Properties of Conductive Oxygen Vacancies and Compact Modeling of IV Characteristics in HfO_2 Resistive Random-Access-Memories

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Abstract

In this work, the HfO_2-based resistive random-access-memory (RRAM) is studied. Three different aspects are investigated. In the first part, the migration barrier of the oxygen vacancy is calculated. Finally, a compact model for the RRAM is implemented and its results are compared with the experimental data.

Introduction

The resistive random-access-memory (RRAM) has been studied intensively. Especially, the HfO2-based RRAMs are widely adopted, because it can be successfully integrated into the modern CMOS technology. Also previous reports based on the FEM/KMC approaches [1] [2] are available.

It is known that the conductive filament plays an important role in the HfO_2-based RRAMs. In this work, properties of oxygen vacancies are calculated with the density-functional theory code (VASP). Moreover, a measured IV curve of a RRAM is reproduced by employing a compact model.

Migration Barrier of Oxygen Vacancies

The switching of the HfO_2-based RRAM is explained by the migration of oxygen vacancies. The migration barrier of oxygen vacancies, the difference between the local maximum and minimum formation energies, is an important material parameter. In Fig. 1, an atomic structure of an amorphous HfO_2 is shown. The structure is obtained by the DFT-MD optimization. The formation energy of the extended Frenkel pair (an oxygen ion interstitial and an oxygen vacancy) [3] is drawn as a function of the position in Fig. 2. For several amorphous structures, the same calculation has been performed in order to improve the fidelity. The crystalline HfO_2 has been also considered for comparison. In Fig. 3, the results are summarized. The extended Frenkel pair has a much smaller migration barrier. An oxygen ion interstitial is lowering the migration barrier of the corresponding oxygen vacancy.

Electrical Property of Oxygen Vacancy Filament

The resistivity of a HfO_2 supercell is calculated. First, a structure is prepared. In Fig. 4, the atomistic structures are shown. Both the crystalline structure and the amorphous one are considered. 296 atoms are included in each supercell. Starting from these structures, oxygen vacancies are introduced to generate an oxygen vacancy filament. The resistivity along the vertical direction is calculated with the Mott formula [4].

In Fig. 5, the resistivity is drawn as a function of the defect density. Each symbol represents a distinct sample. Since the atomistic simulation model is much limited in its size, the defect density is scaled for comparison to a conductive filament model (2nm × 2nm × 5nm). The defect density of two references are determined by the ratio of the filament area and non-conductive insulator area of the simulated model. Amorphous models have relatively high resistivity. When the number of oxygen vacancies increases from 2 to 8, the resistivity of the crystalline HfO_2 increased almost six orders-of-magnitude. Similar trends are found for different samples. These results are in a good agreement with the previous reports [1] [2].

Compact Modeling of IV Characteristics

In Fig. 6, the IV characteristics of a HfO_2-based RRAM measured at the room temperature is shown. The compliance current is 10 mA. By adopting the compact model reported in [5], parameters are extracted. The compliance current is implemented with an ideal MOSFET in the saturation mode. As shown in Fig. 6, it is shown that the compact model with adjusted parameters can reproduce the SET and RESET voltages considerably well. Based on the calibrated compact model, the switching behaviors are predicted at various temperatures, as shown in Fig 7. For lower temperatures, the absolute values of the SET and RESET voltages increase. A similar trend can be found in the previous report [6]. Their slopes are 0.5 V / 50 K and -0.36 V / 50 K, respectively.

Conclusions

In summary, our recent research efforts on the HfO_2-based RRAM are presented. The material modeling and the compact modeling presented in this work will be combined with the FEM/KMC approaches to construct a fully functional modeling environment for the RRAM.

References

[1] S. Ambrogio et al., IEEE TED, vol. 61, 2014.
[2] A. Padovani et al., IEEE TED, vol. 62, 2015.
[3] B. Traore et al, J. Phys. Chem. C, vol. 120, 2016.
[4] S. J. Blundell et al., Concepts in thermal physics, OUP Oxford, 2009.
[5] P.-Y. Chen and S. Yu, IEEE TED, vol. 62, 2015.
[6] R. Fang et al., IEEE EDL, vol. 36, 2015.

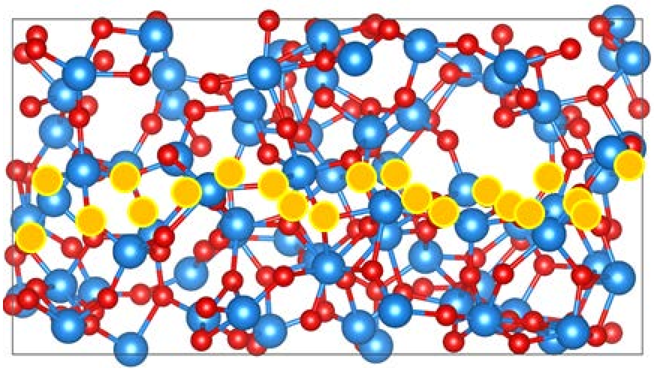

Fig. 1. Atomistic structure of an amorphous HfO_2. Yellow dots represent the possible vacancy locations, considered in Fig 2.

