NEMO5: Multi-Scale, Multi-Physics, Atomistic Modeling of Non-Equilibrium Processes in Nanometer-Scaled Compound Materials For Active Devices and Global Impact on nanoHUB.org

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Abstract

The relentless drive for economic impact has made Moore's law a self-fulfilling prophesy, through ever decreasing device sizes and increasing system integration for over 50 years. Today's commercial devices have nominal gate dimensions of 12 nanometer, critical device active region widths of less than 8 nanometers, and oxide thicknesses of around 1 nanometer. Typical chip level integrations contain over 2 billion transistors. A width of 8 nanometers of Silicon corresponds to roughly 64 atoms, a 1 nanometer thick dielectric layer corresponds to around 8 atoms. These atomic dimensions demand atomistic materials representations, yet a full device still requires 100,000 to 1 million atoms. Going forward it is clear that further reduction in device sizes will ultimately be limited by the physical atom count and the end of the physical downscaling is very near, presumably at the 5 or 7 nanometer device node. The operation of 2 billion such transistors on an area of about 1 square centimeter generates heat to the level of about 100W. This heat level limits the operation speed or clock frequency of these circuits to about 2.5GHz which indeed has not changed for over 10 years now. More's law as we know it for 50 years already slowed down [1] and it will come to a physical limit within a few years.

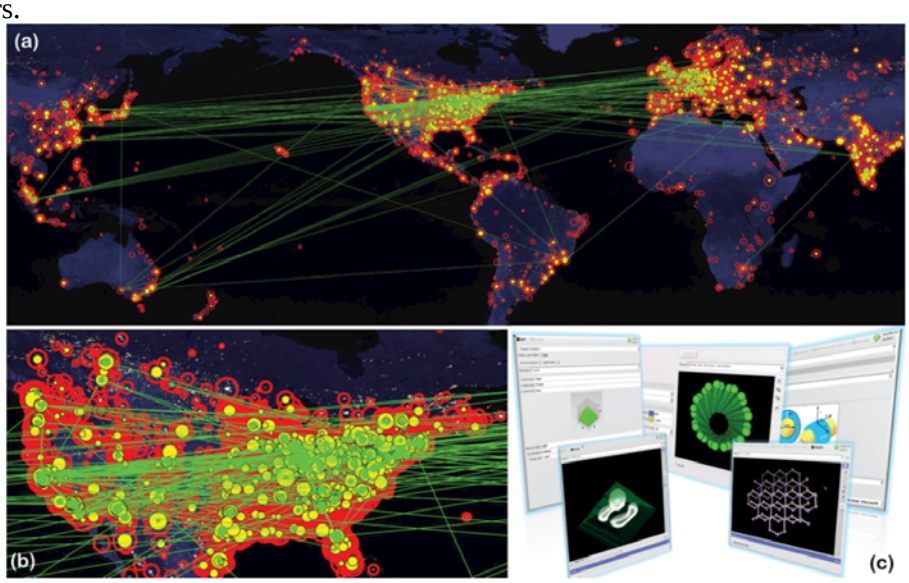

Figure 1 (a) nanoHUB user map 2016. Red dots=content users. Yellow dots=simulation users. Green dots=authors citing nanoHUB. (b) U.S. enlarged. (c) nanoHUB interactive tool sessions and results.

The two rather different scientific communities of solid state device engineers & physicists and the material scientists meet at this nanometer scale. Virtually they can meet on nanoHUB.org where 1.4 million annual users seek information on nanotechnology and over 16,000 users annually run scientific applications through their web browsers powered by significant compute resource. The community members conduct novel research and innovate education through end-to-end user cloud computing resources [2]. Over 1,900 research articles have cited nanoHUB with over 31,000 secondary citations leading to an h-index of 82 [3]. Over 35,000

students have used nanoHUB in organized educational activities in over 1,800 classes at 185 institutions.

This presentation focuses on a modeling and simulation tool suite entitled NEMO [4]. NEMO is an advanced research code that pushes the limits of device modeling at the multi-million atom scale, is actively used in the semiconductor industry, has been accessed by over 200 research groups, and used on nanoHUB without any installation. Over 26,900 users in total have utilized 9 simulation tools that are based on the NEMO tool suite in the past few years. Over 3,756 students have used these 9 NEMO-based tools in 381classes.

