Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

First-principles study on metal-TaO_x-metal heterostructures: response to applied bias voltages[1] SATOSHI WATANABE, TAKUYA MATSUMOTO, ARIHIRO TAWARA, Dept. of Materials Engineering, The Univ. of Tokyo, TINGKUN GU, School of Electrical Engineering, Shandong Univ., TOMOFUMI TADA, Dept. of Materials Engineering, The Univ. of Tokyo — Metal-TaO_x-metal heterostuructures are promising as a novel nonvolatile memory device [1]. The formation of conduction paths in the TaO_x layer is responsible for the low resistance state and the switching mechanism is understood as the electrochemical redox reaction involved with the bias-voltage application. However, microscopic details of the conduction path and switching mechanism have not been clarified yet. We examine electronic states, and electron and ion transport in Cu-TaO_x (x$\sim$2.5)-Pt(or Cu) heterostructures from first principles, focusing on the response to applied bias voltages. We show that Cu interstitials in crystalline Ta_2O_5 enhances electronic conduction considerably [2], while does not in amorphous one. We also show that the potential change due to the bias application is sensitive to the structure of TaO_x layer and/or metal-TaO_x interface: in some case, the potential change may be very small near the Cu/TaO_x interface in the TaO_x layer so that the bias application hardly change the mobility of Cu ions in this region. These results will be discussed in terms of electronic states. [1] T. Sakamoto et al., APL 91 (2007) 092110; [2] T. K. Gu et al., ACS Nano 4 (2010) 6477.

[1]This work was supported by CREST-JST, Low Power Electronics Association and Projects, and Grants-in-Aid by MEXT-Japan.

Satoshi Watanabe
Dept. of Materials Engineering, The Univ. of Tokyo

Date submitted: 11 Nov 2011 Electronic form version 1.4