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First-principles modeling of the electron and ion transport in TiO_2 ReRAM LIANG ZHAO, BLANKA MAGYARI-KOPE, YOSHIO NISHI, Department of Electrical Engineering, Stanford University — Transition metal oxide ReRAM is a promising candidate for next generation non-volatile memories. One of the key challenges in modeling ReRAM operations is the prediction of conduction behaviors. The conduction mechanism was found to vary from metallic in ON state, to quantum tunneling/hopping in OFF state. Since resistive switching is a gradual transition between the two, quantitative prediction of I-V characteristics through arbitrary oxygen vacancy (V_O) configuration is desirable. Here we systematically calculated the electron transport properties of pristine and defective TiO_2, by introducing isolated and clustered V_O in a $TiN/TiO_2/TiN$ device structure. The relaxed atomic structures were obtained from density functional theory (DFT) calculations, and the transport behaviors were calculated by DFT-based non-equilibrium Green's function (NEGF) approach. The I-V characteristics of both ON and OFF states can be well reproduced. It was also found that oxygen diffusion into to the vacancy sites is strongly affected by the interface with metal electrodes. Based on the results of transport calculations, a 3D analytical model is parameterized to allow the detailed prediction of device characteristics.

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