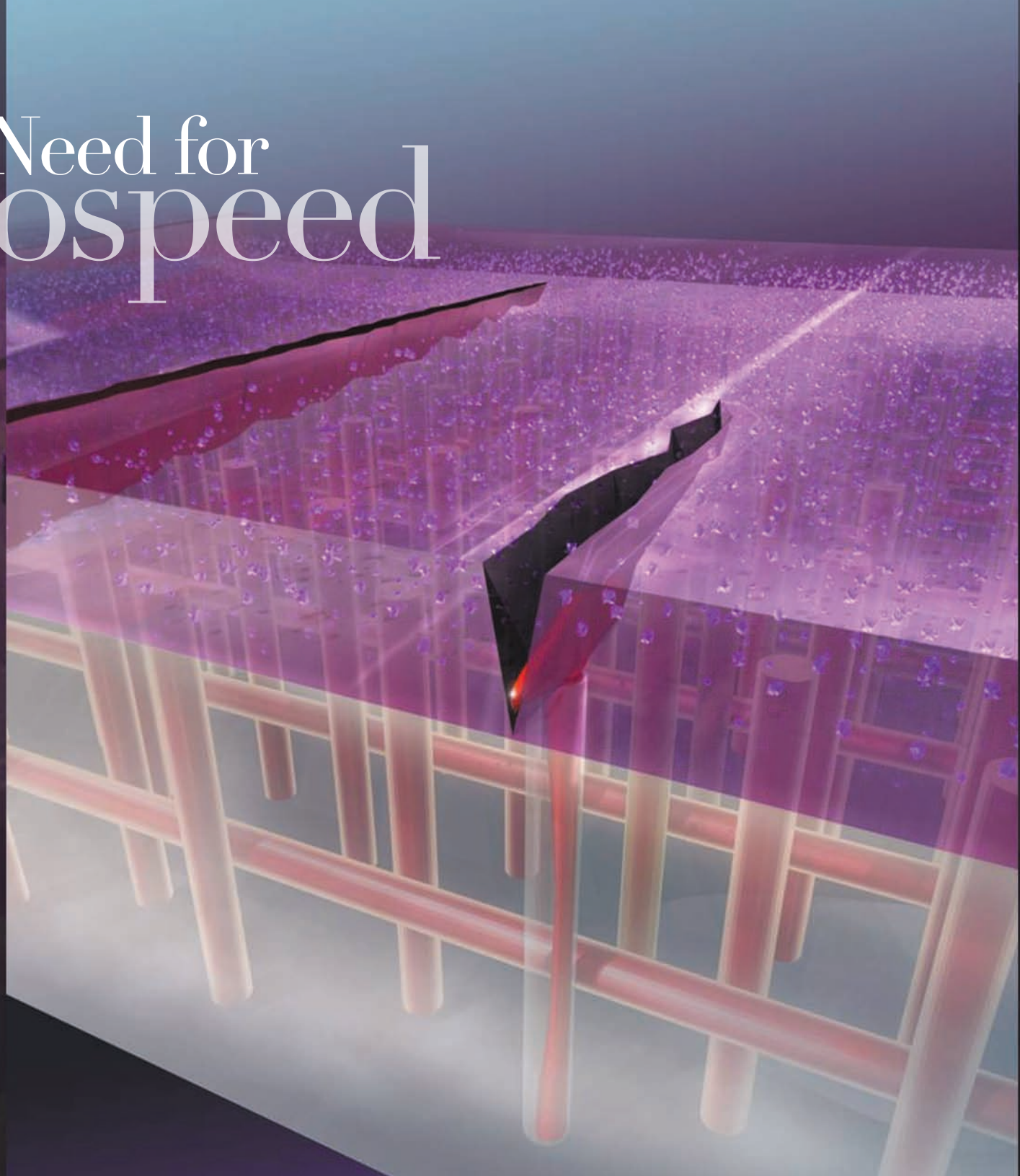
The Need for Nanospeed

Engineers use TeraGrid systems to explore next-generation transistors and new smart materials



For nearly two generations, technology has advanced at an exponential pace, with computers increasing their capability by a factor of two every 18 months, as suggested by Moore's Law. However, this exponential speed-up is now being threatened. The culprit: quantum physics and atomic granularity.

