law to continue well into the 2020s. Among the most promising are wrap-round gate silicon nanowire devices of which several prototypes exist experimentally and for which complete system integration schemes and connectivity architectures have been published\textsuperscript{1}.

In the past few years\textsuperscript{2} we have developed 3D non-equilibrium Green function (NEGF) codes that permit the modelling of such advanced silicon devices by self-consistently solving the Poisson equation and quantum transport equations throughout the full 3D device volume. The methodology has been used to model killer effects such as atomistic impurities and surface/interface roughness scattering, strain inhomogeneities that potentially cause strong variability in performance from erstwhile technologically identical devices. The present paper discusses the 3D NEGF method and its application to silicon nanowire devices with channels of length 4 nm and cross sectional dimensions 2.2 X 2.2 nm, comparable in scale to conjectured carbon nanotube devices. We show that the use of high-k dielectrics, metal wrap-round gate and highly doped source and drain (~$10^{21}$ cm$^{-3}$) leads to highly viable device structures. We note that NEGF methods are well placed to benefit from full-band structure modelling and density functional theory. In the present paper, possible problems in nanowire devices due to the atomistically discrete nature of the source and drain regions are discussed. The strong screening is shown to weaken considerably the effects of unwanted stray dopants and of granularity effects. Further work on developing the non-equilibrium quantum theory of polarisation and image force/screening treating will be needed to underpin the efficacy of the NEGF formalism. We conclude with a brief discussion of how this might be achieved.

\begin{figure}[h]
\centering
\includegraphics[width=0.4\textwidth]{figure1.png}
\caption{Schematic of the wrap-round silicon nanowire transistor aligned in the <100> direction showing coordinate system.}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=0.4\textwidth]{figure2.png}
\caption{Two different slices showing the iso-contours of the current density $j_x(x,y,z)$ source-drain voltage = 0.2 V; gate voltage =0.5 V.}
\end{figure}

\textsuperscript{1} J. Goldberger, et al., (2006), Nano Lett., 6, 973.
This talk is concerned with methods for modelling propagation of light in nanostructures, and their emission properties, at the level of solving Maxwell's equations with dielectrics and sources. Usually this is made more difficult because it is an open boundary problem; we are interested in structures where the internal optical modes are coupled out to the external world, so they are experimentally accessible.

I shall review a number of approaches, focusing in particular on Finite Difference Time Domain (FDTD) methods as a general work-horse. However, FDTD, especially in three dimensions, is very resource hungry, and for specific problems it is usually possible to do a lot better with a bespoke code. Indeed, this is a generally theme: efficiency can be bought at the cost of specificity.

I shall illustrate this proposition with examples from my own work on modelling of photonic crystals. Here we are interested in multi-layer structures, where each layer consists of a periodically patterned dielectric structures. The approach I use is a scattering matrix treatment which stitches together solutions obtained for each layer to calculate the properties of the structure as a whole. For a specific type of photonic crystal, a single layer patterned membrane, even greater efficiency can be obtained using a guided mode expansion method which I shall describe.
Poster Session
Pseudopotential calculations of interband and intraband optical transitions in InAs nanocrystal quantum dots

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An atomistic pseudopotential method is used to calculate the electronic and optical properties of surface-passivated spherical InAs nanocrystals. The calculated intraband (valence-to-valence and conduction-to-conduction) as well as interband (valence-to-conduction) absorption spectra reproduce the features of experimental results [1-3]. However, in contrast to the suggestions of k·p calculations [1, 2], we propose different explanations for the observed optical transitions in InAs quantum dots. The envelope functions of valence band maximum (VBM) and conduction band minimum (CBM) have prevalently p-like and s-like character, respectively. Thus, the absorption from VBM to CBM, which had previously been identified as the $1S_{3/2} \rightarrow 1S_{1/2}$ transition on the basis of k·p calculations [1, 2], is optically forbidden. Instead, our lowest calculated optical transition corresponds to the allowed VBM-1 to CBM transition. Our calculated intraband optical transitions are also in good agreement with recent photoinduced absorption measurements [3]. Starting from these results we propose a new interpretation of the optical features observed experimentally.

