NEMO5, a Parallel, Multiscale, Multiphysics Nanoelectronics Modeling Tool

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Abstract — **The miniaturization of semiconductor devices has reached the point where the number of atoms is countable and geometries are formed in three dimensions. The Nanoelectronic Modeling tool suite NEMO5 is designed to comprehend the critical multi-scale, multi-physics phenomena and deliver results to engineers, scientists, and students through efficient computational approaches.**

Keywords: Atomistic Simulations; Nanoelectronic; Tight-binding; NEGF; Multiphysics; Multiscale; Parallel Computing.

I. INTRODUCTION

The downscaling of electronic devices has reached the condition where the number of atoms in critical dimensions is countable, geometries are three dimensional objects and new materials are introduced. Under these conditions, even a known semiconductor constitutes a new material that cannot be found in nature due to the overall geometry of the device. The interactions of electrons, photons, and phonons are now governed by these new material properties and other longer range interaction effects such as strain at atomistic scale and gate fields. The Nanoelectronic Modeling tool suite NEMO5 [1] is designed to comprehend these multi-scale, multi-physics phenomena and deliver results to engineers, scientists, and students through efficient computational approaches. NEMO5's general software framework can easily include any kind of atomistic model and even semi-classical models if necessary. The software is entirely parallelized and implements advanced models such as the Schroedinger equation and non-equilibrium Green functions (NEGF) in tight-binding formalism, for electronic structure and transport calculations, respectively. It also is able to take into account important effects such as atomistic strain, using valence force field (VFF) strain models. It then allows the calculation of electronic band structures, charge density, current and potential, eigen-energies and wave-functions, phonon spectra, etc., for a large variety of semiconductor materials and devices.

NEMO5 was designed using a dataflow architecture. Components share information with each other using data communication channels. The core is completely written in C++ and uses all the power of the object-oriented paradigm. This means that the code is fast, robust and maintainable. New individual components that perform a specific task/calculation can be inserted even by a non-C++-expert, simply using the well-known Python language [4], [5], [6], without the need to recompile anything. These components interact with NEMO5 as Python library extensions. A Python developer can access structure and geometry definitions, material parameters, and computational flows.

The computational flow is based on the definition and interaction of *solvers* through well defined application programming interfaces (APIs). The interactions are not predefined. They are specified by the user from the input deck. A simulation starts with the parsing of an input deck which provides information about the simulated structure as well as the desired type of simulation flow and the parameters for all required solvers. In a general initialization phase, geometrical domains are constructed. A simulation can incorporate multiple conceptual domains and a mixture of continuum and atomistic representations. Every domain is partitioned into regions of different materials. This enables multi-scale and multi-physics simulations where physically realistic equations are solved on the subsets of the entire domain and simplified models are employed for the remaining regions. If needed, computational directives such as parallelization schemes, general solver iteration schemes, and model optimizations can also be explicitly specified from the input deck. NEMO5 embeds a large variety of well-known packages such as LAPACK, PETSc and SLEPc. These packages provide the great advantage of having updated, advanced, robust and reliable solvers at a fast rate of implementation. NEMO5 also embeds the MPI library for efficient, large-scale parallel computing. It includes a general parallelization class that handles the setup of multilevel parallelization hierarchies and the distribution of problems onto the available processes. This class can be utilized in all simulation types. This enables the solution of large problems using tens of thousands of cores with nearly ideal scaling.

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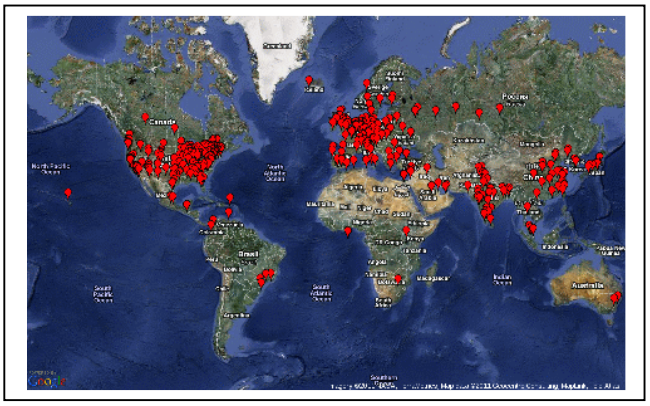

Figure 1. Global usage of 8 NEMO/OMEN powered tools on nanoHUB.org. Over 10,000 users have launched over 160,000 simulations.

