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Quantum Wells, Wires and Dots (QWWAD): Free and open-source simulation tools for semiconductor nanostructures

<u>Alexander Valavanis</u>[1,*] Andrew Grier[1], Jonathan D. Cooper[1], Craig A. Evans[1], and Paul Harrison[2]

[1] Institute of Microwaves and Photonics, School of Electronic and Electrical Engineering, University of Leeds, Leeds LS2 9JT, U.K.
[2] Materials and Engineering Research Institute, Sheffield Hallam University, Sheffield S1 1WB, U.K.
*Contact Email: a.valavanis@leeds.ac.uk

Introduction

A wide range of high-quality software tools is available for simulating the band-structure, charge transport and optoelectronic properties of semiconductor nanostructures, including purpose-made products such as Nextnano [1] and generic finite-element solvers such as COMSOL Multiphysics [2]. While these existing programs are highly regarded as reliable research aids, the vast majority of available software is supplied under a proprietary license, meaning that its source code cannot be studied, modified or redistributed freely by its users. As such, there is currently a lack of free software for researchers and students wishing to study the fundamental physical properties, and the mathematical and computational techniques that underpin intersubband and nanostructure devices and semiconductor materials.

With the intention of creating a free and non-commercial community-driven resource, we present a new open-source project, Quantum Wells, Wires and Dots (QWWAD) [3], which is released under the GNU General Public License 3.0 [4], and which accompanies the new 4th edition of the eponymous textbook [5]. In this paper, we describe the range of physical modelling tools included in the simulation suite, and the design methodology used to improve the robustness, flexibility-of-use and the potential for community-driven code development.
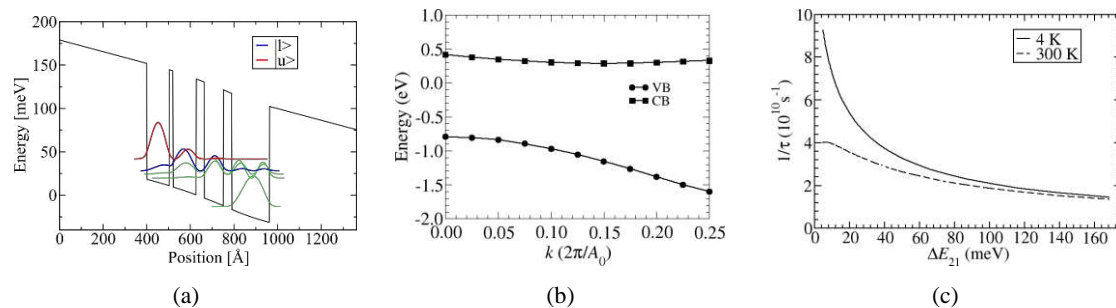

(a) (b) (c)

Fig. 1: (a) Self-consistent Poisson–Schrödinger solution for a single module of a THz QCL using a tight-binding approximation to the boundary conditions. (b) Lowest conduction band (CB) and highest valence band (VB) states computed using an empirical pseudopotential model for a periodic array of Ge quantum dots embedded in a Si host crystal. (c) Impurity scattering rates as a function of subband separation in infinite quantum wells of varying width.

1.   Physical modelling components

The QWWAD simulation suite includes analytical and numerical solvers for the Schrodinger and Poisson equations, enabling rapid computation of the bandstructure both in simple heterostructures (e.g., square or parabolic quantum wells), and in generic one-dimensional potentials [e.g., Fig. 1(a)]. Functionality is also provided for computing impurity and excitonic states and for simulating interdiffusion (e.g., annealing effects) in generic 2D systems. Structures

with higher orders of quantum confinement (quantum wires and dots) can be computed using either simplified quasi-analytical models or empirical pseudopotential calculations [Fig. 1(b)].

A comprehensive set of carrier-scattering calculations is provided, including interactions with impurities [Fig. 1(c)], acoustic and LO phonons, interface roughness, alloy disorder and carrier–carrier processes. A one-dimensional thermal model enables the time-variation of the temperature profile to be computed rapidly for arbitrary multi-layered structures, in response to continuous or pulsed input power sources.

These fundamental physical models can be combined to create full simulations of complex heterostructure systems, for example, self-consistent rate-equation analysis of quantum-cascade lasers.

2.   Software architecture and methodology

The full simulation suite is released under a free-and-open-source license, ensuring that the source-code can be studied, shared, and modified freely (with attribution to the developers). Infrastructure has been put in place for community-driven, collaborative development, coordinated through a project on the Launchpad website [3], which includes project management, community support, bug-management and translation tools. Source-code is managed through the Bazaar distributed version control system, simplifying its sharing, and enabling new features and bug-fixes to be contributed by the community.

A three-tiered hierarchical software architecture has been developed, allowing considerable flexibility in its usage. The core functionality is provided at the lowest level of the hierarchy through an Application Programmers Interface (API) in C++, enabling the QWWAD physical models to be adopted in external custom-made programs by users. The middle tier provides a set of "building-block" programs for running elemental, common modelling tasks (e.g., computing scattering rates within a given bandstructure), which can be combined to generate complete simulations. The highest tier provides a set of example UNIX scripts, which use the QWWAD programs to perform complete "ready-made" simulations of a wide range of systems and physical phenomena. These example scripts can be modified easily by non-expert users, enabling an exploration of the physical systems and rapid development of customised simulations.

The software includes an automated test-suite based on the software-industry standard Google Test infrastructure, which can be configured to ensure that new contributions do not introduce bugs. An automated build system is used to test all new revisions of the code, and to provide ready-made binary packages for the Ubuntu Linux operating system.

3.   Conclusion

We have presented a new free-and-open-source software suite, QWWAD, for simulation of semiconductor nanostructures. This project aims to provide a community-driven resource for collaborative development of a common set of simulation tools for use by researchers and students across a range of institutions. The flexible interface and automated testing infrastructure will enable high-quality functionality to be used in a wide range of custom simulations.

References

[1]   Nextnano, http://www.nextnano.de

[2]   COMSOL Multiphysics, http://www.uk.comsol.com

[3]   Quantum wells, wires and dots (QWWAD), http://launchpad.net/qwwad

[4]   GNU General Public License 3.0, Free Software Foundation (2007),
         http://www.gnu.org/copyleft/gpl.html

[5]   P. Harrison and A. Valavanis, Quantum Wells, Wires and Dots, 4th Ed. Wiley, Chichester (2015).