References:
**Ab initio modelling for advanced gate stack engineering**

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Extensive studies of thin oxide films with high dielectric constant are motivated by their prospective use in the next generation microelectronic devices (primarily, as gate dielectrics in metal-oxide-insulator field effect transistors (MOSFETS) and in volatile memory devices). Major effort in this field is currently focused on the reduction of electrically active defects in these materials and at their interface with silicon. Such defects have a detrimental effect on both device performance and reliability.

I shall review the state of ab initio modelling of defects in high-k materials and its impact on device engineering in view of the following questions:

1. What are the likeliest electrically active defects in the dielectric stack?
2. To what degree the concentration of these defects can be controlled by optimization of chemical composition and deposition/post deposition conditions?
3. How these defects affect device performance and reliability?

I shall discuss the properties of intrinsic defects created during the oxide film deposition on Si substrate (e.g. oxygen vacancies, interstitials and interface defects) as well as extrinsic defects formed as a result of the post deposition treatment (such as various forms of nitrogen, fluorine and hydrogen). A particular attention will be given to the theoretically predicted amphoteric character of oxygen vacancies with the implications for the high-k stacks functionality. Recent modeling of effects of atomic disorder and electron-phonon interaction will also be critically assessed.

Step-graded Hot Electron Injector Gunn Diode Modelling in SILVACO

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This paper presents continuing work on the development of a SILVACO model for a GaAs Gunn diode with hot electron injection based on a step-graded Al_\text{x}Ga_{1-x}As launcher. This device is epoxially grown at the University of Manchester and commercially manufactured by e2v Technologies (UK) ltd. for use in 77GHz Automotive Adaptive Cruise Control (ACC) systems. The device structure has a nominally undoped Al_\text{x}Ga_{1-x}As step-graded barrier (x from 1.7% to a maximum value of ~32%) with the two adjacent spacers to avoid dopant diffusion into the launcher. This is separated from the lightly doped transit region by a doping spike which is required to optimise the downstream electric field.

SILVACO provides a virtual wafer fabrication simulation environment in which two or three dimensional device simulations can be performed using ATLAS virtual Fab software. The initial device model was based on a rectangular 2D structure, whereas the manufactured devices are cylindrical. 3D rectangular and cylindrical models were thus developed and simulated to perform a sensitivity analysis on the injector composition, and to investigate various device characteristics. Simulated forward bias IV characteristics of the 2D device model are shown in figure 1(a) and these are seen to match well to measured data thus validating the choice of the physical models used in the simulations. Simulated results of the models transient response (figure 1(b)) show stable oscillation and confirm that the device is operating in ‘quenched’ mode as expected. The simulated IV characteristics and transient response of all the device models will be presented and compared to measured data. Emphasis will then be placed on discussion of an analysis of injector effectiveness for efficient electron transfer into the transit region conduction band satellite (L) valley. Here the effects of varying doping spike concentration on the electric field profile in the transit region will be discussed in detail. Finally, device simulations at various temperatures will be presented to show the effects of this on various device characteristics.

Physical Modelling of δ-doped GaAs/AlGaAs HEMT

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GaAs/AlGaAs is one the most prevalent material systems for High Electron Mobility Transistors (HEMTs) at cryogenic temperature because of its very high mobilities under these conditions. In this work, physical modelling of a GaAs/AlGaAs HEMT with 1µm gate length geometry is presented. The model is developed based on measurements obtained from a fabricated HEMT grown using molecular beam epitaxy. This model will be used for mixed-mode circuit simulations of mixed-signal designs including a 4 GHz Flash-type ADC. Silvaco ATLAS1 2D simulator is used for simulation and modelling. Models taking into account the effect of transverse and lateral electric fields on mobility, deep-level traps, Fermi-level pinning, carrier generation/recombination and tunnelling have been included.