In the scientific realm device engineers look at the problem of down-scaling from their methods of continuum material descriptions such as bandgaps, effective masses, and dielectrics operated at high bias, out-of-equilibrium, and they find that they can no longer rely on the modeling tools that are agonistic of atoms. Material scientists look at the problem as up-scaling from tiny supercells consistent of typically 16, 32, or 64 atoms that are in equilibrium, and they have in general no tools to up-scale to out of equilibrium concepts that contain 100,000 to 1 million atoms. For the past 24 years a toolset entitled NanoElectronic Modeling or NEMO for short has been developed to fill this modeling and simulation gap and to join these different communities.

Datta [5-7] introduced the Non-Equilibrium Green Function Formalism (NEGF) into the device modeling community in a form that can be intuitively understood. The original NEMO research team established that the empirical tight binding method contains the critical elements of physical sophistication and computational ease to enable atomistic device simulations with quantitative matches to a large set of different devices [8,9]. These two aspects of the modeling puzzle, the foundational treatment of non-equilibrium quantum transport and sufficiently realistic atomistic basis set have now been well established and are widely adopted in the community in modeling tools that follow NEMO's footsteps [10].

There is one aspect in the original NEMO work that has not found widespread adoption in the community yet: the multi-scale, multi-physics partitioning of device regions which enables the fully quantum mechanical modeling of extended device regions subject to strong thermalizing scattering close to equilibrium coupled to domains that are highly out of equilibrium subject to moderate scattering or ballistic transport [11]. In NEMO5 we have generalized the concept and developed a specific model subset that couples multiple domains which individually are considered close to equilibrium to regions that are in non-equilibrium: EqNeq-Model.

This presentation highlights the capabilities of the EqNeq model in two different classes of devices: 1) Tunneling Field Effect Transistors (TFETs) [12] and 2) Multi-Quantum-Well Superlattices for Light Emitting Diodes (LEDs) [13]. Both of these rather different devices share the feature that electrons & holes are injected from man-made quantum-effect dominated reservoirs that are close to equilibrium through complex tunneling barriers into adjoining reservoirs. Through comparison with experimental data we have shown how the EqNeq model enables quantitative understanding of device performance, while typical coherent and incoherent quantum transport approaches fail. The full details of the model, the descriptions, and the modeling results have been published already. Here we repeat some of the multi-scale device partitioning figures and critical results from the previous publications with copyright permissions. The focal point of this presentation is to familiarize the audience with this powerful EqNeq concept for different devices in the GaN material system.

The standard CMOS transistor is fundamentally limited to a turn-on slope of at least 60mV/dec due to the thermionic tail of high energy carriers in the source. With the demand of an on-off current ratio of at least 10^4 and enough margin to withstand device to device fluctuations the industry has basically stopped any further drive voltage scale downs and reached a level of 0.6V – 0.7V. Further voltage reduction to reduce the power consumption requires a steeper turn-on below 60mV/dec. Tunneling Field Effect Transistors (TFETs) are conceptually not limited by the thermionic carrier tail in the source, since bandgaps in the source and the gate region form an energy filter that is clipped by band edges for low *and* high energy carriers. Therefore a whole field of research is exploring TFETs as possible CMOS replacements or augmentations in a variety of different material systems.

The guiding principles in TFET design require very steep electric fields in the tunneling junction that connects the source and the gate regions to maximize the total ON current. Critical concepts in the design of TFETs are discussed in various references [14-16]. Common to all designs is that a high carrier density reservoir is separated by another device region by a tunneling bandgap. Quantum effects such as confinement quantization and band mixing, especially for holes need to be considered. A full band structure analysis is needed to capture band mixing and band non-parabolic effects.

The GaN system offers intriguing possibilities to introduce very large fields in the tunneling region through polarization effects. These built-in fields foster high ON current densities across the tunneling barrier without very tight gate or dopant placement [12]. The band structure and tunneling path of an experimentally realized PIN diode are sketched in Figure 1. Figure 1b shows the conceptual separation of two energy and space regions in which electrons and holes can be considered close to equilibrium (green shading) while the central tunneling region is depicted as white.