NEMO5 represents the culmination of about 18 years of development and now encompasses all the capabilities of its predecessors for transport (NEMO1D and OMEN) and electronic structure (NEMO3D and NEMO3D-peta). Today this code is used for electronic structure and transistor research in academia and industry. NEMO5, along with NEMO3D and OMEN, also powers 8 applications on nanoHUB.org and has served already over 10,000 users with over 160,000 simulation runs (see for example Fig. 1).

II. Physical Models

In the following, a description of only several models implemented in NEMO5 is reported. NEMO5 represents a huge base of models and methods. All details and models cannot be reported. For the sake of completeness, references are reported for the interested user.

Crystal structures: Atomistic simulations are at the core of the current capabilities of NEMO5. Diamond and zincblende structures are the most common materials in nanoelectronics but simple-cubic, wurzite and rhombohedral (triagonal) crystal structures as well as carbon nanotubes and graphene are other available choices in NEMO5. The code is open for extensions to other crystal structures by specification of their primitive unit cell. As examples, a disordered quantum well calculation is shown in Fig.2 and a graphene band-structure is reported in Fig.4. Another example that clearly shows the capabilities of NEMO5 to deal with complex crystal structures is the topological insulator Bi_2Te_3. Topological insulators are a new class of materials that combines the properties of insulators and conductors. Topological insulators possess an insulating bulk while their surfaces host bound Dirac fermion like spin-polarized particles with high mobility. NEMO5 quantitatively predicts the electronic properties of these materials. The warped snow-flake like Fermi surface of Bi_2Te_3 is shown in Fig. 6.

Multi-scale and multi-physics approach: Models implemented in NEMO5 can exhibit different length scales and different computational complexities. For example, a calculation of an atomistic strain profile can be achieved for structures of sizes such as 100 nm^3 using a few hundred cores. As shown in [7], the long-range strain critically affects the central device domain (see also Fig. 2). On the contrary, an investigation of incoherent carrier–carrier scattering mechanisms on a micrometer length scale is neither feasible nor desirable, as most of the system is more adequately described by an incoherent and equilibrated carrier population. NEMO5 has the ability to couple together results obtained for domains of varying size, allowing for multi-scale and multi-physics simulations. Electrostatics and effective-mass band structure models are continuum theories that have no concept of atoms as such, but they can be mixed with charges discretized over an atomic lattice. Conversely, an atomistically resolved electrostatic potential, necessary for tight-binding calculations, can be obtained by interpolation from a coarser grid. A coupling of quantum transport with drift-diffusion has been demonstrated in [8].

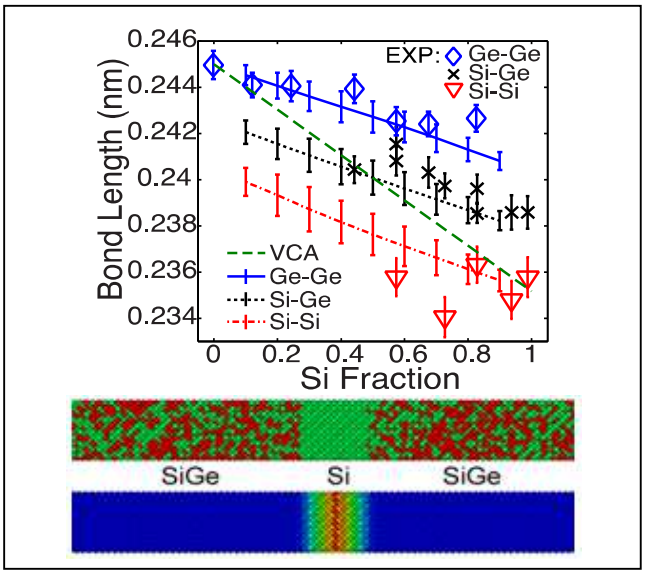

Figure 2. (a) Statistical bond distribution of Si_xGe_{1-x} as a function of Si concentration (x) for NEMO5 vs. experimental data [2,3]. Bond distribution is trimodal with distinct peaks associated with Ge-Ge, Ge-Si, and Si-Si bonds. Si in green, Ge in red. (b) Random alloy SiGe/Si/SiGe quantum well and (c) wavefunction for lowest conduction band state.

