

Frenkel pair formation in Ta₂O₅ for ReRAM devices

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Resistive random access memory (ReRAM), characterized by a simple metal–insulator–metal (MIM) device structure, holds promise for diverse applications, including non-volatile data storage [1], in-memory logic [2], and neuromorphic devices [3]. Among potential memristor candidates, Ta₂O₅ stands out as the most favourable material. It is widely accepted that applying a sufficiently high voltage initiates the formation of a conduction path, driven by mechanisms such as vacancy migration (fig 1). [4] Once established, this conduction path can be reset (broken, resulting in high resistance) or set (re-formed, resulting in lower resistance) by applying another lower voltage.

Using density functional theory, we investigate the possibility of oxygen vacancy formation as a plausible mechanism for filament formation. The atomistic mechanisms of these processes remain partially unexplained with the initial generation of oxygen vacancies within Ta₂O₅ remains unclear. Vacancy formation may produce different charged species depending on the charge being trapped by the defect. When hole trapping is involved, a positively charged vacancy and a neutral interstitial oxygen atom is formed. Conversely, when electrons are trapped a neutral oxygen vacancy and negatively charged oxygen interstitial ions are produced instead. The charged species in either mechanism is responsible for filament formation. We propose electron/hole trapping in crystalline and amorphous Ta₂O₅ followed by bipolaron trapping in amorphous Ta₂O₅ for oxygen vacancy formation. Under zero bias we report a high energy barrier for Frenkel pair formation but a reduced energy barrier for bipolaron assisted Frenkel pair formation as a more feasible mechanism for filament formation.

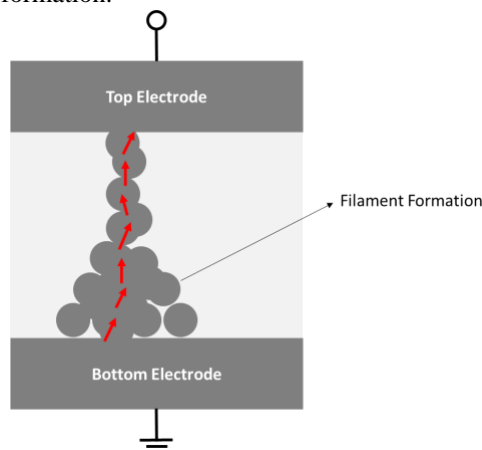


Figure 1. Filament formation during bias application (SET). When bias is applied oxygen vacancies are formed creating a filament (Grey spheres) allowing current (red arrows) to pass through the device.

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