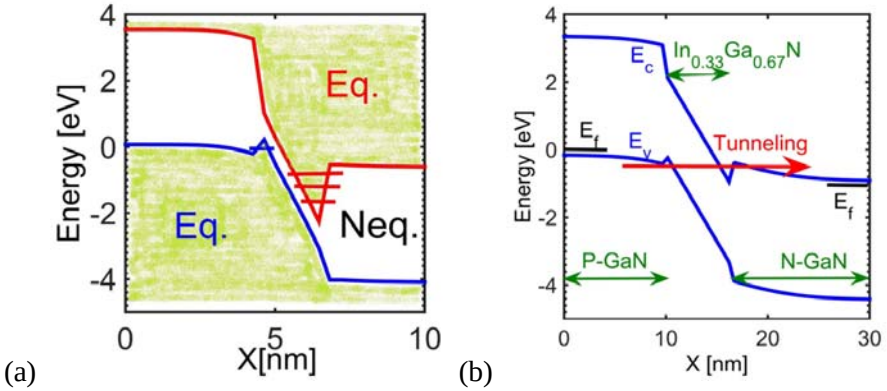

Figure 2. Band to band tunneling in a GaN system PIN diode. a) Schematic showing the boundaries between equilibrium (Eq.) (green shaded) separated from an spatially and energy dependent non-equilibrium (Neq.) region (white). (b) Energy band diagram of a tunneling heterojunction. The band diagram corresponds to the InGaN/GaN tunneling diode reported in [17]. Figures taken from reference [12] with permission.

The computation of thermalizing scattering within NEGF is extremely computationally intensive and for the class of device sketched in Figure 2 is really not needed. A much better entry assumption into the problem is to consider the source and the drain to be at or close to equilibrium, which effectively includes any and all scattering processes. These close-to-equilibrium reservoirs can the inject and receive carriers through the low-carrier density non-equilibrium tunneling regions.

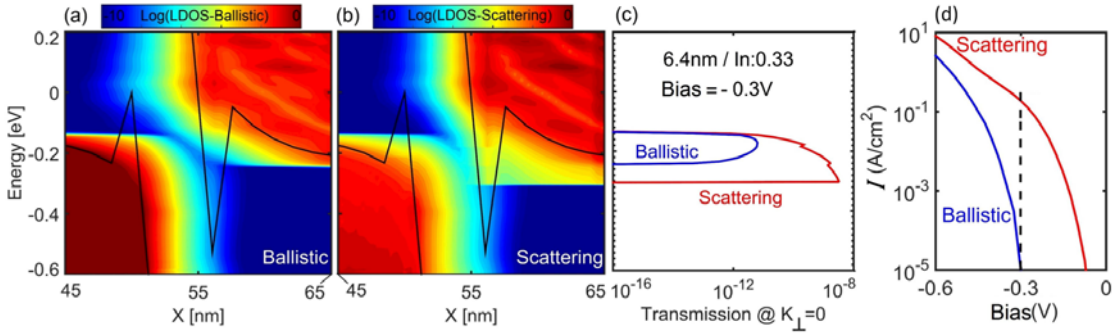

Figure 3) (a) Ballistic Local Density of States (LDOS) in the quantum-well region of the device measured in [Tarek 6] at −0.3 V. (b) Corresponding scattering LDOS in the quantum well showing significantly larger DOS than the ballistic case. (c) Ballistic versus scattering transmission. (d) Ballistic versus scattering current. Ballistic transport significantly underestimate the LDOS and the transmission inside the quantum well resulting in a significantly smaller tunneling current. Figure copied from reference [12] with permission.

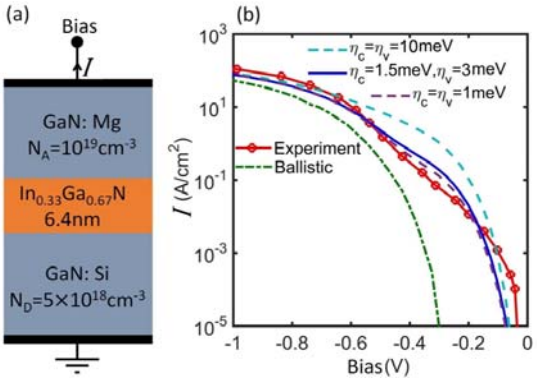

Figure 4) (a) Schematic of the device measured in [6]. (b) Computed current–voltage characteristics for the device of [Tarek 6]. The scattering model reasonably matches the experimental measurements unlike the ballistic model that significantly underestimates the current. Figure copied from reference [11] with permission.

The EqNeq model presented in Figures 2-4 from reference [12] goes beyond the original 1995 model [11] by introducing a separation of the Equilibrium-NonEquilibrium-Equilibrium regions that are not "simply" length/layer dependent but space and energy dependent. This energy and physical space separation is actually more complicated since the band edges, or modes are also k-dependent if an ultra-thin body is considered [12].

Another expansion of the 1995 model [11] has been introduced in reference [13] to model superlattice LEDs. Realistic LEDs separate multiple quantum wells that are strongly filled with electrons and holes by tunneling barriers to generate significant electron-hole recombination to harvest photons. Again, the explicit computation of all scattering processes that equilibrate the LED quantum wells is excessively computationally expensive. A multi-domain decomposition into regions of high carrier densities that are close to equilibrium that can inject carriers into adjacent regions that are in non-equilibrium regions constitutes a breakthrough in quantum well LED modeling.