Atomistic Strain: Nanostructures composed of materials with different lattice constants exhibit strain. NEMO5 is able to compute the strain induced displacements of atoms using an extended version of the valence force field (VFF) model [9] in which the lattice energy is expressed in terms of atomic bond angles and lengths together with various microscopic spring constants. The energy functional implemented in NEMO5 features contributions from stretching, bending, cross-stretch, stretch-bend, and second-nearest-neighbor angle-angle interactions. These contributions can be turned on and off by the user in a mix and match fashion. For polar materials, the long-range Coulomb interaction can be added in the case of 0-D (bulk) and 3-D (confined) simulations. Energy minimization is performed by a Newton optimization method that minimizes

the total elastic energy of the crystal expressed in terms of atomic displacement coordinates. The Jacobian and Hessian matrices consist of first and second derivatives of the total elastic energy functional and need to be calculated at every iteration. This ensures quadratic convergence in the proximity of the solution (see [10]).

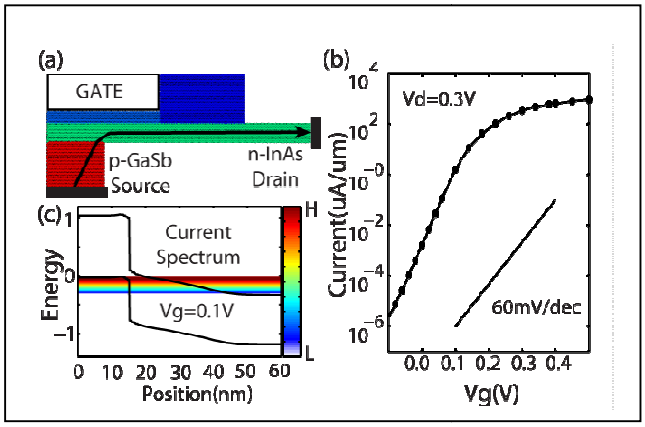

Figure 3. Simulation of band-to-band Tunneling FET. (a) 2D simulation domain of TFET. (b) Coherent IV characteristic of TFET at Vd=0.3V. (c) Current spectrum at Vg=0.1V.

Electronic Structure and Tight-Binding parameters: NEMO5 aims at the simulation of realistically extended nanoscale devices. The semi-empirical tight-binding formalism [17] using nearest-neighbor coupling offers an attractive compromise between computational cost and accuracy of the obtained results. It has been the workhorse of NEMO-1D, NEMO-3D, and OMEN and has been extensively validated. The atomistic representation of this method allows for an accurate treatment of material interfaces, alloy disorder and randomness, and structural roughness. Crystal symmetries are represented correctly and the obtained equations are much less numerically expensive. An important aspect in tight-binding calculations of states in finite structures is the passivation of dangling bonds at physical surfaces. NEMO5 generalizes the passivation scheme of [11] to apply to all crystal structures. The method is also able to treat non-trivial passivation atoms or molecules. Recently, [21] a method to extract Empirical Tight-Binding (ETB) parameters from *ab-initio* calculations has been developed in which the ETB basis is parameterized by means of analytical functions. The density functional theory (DFT) Hamiltonian is then transformed into the ETB basis. ETB parameters such as onsite energies and two center integrals are obtained from the transformed Hamiltonian. Targets such as band structure, effective mass and wave functions are then evaluated. To match ETB targets with the DFT ones, ETB basis functions are adjusted iteratively. The DFT starting data are obtained from the software ABINIT and the results for bulk Silicon are shown in Fig. 5.

Quantum Transport: NEMO5 currently implements two approaches to quantum transport. The first approach [13] uses open-boundary wave functions and can be applied in ballistic simulations. In the absence of scattering, this formalism is physically equivalent to Green's functions and outperforms NEGF simulations as only linear solves of a sparse matrix with multiple right-hand-side vectors are needed [13]. The second implemented approach to quantum transport uses NEGF [14] which is a many-body formalism capable of incorporating scattering and coherence loss. When used in conjunction with a tight-binding Hamiltonian, the resulting computational cost is very large [15] and must be tackled with multilevel parallelization techniques. The recursive Green's function (RGF) algorithm, a numerical technique to compute necessary components of Green functions in two-terminal devices while avoiding explicit full matrix inversion, was generalized during the development of NEMO5 to multiple terminals and arbitrary geometric shapes and implemented in a highly parallelizable way. Very recently a novel technique called low rank approximation (LRA) [19] [20] has been developed and implemented in NEMO5. NEGF involves many matrix-matrix multiplications and matrix inversions which all scale with the rank of the matrix to the third power. This rank equals the number of degrees of freedom in the system (up to 20 per atom) and can insofar hardly be changed. The LRA method approximates all NEGF matrices with matrices of much smaller rank (down to 10% of the original rank). In this way, all calculations of can be done in much shorter time and with much smaller memory load. The numerical load of the approximate calculation is several orders of magnitude smaller, while the predictive power of NEGF is still preserved. In this way, the quantum transport equations of the NEGF method can be applied on various devices of realistic extensions – in atomistic resolution. This opens up the investigation of structures with advanced geometries. Fig.3 shows an example of quantum transport simulation in a band-to-band tunneling FET.