To accurately model 2DEG carrier concentration to match the measured value of 5.4x10¹¹/cm², Fermi-level pinning was incorporated and conduction and valence band discontinuities were adjusted using the align parameter of the simulator. Furthermore, the δ-doping profile and level were adjusted and a deep-level trap density of 3x10¹⁶/cm³ was introduced in the AlGaAs layers while keeping the band diagram comparable to theoretical computations². Yamaguchi’s model³, which is specifically developed to model mobility in MOS inversion layers, has successfully been adapted for HEMTs, taking into account saturation velocity and the effect of lateral and transverse electric fields. Parasitic resistances were introduced to closely model the ohmic region of measured DC curves and extracted AC parameters.

DC and RF measurements, used to compare with the model, have been obtained using an HP8510C network analyzer over a frequency range of 45 MHz to 20 GHz. An ADS⁴ application is developed to extract intrinsic and extrinsic parameters through linear modelling of measured and simulated S-parameters.

Including the physical phenomena as discussed above culminated in the model giving good fit of DC IV curves (figure 1) and excellent fit between measured and simulated RF results (figure 2). However, further enhancement is required to accurately model the knee region (as encircled in figure 1).

Theoretical analysis of 1.55 µm emitting GaInNAs quantum dots

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The GaInNAs semiconductor quantum dots (QD) with dilute amount of nitrogen are promising candidates for the active region in the next generation of optoelectronic devices. It has been found that isovalently substitutionally replaced a small amount of the group V element by nitrogen in a III-V compound reduces the energy gap and increases the electron effective mass, a trend that is quite opposite to the most common III-V compounds, thus offering an alternative route to band structure engineering and improved optoelectronic properties. Recent advances in growth techniques facilitate the fabrication of self-assembled QDs with a very small amount (less than 5%) of nitrogen substitutional impurities in the QD region or in the capping layer. With appropriate tailoring of the QD morphology, this opens the possibility of GaAs-based optoelectronic devices emitting at 1.55 µm and beyond. We present here a theoretical study of the electronic and optical properties of the dilute nitrogen GaInNAs/Ga(N)As quantum dot (QD) structures. The calculations are based on a 10 band \(k\cdot p\) band-anti-crossing (BAC) Hamiltonian, incorporating valence, conduction and nitrogen-induced bands, strain and piezoelectric field. Numerical results for the model system of capped pyramid and truncated cone shaped quantum dots on a thin wetting layer are presented. Our analysis shows that the influence of nitrogen induces more confined states in the CB than in equivalent N-free QDs, reducing the energy of the fundamental optical transition. The better confinement in dilute nitrogen QD is due to both significantly reduced compressive strain, which was one of the major obstacle for a long-wavelength emission from InAs/GaAs QDs, and BAC effect. These effects, in conjunction with QD size variation can be of great benefit for the design of devices emitting at longer wavelengths. Furthermore, in contrast to N-free QDs, dilute nitrogen QDs exhibit reduced dipole matrix element and larger Coulomb interaction energy. Our analysis shows advantages of Ga\(_{0.3}\)In\(_{0.7}\)N\(_{0.04}\)As\(_{0.96}\) over equivalent InAs:N QD material system in the design of QD devices operating at 1.55 µm and at RT. We briefly discuss possibilities of the 1.55 µm and at RT emission from the dilute nitrogen QD grown on different substrates like InP.

![Variation of the optical matrix element dependence on the QD size for the three material systems given in the figure legend; (inset) evolution of the e\(_0\) to h\(_0\) charge densities overlap with the QD size in In=70%, N= 4% QD. All results are for QD on GaAs substrate.](image)

Fig. 1 Variation of the optical matrix element dependence on the QD size for the three material systems given in the figure legend; (inset) evolution of the e\(_0\) to h\(_0\) charge densities overlap with the QD size in In=70%, N= 4% QD. All results are for QD on GaAs substrate.

