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Switching Mechanism of Resistance Random Access Memory Based on the First-Principles Calculations

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Conducting Bridging Random Access Memory (CB-RAM) categorized in Resistance Random Access Memories (ReRAMs) forms conducting paths with metal atoms in the oxide layer sandwiched between metal electrodes, e.g., paths of Cu atoms in the HfO_2 layer in a Cu/HfO_2/Pt-structure, when in a low resistance state, and the paths are ruptured when in a high resistance state. It is reported [1,2] that water molecules contained in the atmosphere play a crucial role to the switching and conducting characteristics. For elucidation of resistive switching mechanism and of influence of water, we focus on diffusion properties of Cu atoms in the HfO_2 layer. Assuming that the conducting Cu paths are formed in boundary regions among polycrystalline HfO_2 and each of them are vast enough with the atomic scale, we have prepared several kinds of surfaces of a monoclinic HfO_2 crystal and have investigated Cu atom diffusion properties on them by using the first-principles program PHASE [3]. Influences of surface oxygen vacancies and of water molecules have been also investigated. Based on the calculation results, we will discuss the resistive switching mechanism.

The role of oxygen vacancies in conventional ReRAMs will also be reviewed based on first-principles calculations for vacancies in TiO_2.

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