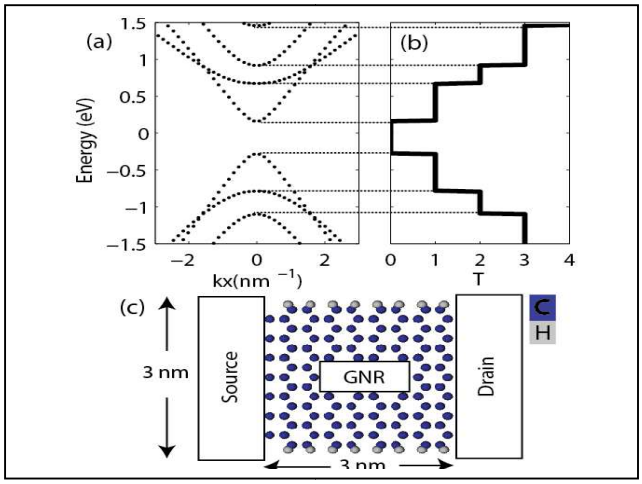

Figure 4. (a) The bandstructure (E-k) and (b) the transmission of (c) a graphene nanoribbon (GNR) with the width 3 nm, the length 3 nm, and no bias.

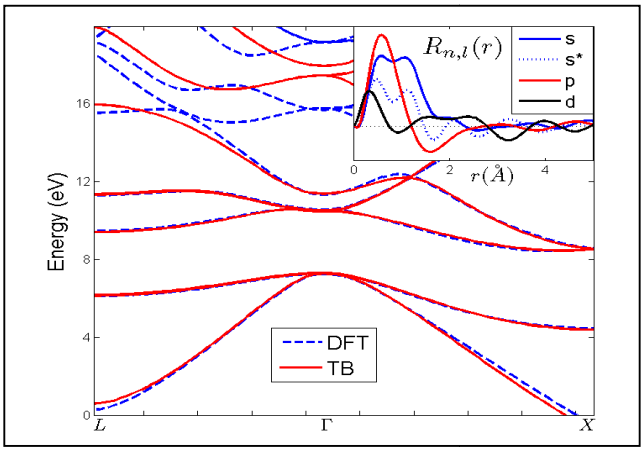

Figure 5. Silicon band structures DFT vs. Tight Binding (TB), and TB basis functions (insert). Both TB parameters and TB Basis functions can be obtained from DFT calculations.

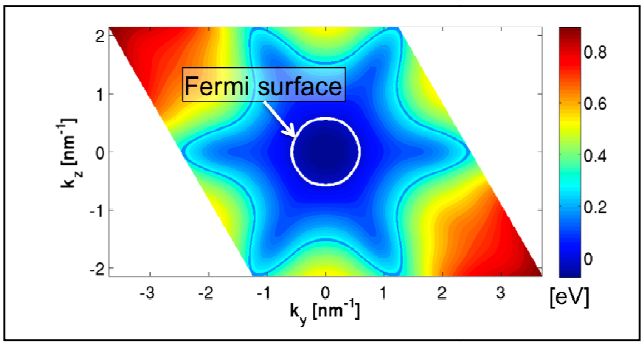

Figure 6. Hexagonal (snowflake-like) warping of the Fermi surface of topological insulator Bi_2Te_3.

CONCLUSIONS

In this paper, the innovative NanoElectronic Modeling Tool suite, NEMO5, has been presented. It has been shown that NEMO5 is able to deliver reliable and robust simulation results for technologically relevant novel devices. The tool can also simulate a variety of materials and technologically relevant structures with a atomistic resolution. NEMO5 exploits the paradigm of object oriented coding (C++ and Python) which makes it easily maintainable. New solvers can be added easily to the existing framework using Python scripts. Currently new capabilities are being added and will be released as soon as available.

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