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Theoretical modelling of manipulation of covalently bound molecules using atomic force microscopy

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Controlled manipulation of atoms and molecules is the route to the assembly of complex molecular and atomic patterns in nanotechnology. Scanning tunnelling microscopy (STM) has been widely used to manipulate atoms and molecules vertically and laterally across the surface. Vertical manipulation of atoms has been achieved by atomic force microscopy (AFM). Manipulation of molecules with AFM, however, has not been thoroughly studied either experimentally or theoretically.

We present the results of our theoretical modelling of manipulation of a large molecule, the C_{60} fullerene, covalently bound to the Si(001) surface. We first discuss the manipulation of this molecule using STM, i.e. its lateral manipulation via an intermediate pivoting point and a possibility of its vertical manipulation from a precursor state where its bonding to the surface is minimised [1,2]. This type of manipulation is possible in STM but not in AFM, where the cantilever oscillation period is much longer than atomic relaxation times, and the molecule would relax from the metastable precursor state to a stable site. However, a different mechanism can be employed in AFM: the lowering of a manipulation barrier due to the tip-molecule interaction. We incorporate kinetic Monte Carlo simulations in the virtual AFM simulation program [3,4] to model the manipulation of the C_{60} molecule a result of its interaction with an oscillating AFM tip. A novel fixed-time step kinetic Monte Carlo scheme [5] is used to determine the probabilities of the molecule jumping to a new adsorption site, while the virtual AFM predicts the response of the AFM during manipulation of the molecule.

References

**Applicability of k·p Method for Modelling of Type-II InAs/GaSb Superlattices**

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InAs/GaSb superlattice has unique type-II “broken gap” band alignment, where the conduction-band minimum in InAs is below the valence-band maximum in GaSb. By tailoring the superlattice period, this antimonide-based system provides great potential for optical devices of wide wavelength range, in particularly within the 3-5µm mid-infrared atmospheric window. Recently, some promising results have been reported for short period InAs/GaSb superlattices operating at this wavelength range.

Most commonly, the calculations of electronic and optical properties of semiconductor heterostructures are based on the k·p method. Recent theoretical calculations, however, could not correctly predict the band structure of the short period InAs/GaSb superlattices. Instead, they systematically overestimated the superlattice band gap energy (between the conduction and heavy hole minibands). This has led to suggestion that the k·p method is not adequate for these heterostructures because of the specific interface condition due to the lack of a common atom at the interface. Effects due to interfacial atomic segregations were also suggested. The atomistic simulations, such as pseudopotential method, have been suggested as the only viable alternative. However, the amount of calculation involved is massive; in addition, some fitting parameters are required. Simultaneously, some modifications of the standard k·p model were proposed. In some publications, introduction of artificial delta-function potential at interface within the standard k·p model was suggested, as an approximation for the effect of no-common-atom. The results were in better agreement with experimental data, even within the single-band model.

Here, we investigate the effect of interfacial segregation on the electronic structure of a short period InAs/GaSb superlattice in the framework of standard multi-band k·p method. We use experimental observations, such as TEM images and STM-measured segregation profile, to simulate the interface profile. The segregation was approximated by a graded composition of InAs\(_{(x)}\)GaSb\(_{(1-x)}\) at the interface. The calculations were performed with Finite Element Method, using strain-dependent eight-band k·p Hamiltonian within the envelope function approximation framework. The strain calculations were based on the continuum elastic approximation.

The calculations show that, by taking into account the segregation in the potential profile, there is a significant reduction in the superlattice band-gap energy, as large as 70meV. This is in a much better agreement with the experimental data, as compared to a model with an abrupt potential step at the interface. Our results show that the k·p method can be used as a tool for designing of InAs/GaSb superlattices with a good predictive ability, as long as the physical structure of the interface is correctly approximated.

