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Computational Materials Design (CMD®: Realization of the Switching Mechanism in RRAM HIDEAKI KASAI, SUSAN ASPERA, Osaka University, YUKIO TAMAI, NOBUYOSHI AWAYA, Sharp Corporation, KOUKOU SUU, ULVAC Inc., HIRO AKINAGA, National Institute of Advanced Industrial Science and Technology — Recent developments in computational techniques, coupled with the rapid progress in computer efficiency, make first principles-based COMPUTATIONAL MATERIALS DESIGN (CMD®) a relevant field in the world of surface science and condensed matter physics. In this scheme, quantum mechanical calculations are performed to design promising materials and, understand the necessary mechanisms for the realization of an efficient technological device. Among the many systems our group is engaged with is on the elucidation of the switching mechanism of resistance random access memory (RRAM) devices. In this study, we propose a mechanism of resistive switching based on the change in the electronic properties of a metal-insulator-metal type of RRAM brought about by pulse voltages and presence of aligned oxygen vacancies. In this kind of RRAM, the presumed change in the electronic properties of the transition metal oxide (TMO) insulating layer is attributed to the presence of aligned oxygen vacancies with charge carrier trapping, and oxygen vacancy movement near the TMO-metal electrode interface. These results were further experimentally verified in an academe-industry joint collaboration through the NEDO project.

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