Simulations provide new insight into emerging nanoelectronic device

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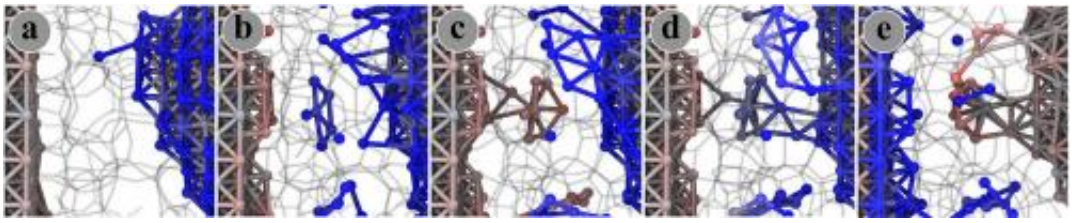

This image sequence is from a simulation that shows in unprecedented detail the switching action of devices that might replace conventional memory for electronics applications, with the potential to bring faster and higher capacity computer memory while consuming less energy. Credit: Purdue University

Researchers have used an advanced model to simulate in unprecedented detail the workings of "resistance-switching cells" that might replace conventional memory for electronics applications, with the potential to bring faster and higher capacity computer memory while consuming less energy.

These electromechanical "metallization cells" rapidly switch from high resistance to low resistance - a two-state operation that could be used to represent the ones and zeros in the binary code needed to carry out software commands and store information in computers.

Researchers at Purdue University developed a new method to simulate the electrochemical processes that govern the operation with atomistic

detail. The researchers used the model to simulate the performance of a type of resistance-switching cells also called conductive bridging cells.

"Despite their importance, the mechanisms that govern their remarkable properties have been poorly understood, limiting our ability to assess the ultimate performance and potential for commercialization," said Alejandro Strachan, a professor of materials engineering at Purdue. "Now, an atomic-level mechanistic understanding of the switching process provides new guidelines for materials optimization."

The resistance-switching cells are being considered as a possible replacement for current non-volatile memory, which is reaching its technological limits and could also be used for logic applications. The conductive bridging cells can switch in a matter of nanoseconds - making them potentially capable of ultra-fast operation - and they are extremely small, possibly allowing for more compact, powerful computer memory, Strachan said.

Findings are detailed in a research paper appearing this week in the journal *Nature Materials*. The paper was authored by Purdue postdoctoral research associate Nicolas Onofrio, graduate student David Guzman and Strachan.

The devices contain two metallic electrodes separated by a dielectric, or insulating material. As a voltage is applied, the active electrode - made of copper in this case - dissolves in the dielectric and the ions start moving toward the inactive electrode. These ions eventually form a conductive filament that connects the two electrodes, reducing the electrical resistance. When the voltage is reversed, the filaments break, switching back to the high-resistance state. An animated gif shown in this video depicts the action:

The researchers were able to simulate for the first time what happens at

the actual nanoscale size and time regimes of the devices, yielding new information about how the filaments form and break. Findings provide new insights into the electrochemical reactions leading to the formation of the filaments and their breakup, predicting the ultrafast operation observed in previous experiments with larger devices, with switching as fast as a few nanoseconds.

The emergence of such advanced simulations is making it possible to predict the precise behavior and performance of new devices before they've been constructed, a goal of the Materials Genome Initiative formed in 2011.

"The goal of the MGI is to discover, develop and deploy materials twice as fast at half the cost," Strachan said. "Now it takes 20 years from the time we discover a material in a lab until we put it in a product, and that's too long. We foresee that the next decades will witness a revolution with the incorporation of multiscale simulation and experiments leading to dramatic gains in performance and reduction in development costs and time."

The research is based at the Birck Nanotechnology Center in Purdue's Discovery Park and is affiliated with the Network for Computational Nanotechnology, the Center for Predictive Materials and Devices (c-PRIMED) and nanoHUB. The simulations are carried out using supercomputers through Information Technology at Purdue's (ITaP) research computing division.

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Future work will involve research to find better materials for the

devices.

More information: Atomic origin of ultrafast resistance-switching in nanoscale eletrometallization cells, *Nature Materials* (2015) DOI: 10.1038/nmat4221

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