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New model explains how single electrons cause damage inside silicon chips

Researchers in the UC Santa Barbara Materials Department have uncovered the elusive quantum mechanism by which energetic electrons break chemical bonds inside microelectronic devices — a detrimental process that slowly degrades performance over time. The discovery, published as an Editors' Suggestion in Physical Review B, explains decades-old experimental puzzles and moves scientists closer to engineering more reliable devices.

Modern electronics — from smartphones and laptops to solar cells and medical implants — depend on semiconductor materials being stable and dependable for many years. Yet even the most advanced devices suffer gradual wear that eventually limits their performance. The leading culprit is "hot-carrier degradation," a phenomenon that causes electrically energized electrons to trigger chemical changes deep inside the device. Until now, the precise physical mechanisms behind that process were unknown, limiting engineers' ability to suppress the phenomenon.

Professor Chris Van de Walle's Computational Materials Group has uncovered the quantum mechanism that triggers bond breaking. The team focused on the silicon-hydrogen bonds that are present near the silicon-oxide interface at the heart of each transistor. Hydrogen is intentionally introduced during manufacturing to passivate any broken silicon bonds — that is, to prevent the broken bonds from acting as electrically active defects that degrade performance. However, when constantly exposed to electrons flowing through the transistor, the hydrogen occasionally detaches, re-exposing the broken silicon bonds and degrading the device's performance.

The accepted wisdom in the field was that this bond breaking was the cumulative result of many electrons hitting the bond. Van de Walle's team used advanced quantum simulations to demonstrate that the process is actually triggered by a single electron. They identified a previously hidden electronic state that plays a key role in the mechanism: when a high-energy electron briefly occupies this state, it weakens the silicon–hydrogen bond and pushes the hydrogen atom out of position.

In a second breakthrough, the team revealed that hydrogen follows quantum-mechanical laws rather than classical ones as it detaches from the bond. If hydrogen were behaving as a classical particle, we could define a simple criterion for bond breaking, based on the distance between the silicon and hydrogen atoms. But hydrogen is not a classical particle; it behaves more like a cloud or a "wave packet." Bond breaking is then defined by the probability that the hydrogen wave packet extends beyond a certain distance.

The newly discovered mechanism explains multiple experimental observations that have puzzled scientists for years. For instance, it was not understood why bond breaking is most detrimental when the electron energy is around seven electron-volts; the new results show that this value corresponds to the energy of the previously unidentified electronic state. Experimentalists had also observed that the process is temperature independent and is significantly slower (by a factor of one hundred) when using deuterium as a substitute for hydrogen — deuterium being an isotope that is electronically identical to hydrogen but twice as heavy. The new quantum model explains all of these effects, confirming that the underlying physics have finally been elucidated.

"Our results show that the interplay between electrons and nuclei in a highly non-classical regime is what drives bond breaking," said Woncheol Lee, a postdoctoral researcher in the Van de Walle lab and the study's first author. "This process doesn't fit into the usual picture of heating-induced damage; it's a short-lived quantum event that we can now model without needing to fit it to an experiment."

The breakthrough has relevance beyond silicon technology. Electron-induced bond breaking occurs in many materials, including semiconductors used for light-emitting diodes (LEDs) and power electronics. Device degradation is currently a huge problem for ultraviolet LEDs, which engineers hope to commercialize for important applications such as disinfection and water purification.

“The quantum framework we developed gives materials scientists a predictive tool to assess which chemical bonds are most likely to break in extreme conditions,” said Van de Walle, “thus opening the door to engineering more stable materials with longer lifespans.”

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