LEADING FUTURE ELECTRONICS INTO THE NANO REGIME USING QUANTUM ATOMIC SIMULATIONS IN NEMOS

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PI: Gerhard Klimeck
Co-PI: Tilmann Kubis
Collaborators: Tarek Ameen1, Daniel Valencia1, Pengpeng Long1, James Charles1, Daniel Lemos1, Hardrud Saharabudhe1, Kuang-Chung Wang1, Junzhe Gong1, Ching-Chen Yang, Zhe Zhang, Prasad Sarangapani1, Yuanchen Chu1, Tilmann Kubis1

Purdue University

EXECUTIVE SUMMARY

With a revenue of $338.9 billion in 2016, and as an enabler for larger economy chains (i.e., electronic systems), the semiconductor industry influences approximately 10% of the world GDP [1]. The transistor is at the heart of this enormous industry and continuous improvements of transistors in terms of speed and power consumption are essential for the stability and growth of the semiconductor industry as well as the dependent product chains and economics. Needed improvements in transistors’ performance have driven the semiconductor industry to push for smaller transistors, reaching 14 nanometers (nm) in the latest technology node, while development is ongoing for 10 nm technology and beyond. Such aggressive downscaling into a countable number of atoms in the critical dimensions makes atomic simulations necessary for modeling new generations of nano-electronic devices even beyond transistors [2–3].

RESEARCH CHALLENGE

The U.S. has always been a world leader in the semiconductor industry with 40% of the worldwide semiconductor device-related patents originating in the U.S. [4]. The U.S. semiconductor industry is one of the nation’s largest and most strategic industries, and the U.S. holds one-third of the global semiconductor device market worth over $300 billion per year. Simultaneously, a relentless drive for smaller semiconductor devices is occurring, with devices expected to be about 5 nm long in their critical active region within 10 years. Further improvements in shrinking dimensions will come only through the detailed study of device designs, materials, and of quantum effects such as tunneling, state quantization, and atomic disorder. Fundamental questions remain about the downsizing of the CMOS (complementary metal-oxide-semiconductor) switch and its eventual replacement. What is the influence of atomic local disorder from alloy, line-edge roughness, dopant placement, and fringe electric fields? How do lattice distortions due to strain affect carrier transport in nanometer-scale semiconductor devices such as nanowires, finFETs, quantum dots, and impurity arrays? What are the effects of interconnects’ sidewall roughness, grain boundaries, electron-phonon scattering, and roughness of metal-dielectric interfaces? Can inserting new materials and device concepts reduce power consumption?

NEMOS is designed to comprehend the critical multiscale, multi-physics phenomena for nano-scale technology through efficient computational approaches, and enables quantitative study of new generations of nano-electronic devices even beyond transistors [2–3].

RESULTS & IMPACT

For nitride devices, the I–V characteristics produced from these simulations agree quantitatively with experimental measurements. The simulations have been used to suggest improvements in the multi-quanta-well nitride-based light-emitting diode. In addition to this, a new alloy engineered Nitride TFET is proposed as a novel low-power transistor design.

Regarding transistor simulations, the tunneling from the valence to conduction band has the potential to yield significantly improved subthreshold slopes to allow lower supply voltages and much-needed lower power consumption compared to MOSFETs. Electron transport through the overall device, including the source and drain, entails significant amounts of computational demanding scattering, which cannot be ignored in realistic device performance predictions. A new method on the rank reduction of matrices through basis transformations that retain key physical information for modeling incoherent scattering phenomena has been implemented in NEMOS. These low-rank approximations provide shorter times-to-solution and smaller memory footprints. Blue Waters was used for assessing these times-to-solution and memory improvements. Using these low-rank approximations on nano-wire with a width of 5 nm shows a speed-up of 200 and needs only 7% of the memory.

WHY BLUE WATERS

Quantum transport simulations are very computationally expensive, and memory demanding due to the high degree of complexity of the equations used, especially if incoherent scattering of particles is needed. A toy quantum transport calculation of a 50 nm long wire with a 3 nm diameter requires around 1 teraflop for a single energy point where more than 1000 energy points are needed. And this calculation must be repeated perhaps hundreds times for a full current-voltage sweep. The treatment of a realistic device would require an atomic resolution of a device with a cross section of more than (20x20) nm², which includes the core semiconductor and the surrounding gate material. Such devices of larger sizes are especially an issue due to the O(ε) scaling of matrix operation time-to-solution and O(ε) scaling of memory. Blue Waters was used for running such simulations on up to 16,384 cores per simulation. In many cases the work could not be accomplished in a reasonable amount of time without Blue Waters, and for the larger simulations the work could not be accomplished on other available systems. Blue Waters staff provide exemplary support and user outreach to guide system usage, help with issues as they arise, and assist in code performance and scaling.

PUBLICATIONS AND DATA SETS


Figure 1: 3D visualization of a typical sub-10 nm novel transistor design made from blyer phosphorene that is being investigated using NEMOS. (Credit: Tarek Ameen)

Figure 2: Energy-resolved electron, hole density of states (contour lines) (Red with electrons and blue (color contours) of energy efficient multi-quantum well light-emitting diode simulated by NEMOS. (Credit: Junzhe Gong, Gerhard Klimeck)