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Interacting electrons in semiconducting carbon nanotube quantum dots: a 2-band effective mass approach.

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Quantum dots have recently been formed on a semiconducting carbon nanotube\textsuperscript{1}. We develop a new 2-band effective mass Hamiltonian to describe this novel system and calculate the states of up to 6 interacting electrons in a nanotube dot by exact diagonalisation.

We are interested in gated nanotube dots: in our model, electrons are confined electrostatically near the tube centre and the 1D confinement is harmonic. We describe the states of such a dot with an effective mass theory and there are new features in the theory that arise from the nanotube band structure. In all semiconducting nanotubes there are two equivalent conduction bands which, within the zone folding approximation, come from the equivalence of the $K$ and $K'$ points in the graphene BZ. The Coulomb interaction couples these bands and, to investigate this coupling, we derive a new 2-band effective mass theory for nanotubes starting from the Hamiltonian of a graphene sheet.

We calculate the ground state energy of 2 to 6 interacting electrons by exact diagonalisation of this Hamiltonian. We see evidence of a 4-electron periodicity in the dot addition energy and interestingly, we predict that the 2-electron ground state can be ferromagnetic. If we remove the band degeneracy, for example by deforming the nanotube, we recover the 2-electron periodicity in the dot addition energy that has been observed experimentally\textsuperscript{1}.

![Figure 1. Addition energy for a 35,0 nanotube quantum dot. 2-band calculation: solid line with circles, single band calculation: dotted line with squares.](image)

Plane wave methodology for electronic structure of single quantum dots

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The development of the plane wave methodology for the calculation of the electronic structure of single quantum dots within the framework of multiband envelope function theory was presented.\(^1\)

The plane wave method inherently assumes periodic boundary conditions. This is an excellent feature if one wishes to study the behavior of quantum dot superlattices. However, if one wants to study a single quantum dot, this is a drawback as periodic boundary conditions introduce artificial physical interactions with neighboring quantum dots in a superlattice. The methodology developed enables one to use a small embedding box, sufficient to eliminate electronic coupling, without introducing the artificial interaction with periodically replicated array of quantum dots caused by periodic boundary conditions. The appropriate formulas for Fourier transforms of strain tensor components on the embedding box that eliminate the strain field of neighboring dots were derived. The expressions that enable the evaluation of Coulomb integrals in inverse space without the introduction of artificial electrostatic interactions with surrounding dots were presented.\(^2\) The degree of accuracy can be systematically improved by increasing the embedding box that defines the k-space grid or by introducing the several lowest order corrections in the multipole expansion of the Coulomb integral.\(^3\) It was also shown how Hamiltonian symmetry can be exploited to further reduce the computational effort in the case of quantum dots of symmetric shape.\(^4\) Numerical results illustrating the application of the methods to the calculation of single-particle states, as well as the configuration interaction calculation of exciton, biexciton, and negative trion states in InAs/GaAs quantum dots were given. The method described has been incorporated into the existing parallel kppw code for quantum dot electronic structure calculations, where single-particle states are calculated within the framework of the 8-band $k\cdot p$ method including the effects of strain and piezoelectricity.\(^5\)

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\(^1\) N. Vukmirović and S. Tomić, submitted.
\(^2\) N. Vukmirović and S. Tomić, Physica E (in press)
**Investigations of the Kink effect in InAlAs/InGaAs pHEMTs**

Shahzad Arshad, M. Mohiuddin, A. Bouloukou and M. Missous, School of Electrical and Electronic Engineering, University of Manchester, UK

The InAlAs/InGaAs material system provides one of the highest transconductance pHEMT devices because of its large conduction band discontinuity, high electron mobility and very good carrier confinement in the channel. The DC characteristics, however, show a sudden rise in drain current at fixed value of drain voltage, resulting in high drain conductance and reduced voltage gain. This undesirable phenomenon is usually referred to as the Kink Effect. In this work a comprehensive understanding of the causes of this effect is developed using SILVACO ATLAS[1] 2-D physical simulator.