Technology's rapid growth is based on engineers' ability to shrink transistors—built generally from silicon—to seemingly impossible small scales. However, when silicon reaches a certain size—10 nanometers, or 5,000 times thinner than a strand of hair—new factors related to the discreteness and quantum behavior of atoms make a considerable impact.

As a consequence, nano-transistors heat to combustion, and particles display exotic traits. Materials we thought we understood need to be evaluated through this new nano-lens, and quantum mechanics must be considered when designing ultra-small systems.

Researchers using TeraGrid systems at the Texas Advanced Computing Center (TACC), the National Institute for Computational Sciences (NICS), and Purdue (Network for Computational Nanotechnology or NCN) are pushing the limits of our knowledge by developing a new generation of nano-transistors and "smart" materials.

Because electrons don't move quickly through silicon, there are intrinsic limits to the speed at which silicon-based transistors can calculate. Therefore, scientists are searching for alternatives. Mathieu Luisier and Gerhard Klimeck of Purdue University are collaborating with Jesus Del Alamo at the Massachusetts Institute of Technology to explore ultra-small, high-mobility transistors that use a promising alternative to silicon: gallium arsenide, or GaAs.

Gallium arsenide has high electron mobility and is able to convey energy from one electron to another at the nanoscale—good qualities for a transistor. Using the nanoelectronic simulation tool, OMEN, the researchers

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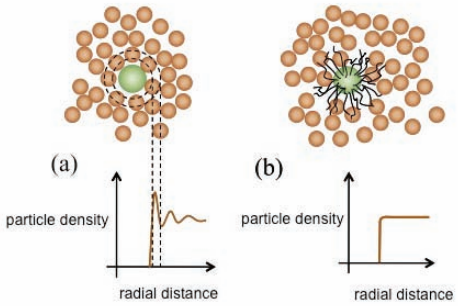

Typical structure surrounding (a) a bare nanoparticle and (b) a nanoparticle with polymers grafted its surface. In the latter case, the polymers disrupt the "cage" of neighboring particles that otherwise form and inhibit nanoparticle motion. Courtesy: Thomas Truskett, The University of Texas at Austin

simulated the quantum behavior of atoms in experimental nano-scale transistors and, for the first time, replicated the observed currents passing through the device.

"We reproduced their experimental data in both the 'on' and 'off' states of the device, which could only be achieved by properly accounting for the tunneling currents flowing through the insulator layers of the devices," says Luisier. "OMEN is the only device modeling tool that is capable of such physical accuracy and scaling."

The simulations used more than 70,000 processors simultaneously, and are helping to determine the optimal size and atomic configuration for this new transistor, which researchers hope will drive computer advances for decades.

"How many atoms thick should you make each of several layers? How long should the channel be to get the best performance?" asks Luisier. "What kind of metal alloy should be used for the transitor gate? These are some of the technology and design challenges where we can help."

Semiconductors aren't the only nano-materials worth studying. Thomas Truskett, a chemical engineer at The University of Texas at Austin, is investigating a related, but different question: How do you get molecules to line up faster in new nano-materials?

Truskett is interested in making "smart materials" whose purpose is embedded into their very structure. Examples include gels that harden on impact to become stronger than Kevlar, or metals that "heal" themselves.

Designing smart materials requires an understanding of the processes materials undergo at the smallest scales, and a theory of how to control these processes. Through a series of computational experiments using TACC's *Lonestar* supercomputer, Truskett accelerated the movement of virtual particles by grafting a "fuzzy layer" of polymers to the material's surface.

"If you provide a gentle force, you can break the structure around the particle enough for it to move quickly through the crowd," says Truskett.

Allowing particles to pass each other faster accelerates the reaction rate of materials, which means the difference between a viable nanoparticle for industry and one that is impractical. Truskett's theories have been subjected to atomistic simulations and laboratory experiments to test their validity. The findings were published in the *Journal of Chemical Physics* in September 2009.

For more information: http://www.che.utexas.edu/-truskett/

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