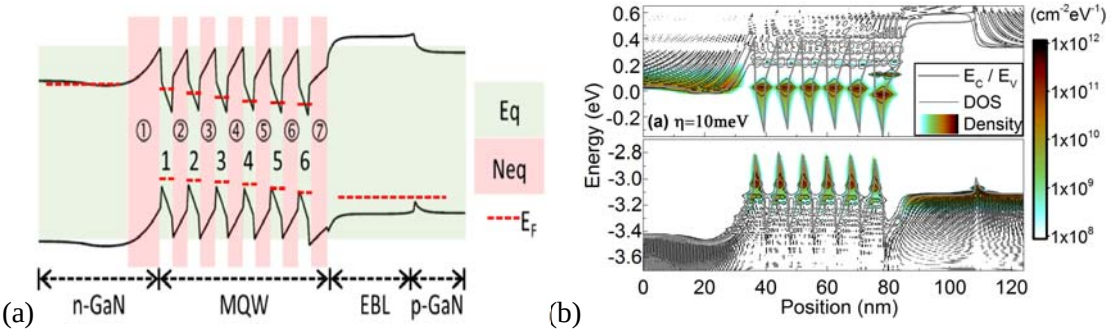

Figure 5a) LED structure that consists of an n-GaN layer; a low-doped active region made of InGaN/GaN MQW; an AlGaN electron-blocking layer and a p-GaN layer. The equilibrium (eq - green) and non-equilibrium (Neq-red) regions are marked in different colors. Each equilibrium-region has a unique quasi Fermi level, for holes and electrons as indicated by a red dashed line. The Fermi level drops across the device are depicted not to scale to emphasize that they are different from one QW to the next. The actual Fermi level drop across the 6 QWs at normal operation of 2.9V is only 25meV for electrons and 176meV for holes. (b) Energy-resolved electron, hole density of states (contour lines) filled with electrons and holes (color contours). The bulk-based conduction and valence band edges serve as a guide to the eye and only enter the calculation in the definition of the empirical scattering strength η. States in the QW are broadened due to η and coupled to each other. Figures copied from reference [13] with permission.

The device partitioning with the EqNeq model enables a quantitative agreement with experiment and theory/modeling which typically deviates from on the actual Voltage scale by a Volt. The model presented here enables understanding of device performance as a function of carrier temperature as discussed in more detail in reference [13].

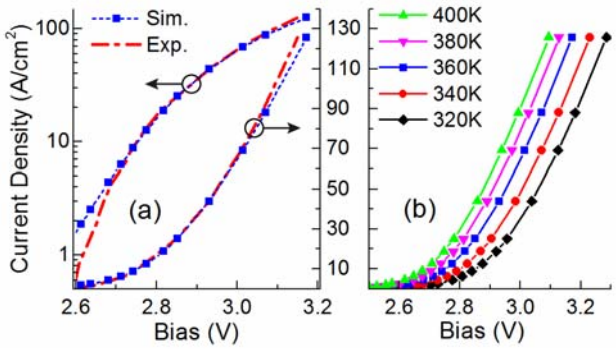

Figure 6a) I-V comparison with experiment shows good quantitative match on a linear and a log scale. A 2.0 mΩ·cm2 series resistance, 360K electron temperature, and 100meV spectral broadening in the quantum wells are assumed in the simulation 28-29. (b) I-V Simulations for various temperatures ranging from 320K to 400K result in a variation of ~170meV in turn-on voltage. Copied from reference [13] with permission.

The physical partitioning of these nanoelectronic devices corresponds to a computationally efficient matrix partitioning. This partitioning enables comparatively rapid computations of electron flow through complex physical structures. The mathematical details are provided in the referenced original papers.

Acknowledgements

The authors are grateful to the 30+ students, post-docs, and research faculty that have been involved in the development of NEMO5. Financial support for this development by Intel, TSMC, Philips/Lumileds, IBM, GlobalFounries, Samsung, and TSMC is acknowledged. This work uses nanoHUB.org computational resources operated by the Network for Computational Nanotechnology funded by the U.S. National Science Foundation under Grant EEC-0228390, Grant EEC-1227110, Grant EEC-0634750, Grant OCI-0438246, Grant OCI-0832623, and Grant OCI-0721680. NEMO5 developments were critically supported by an NSF Peta-Apps award OCI-0749140.

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