The modelled pHEMT is a layered structure that simulates the epitaxial layers of the fabricated device grown on MBE[2]. A Gaussian doping profile for the δ-doped layer, Fermi-level pinning and conduction band alignment parameters have been used to achieve comparable energy band diagram and sheet charge density with the experimentally measured data. Furthermore physical models incorporating field dependent mobility, generation-recombination mechanisms and deep-level traps are used. With the help of these physical models, threshold voltage, drain saturation and gate leakage current are successfully simulated and agree very well with the measured data.

This work involves extensive study of the interaction and effect of electric field on the release of carriers from deep-level traps of InAlAs buffer layer which are transferred to the channel. These carriers, combined with carrier generation mechanism due to impact ionization, increase the electron concentration and hence appreciably boost the drain current (figure 1). The kink phenomena can also be seen in the DC simulations of the device when deep-level traps are introduced in the model and impact ionisation is enabled (figure 2).

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Faraday Effect in Coherent Pulse Propagation in Quantum Nanostructures

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The investigation of the Faraday effect and the related coherent dynamics of light-matter interactions in Quantum Nanostructures (QNs), such as quantum dots and carbon nanotubes, can reveal their microscopic properties and therefore represents a powerful tool to study QNs. Here, we propose a model\(^1\) that can be used to describe the Faraday effect in QNs subject to an ultra-strong magnetic field.

Most analyses on Faraday effect in resonant medium consider the situation of a weak magnetic field, so that the width of the Zeeman splitting, \(\hbar \omega_L \ll d\), where \(d\) is the bandwidth of the incident light pulse. However, if \(\hbar \omega_L \gg d\) and the line widths of the relevant transitions, the level degeneracy is lifted and the light can not be resonant with more than one transition. We refer to such a magnetic field as an ultra-strong. Under an ultra-strong magnetic field parallel to the light propagation direction, if the central frequency of the incident light is tuned with the resonant frequency of a transition with \(\Delta M = 1\) or \(\Delta M = -1\) (\(\Delta M\) represents the magnetic quantum number difference between the relevant quantum levels of the transition), the effect from this transition on the incident light will be much larger than the one from other transitions, so that the interaction of the light with the medium can be effectively considered as an interplay of the light with a two-level quantum system.

\[\text{Fig. 1.} \quad \text{Time evolution of a linearly-polarised } 2\pi \text{-pulse at } z=280 \text{ \mu m for resonant dipole density: (a) } N=2\times10^{19} \text{ m}^{-3} \text{ (showing elliptic polarisation); (b) } N=2.5\times10^{20} \text{ m}^{-3} \text{ (showing circularly-polarised stimulated coherent emission).}\]

In this paper, we investigate the Faraday rotation of a linearly-polarised \(2\pi\) pulse in a resonant absorptive medium under an ultra-strong magnetic field and show that its characteristics are significantly different from those in a weak magnetic field.\(^2,3\) New phenomena have been predicted and conditions for their experimental observation have been identified. Investigations of the dependence of the coherent emission on the system parameters and how it destroys the Self-Induced Transparency are under way.

The development of atomistic empirical potential methods for molecular dynamics (MD) and molecular statics (MS) has allowed structural simulations of low dimensional III-V semiconductor materials to become a field that has attracted a substantial amount of interest in recent years. There are three main reasons for this. First, the electronic properties of lattice mismatched epitaxial semiconductor layers are strongly affected by their structural properties. Hence the reliable determination of quantities such as the elastic properties and the resulting strain is a fundamental prerequisite for implementing any accurate description of the bandstructure and the associated energy levels. Second, in, e.g., epitaxial quantum dot islands the stochastic variations of the local stoichiometry are often on a nanometer scale, precluding the use of less accurate continuum models. Third, the use of other atomistic approaches is precluded by the volume of the average nanostructure which is normally several orders of magnitude larger than that of the largest simulation cell of a typical ab initio calculation. In this work we will show that properly parameterized empirical potentials (EPs) that can capture the essential elastic and cohesive properties of a material, with the same accuracy as an ab initio calculation but with a substantially lower computational demand, can be used to obtain a deep level of insight into the properties of the epitaxially grown quaternary alloy InGaAsSb. We will show how the strain energy as a function of composition does not follow intuitive averages between the binary constituents, and that the theoretical behaviour appears to be substantiated by experimental evidence of growth of InAs QDs capped by GaSbAs.