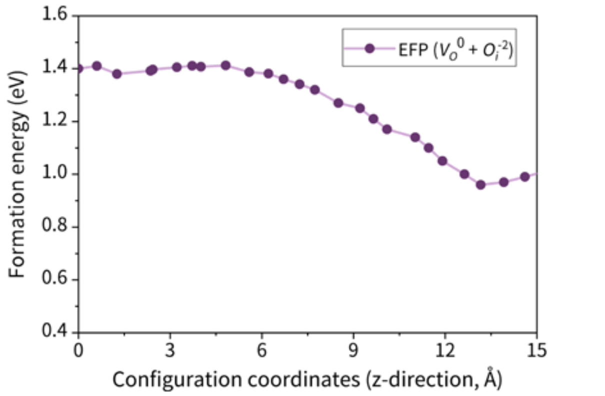

Fig. 2. Formation energy of the extended Frenkel pair for the structure shown in Fig. 1.

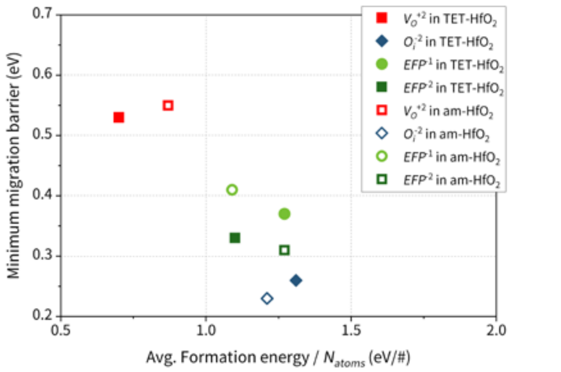

Fig. 3. Migration barriers of various defects in HfO_2. Both the crystalline and amorphous structures are considered.

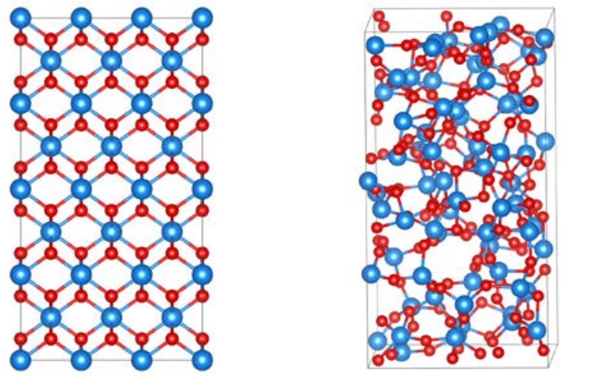

Fig. 4. HfO2 supercells for the conductivity calculation. (Left) A crystalline structure and (Right) an amorphous structure.

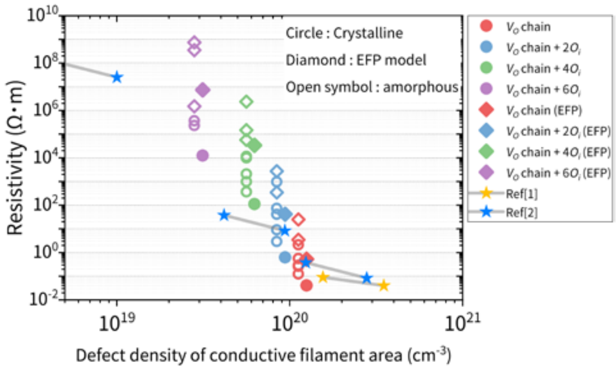

Fig. 5. Calculated resistivities of various HfO_2 structures. When the number of oxygen vacancies increases, the resistivity decreases exponentially.

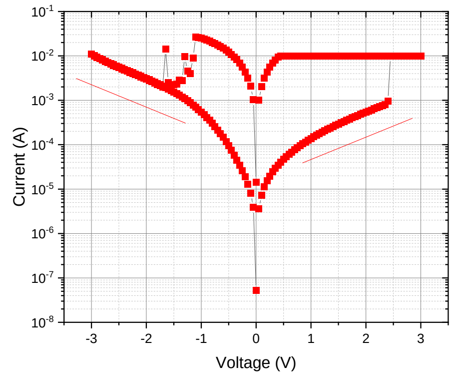

Fig. 6. Measured IV switching charactersitics of a HfO_2-based RRAM. Thickness of the HfO2 layer is 15 nm. The SET and RESET voltages are 2.5 Vand -1.1 V, respectively.

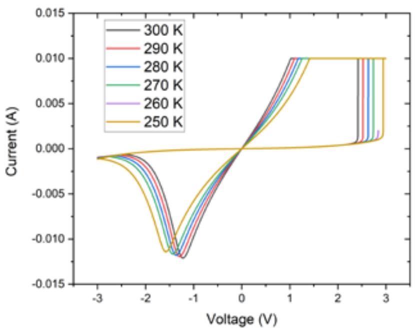

Fig. 7. Simulated switching charactersitics of a HfO_2-based RRAM at various temperatures.

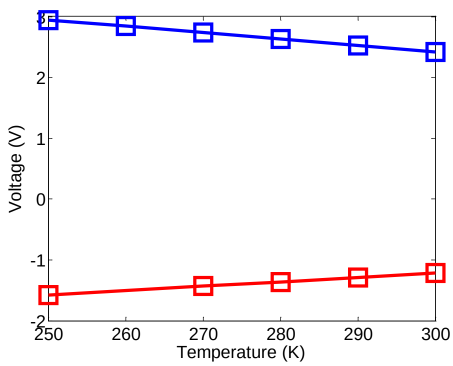

Fig. 8. SET (Blue) and RESET (Red) voltages of the RRAM in Figs. 6 and 7 as functions of the temperature.