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Atomistic simulations of novel nanoscale semiconductor devices: resistance switches and two-dimensional transistors

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ABSTRACT

As transistors get smaller, we are achieving record levels of memory density. However, there is a limit to how small transistors can be made before their functionality breaks down. Thus alternatives to traditional transistor technology are needed. The two such technologies we examined are: resistance switching devices, which reversibly grow metal filaments through a dielectric, and two-dimensional transistors, which are capable of breaking through the scalability limit of traditional transistors. In order to design resistance switching devices which create filaments with some level of consistency, the dynamics of the filament formation need to be explored. Herein we model this process using molecular dynamics (MD) simulations under the influence of external electric fields. We examined a configuration using an atomically sharp microscope tip as the active electrode and polyethylene-oxide and silica as the dielectrics. We observed localized filament formation propagating from the tip. Due to their size, two-dimensional transistors cannot be doped by traditional means. One method of doping is to use electrostatic energy from free ions in an electrolyte solution on the surface of a material. To examine the levels of doping in the system, we investigate the diffusion of free ions in a polyethylene-oxide electrolyte as a function of electric field and ion concentration. We expect our simulations of resistance switches and 2D transistors to guide fabrication of future devices by providing a better understanding of the effect initial parameters have on the evolution of the system.

KEYWORDS

Atomistic simulation, Electrochemical, molecular dynamics, resistance switching, two-dimensional materials