Ab initio calculations of electron energy loss near edge structure of ternary alloys: AlGaN

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In this paper we present results of N K-edge electron energy loss near edge structure (ELNES) calculations for Al$_x$Ga$_{1-x}$N ternary alloys. Such calculations are needed for correct interpretation of experimental data that can now be obtained with a high spatial and energy resolution in modern transmission electron microscopes. It is known that better agreement with experiments is obtained for simulations using a core-hole.

For this reason we used a full potential Wien2k code which treats all electrons explicitly, and thus allows a straightforward implementation of core-holes. Ab initio calculations are very time expensive when high numbers of atoms are used. Therefore, we use 2x2x2 supercells (32 atoms in total) to model various compositions. Atomic positions in the supercells were derived using special quasi-random structures methodology. A detailed analysis of available experimental data and calculated N K-edges of AlN and GaN proved that a partial core-hole of 0.5e is an ideal compromise for the whole range of compositions of Al$_x$Ga$_{1-x}$N.

We also studied variations of ELNES spectra with different neighbourhoods of nitrogen atoms. Our results imply that the four nearest neighbours of a N atom have a principal influence on the ELNES. This conclusion justifies the use of the 2x2x2 supercells which are usually regarded as too small. We showed that in our case, the supercell of this size is capable of a successful reproduction of the ELNES N K-edge evolution with composition $x$, and at the same time remains computationally affordable.

Multi-Band $k\cdot p$ Calculations for Valence Band Structure of Strained Type-II InSb/InAs Quantum Dots

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Self-assembled quantum dots (SAQDs) promise a new generation of novel optoelectronic devices. Due to high optical efficiency, they possess potential for dramatic improvement in performance in terms of threshold currents, thermal behavior, differential gain and device lifetime. The most studied system is InAs/GaAs but antimonide-based systems have received much attention due to potential for optical devices in the 3-5 µm spectral region. InSb/InAs SAQDs offer a system with expected type-II band alignment. Recently, successful growth of InSb/InAs SAQDs has been reported. They have shown intense photoluminescence at room temperature in the 3.9-4.3 µm wavelength range. To our knowledge, there has been no theoretical modelling of InSb/InAs SAQD system in the literature. These quantum dots are very small (2.5-3 nm); because of that, it is very difficult to either control or assess their composition, size and/or shape. Therefore, analysis of the effect of these parameters on the electronic structure is crucial for meaningful characterization of these dots using optical methods. We have modelled the electronic structure of InAsSb dots of various shapes, aspect ratios and composition. The calculations of the band profile were performed by the Finite Element Method using standard deformation-potential theory and the continuum elasticity approximation. The InSb/InAs SAQDs exhibit a type-II broken-gap alignment. Our calculations confirm that strong confinement only exists for holes, with confinement potential of $\approx 0.8$ eV. Hence, the valence band structure of this SAQD system needs to be studied in detail. For theoretical modelling of the electronic structure near the band edges, the $k\cdot p$ method is a credible tool. Therefore, the size-quantization energies were obtained within the envelope function approximation using a 6-band $k\cdot p$ Hamiltonian. The influence of strain on band energies is examined and the single-particle bound-state energies are calculated as a function of aspect ratio and composition. Our calculations demonstrate that the confinement potential is mainly governed by the dot aspect ratio, being insensitive to other shape details. With increasing aspect ratio for a given lateral size of the dots, strain-induced splitting of the valence-band increases, and a deeper Confinement potential for holes is formed. However, the transition energy increases due to the size-quantization effect of the reducing dot height. We also found that effect of variation in the dot composition is comparable to that of the aspect ratio. The calculated transition energies were compared to the available experimental data. Our analysis shows that the dot composition can be estimated if the aspect ratio is known, and vice versa.

