Molecular dynamics study of resistance-switching in nanoscale electrometallization cells

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ABSTRACT

In the search of new memory devices, conductive bridge random access memory have been of particular interest due to their low power consumption, fast write/read capability, high endurance, and scaling limits reaching nanometers. These devices consist of a metal–insulator–metal structure and switch between high and low conductivity states with the application of voltage due to the formation and dissolution of a metallic conductive bridge. We present the first molecular dynamics simulations of switching in nanoscale devices based on Cu as the active electrode and amorphous SiO$_2$ electrolyte. The interactions between atoms are described by the reactive force field (ReaxFF) and the charges are calculated self-consistently at each step of the simulation using a modified charge equilibration method. This last method describes the voltage applied between two electrodes and the electrochemistry that occurs at the interfaces by adjusting of the local electronegativities of the atoms, identified on-the-fly during the simulation. The simulations predict the ultrafast switching observed in these devices. We find that single-atom-chain bridges often form during device operation but they are metastable with lifetimes below a nanosecond. We propose an atomic-level mechanistic understanding of the switching and provide insight into their ultimate scaling and performance. Finally, the method proposed to describe electrochemical processes is generally applicable and can also be used to study nanoscale batteries and capacitors.