AN ATOMISTIC UNDERSTANDING OF THE OXYGEN VACANCIES IN Pt/TiO_2/Ti RESISTIVE RANDOM ACCESS MEMORY: *AB INITO* STUDY

Jung-Hae Choi, Electronic Materials Research Center, Korea Institute of Science and Technology, Korea
choijh@kist.re.kr
Taeyoung Jeong, Electronic Materials Research Center, Korea Institute of Science and Technology, Korea
Cheol Seong Hwang, Department of Materials Science and Engineering and Inter-University Semiconductor Research Center, Seoul National University, Korea

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Resistive random access memory (ReRAM) is a promising next-generation device. However, the mechanism of the resistive switching is still under debate. In the resistive switching metal oxides, it has been generally known that oxygen vacancies are the mobile species and that the conducting filaments (CFs) are composed of the concentrated oxygen vacancies. The atomistic behavior of these concentrated oxygen vacancies is expected to be different from that of an isolated oxygen vacancy, but it has not been intensively considered in most studies. Therefore, we performed *ab initio* calculations on a model system of Pt/TiO_2/Ti device to elucidate the characteristics of the oxygen vacancies, such as the cohesive energy, oxidation number, and diffusion barrier energy, according to the concentration and configuration of the oxygen vacancies. We revealed that the charge transition of the oxygen vacancies occurs during resistive switching. In the high resistive state (HRS), the stable oxidation number of an isolated oxygen vacancy is 2+. During the set process of a transition from the HRS to the low resistive state (LRS), the stable oxidation number of the concentrated oxygen vacancies becomes 0, resulting in the formation of the neutral CF. Conversely, during the reset process of a transition from the LRS to the HRS, the stable oxidation number of oxygen vacancies returns to 2+, accompanying the CF destruction. Using this mechanism, we will explain the causes of the eight-wise (8w) polarity in TiO_2-based ReRAM, which has not yet been well understood. Furthermore, we will discuss the coexistence of the two opposite bipolar resistive switching, 8w and counter-eight-wise (c8w) polarities.