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Recombination driven vacancy motion - a mechanism of memristive switching in oxides[1] XIAO SHEN, YEVGENIY S. PUZYREV, Vanderbilt University, SOKRATES T. PANTELIDES, Vanderbilt University, ORNL — Wide-band gap oxides with high O deficiencies are attractive memristive materials for applications. However, the details of the defect dynamics remain elusive, especially regarding what drives the defect motion to form the conducting state. While the external field is often cited as the driving force, we report an investigation of memristive switching in polycrystalline ZnO and propose a new mechanism [1]. Using results from density functional theory calculations, we show that the motion of O vacancies during switching to the conductive state is not driven by the electric field, but by recombination of carriers at these vacancies, which transfers energy to the defects and greatly enhances their diffusion. Such mechanism originates from the large structural change of O vacancies upon capturing electrons. In addition, contrary to the hypothesis that memristive switching in polycrystalline materials is facilitated by the defect motion along the grain boundary (GB), we show in our system the vacancies move perpendicular to the GB, attaching and detaching from it during the switching process. We call it recombination driven vacancy breathing.

[1] X. Shen, Y. S. Puzyrev, and S. T. Pantelides, MRS Commun. 3, 167 (2013).

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