Two-dimensional physical modelling of InP-Based Single Heterojunction Bipolar Transistors (SHBTs)

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Introduction
State-of-the-art SHBTs were designed, grown, fabricated and tested in-house. A self-aligned transistor with an emitter area of 5x5 µm² and low offset voltage of 150mV is simulated. The device (Table 1) shows an excellent DC current gain of 78. Microwave S-parameters were measured on wafer and a cut-off frequency (fₜ) and maximum oscillation frequency (fₘₐₓ) were measured to be 71Ghz and 60Ghz respectively at Iₑ=14.6 mA and Vₑₑ=1.5V. This paper reports on the continuing research into the design and two-dimensional physical modelling of InP/InGaAs HBTs in ATLAS using SILVACO².

Device Simulation
The device was carefully layered and meshed in DEVEDIT to improve simulation performance and to avoid convergence errors. A concentration dependent Analytic mobility model was included in the simulation to approximate the effect of doping on the mobility of electrons and holes in the material. Due to high base doping concentration, Bandgap Narrowing model is also required. Recombination mechanisms are approximated by concentration dependent Schokley-Read-Hall, Auger and Band to Band models. In order to simulate the break down voltage and the effect of the impact ionization, Selberherr’s Model is implemented. Thermal effects are not considered in the simulations.

Comparison of Results
The effects of the spacer layer on the turn-on voltage and the energy band diagram are simulated. A close agreement between simulated and measured data (Figure 2) is demonstrated in the presented work. Further improvements and comparisons will be shown in the future.

Table 1: SHBT Epilayer Structure

<table>
<thead>
<tr>
<th>Layer</th>
<th>Material</th>
<th>SHBT</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cap</td>
<td>In₀.₄₇Ga₀.₅₃As</td>
<td>n⁺=1x10¹⁹ cm⁻³, 1500 Å</td>
</tr>
<tr>
<td>Emitter 1</td>
<td>In₀.₄₇Ga₀.₅₃As</td>
<td>n⁻=1x10¹⁷ cm⁻³, 1500 Å</td>
</tr>
<tr>
<td>Emitter 2</td>
<td>InP</td>
<td>n=1x10¹⁷ cm⁻³, 400 Å</td>
</tr>
<tr>
<td>Spacer</td>
<td>In₀.₄₇Ga₀.₅₃As</td>
<td>Intrinsic, 50 Å</td>
</tr>
<tr>
<td>Collector</td>
<td>In₀.₄₇Ga₀.₅₃As</td>
<td>p⁺=1.5x10¹⁵ cm⁻³, 860 Å</td>
</tr>
<tr>
<td>Subcollector</td>
<td>In₀.₄₇Ga₀.₅₃As</td>
<td>n⁺=1x10¹⁷ cm⁻³, 6300 Å</td>
</tr>
<tr>
<td>Buffer</td>
<td>In₀.₄₇Ga₀.₃As</td>
<td>n⁻=1x10¹⁷ cm⁻³, 5000 Å</td>
</tr>
<tr>
<td>Substrate</td>
<td>Semi-Insulating InP</td>
<td></td>
</tr>
</tbody>
</table>

Conclusion
Accurate physical modelling of complex InP-based HBTs has been presented which not only provides inexpensive, reliable and efficient prototyping, but also aids with the understanding of the underlying device physics. Further work on improving simulation and epilayer design of subsequent InP-based HBTS is in progress.
