Journal of ELECTRONIC MATERIALS, Vol. 42, No. 1, 2013
DOI: 10.1007/s11664-012-2270-8

Realization of the Switching Mechanism in Resistance Random Access Memory™ Devices: Structural and Electronic Properties Affecting Electron Conductivity in a Hafnium Oxide–Electrode System Through First-Principles Calculations

SUSAN MEÑEZ ASPERA,[1] HIDEAKI KASAI,[1,3] HIROFUMI KISHI,[1] NOBUYOSHI AWAYA,[2] SHIGEO OHNISHI,[2] and YUKIO TAMAI[2]

1.—Department of Applied Physics, Osaka University, Suita, Osaka 565-0871, Japan. 2.—Corporate Research and Development Group, Sharp Corporation, 1 Asahi, Daimon-cho, Fukuyama 721-8522, Japan. 3.—e-mail: kasai@dyn.ap.eng.osaka-u.ac.jp

The resistance random access memory (RRAM™) device, with its electrically induced nanoscale resistive switching capacity, has attracted considerable attention as a future nonvolatile memory device. Here, we propose a mechanism of switching based on an oxygen vacancy migration-driven change in the electronic properties of the transition-metal oxide film stimulated by set pulse voltages. We used density functional theory-based calculations to account for the effect of oxygen vacancies and their migration on the electronic properties of HfO_2 and Ta/HfO_2 systems, thereby providing a complete explanation of the RRAM™ switching mechanism. Furthermore, computational results on the activation energy barrier for oxygen vacancy migration were found to be consistent with the set and reset pulse voltage obtained from experiments. Understanding this mechanism will be beneficial to effectively realizing the materials design in these devices.

Key words: Resistance random access memory (RRAM™), DFT, HfO_2, switching mechanism, electronic properties, oxygen vacancy

INTRODUCTION

Technological advances in materials design are apparently geared towards the development of materials for devices that are small but perform their intended functions faster, are more cost-effective to produce, and that can be operated with low power. In the development of nonvolatile memory, a metal–insulator–metal device, usually called resistance random access memory (RRAM™),[1–8] appears to be very promising due to its scalability and ability to be operated with low power. Materials such as transition-metal oxides (TMOs), which are used as the insulator that is sandwiched between two metallic electrodes, can switch properties from an insulating material (high resistance, OFF state) to a metallic material (low resistance, ON state), and vice versa.[9–11]

Studies related to the RRAM™ switching mechanism suggest that the ON–OFF mechanism is related to the creation of a conduction path by either cation migration or anion migration within the insulator, thereby connecting one electrode to the other.[7] The switching mechanism based on anion migration suggests that the creation of a conduction path through defect formation and charge carrier trapping might be responsible for the switching,[12–16] although this has not yet been conclusively clarified. Theoretical understanding behind this mechanism is of great interest to our research group, which has also carried out investigations on the oxidative reaction of the anode through experimental and theoretical approaches.[17–21]

In this study, we investigated the formation of a conduction path through anion migration, and the

(Received October 13, 2011; accepted September 15, 2012; published online October 2, 2012)