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The effect of Ta "oxygen scavenger layer" on HfO_2-based resistive switching behavior: termodynamic stability, electronic structure, and low-bias transport XIAOLIANG ZHONG, Argonne Natl Lab, IVAN RUNGGER, Materials Divison, National Physical Laboratory, TW11 0LW, UK, PETER ZAPOL, Argonne National Laboratory, HISAO NAKAMURA, YOSHIHIRO ASAI, National Insitute of Advanced Industrial Science and Technology (AIST) Japan, OLLE HEINONEN, Argonne National Laboratory and Northwestern University — Metal-oxide-metal heterostructures are promising candidates for next-generation random access memories, which exhibit reversible resistive switching between high- and low-conductance states. Recent experimental work showed that inserting a metallic 'oxygen scavenger layer' between TiN electrode and HfO2 significantly improves device switching performance. We show, using atomistic modeling within the GGA+U scheme of Density Functional Theory, that a Ta oxygen scavenger layer significantly enhances the thermodynamic stability of depleting oxygen from the oxide. Furthermore, the presence of a Ta layer reduces the dependence of the Schottky barrier heights on the location of the oxygen removed from the oxide matrix. Finally, the Schottky barrier height has a very small effect on the on-state low-bias conductance; this is more sensitive to the location of the depleted oxygen. We gratefully acknowledge the computing resources provided on Blues, a high-performance computing cluster operated by the Laboratory Computing Resource Center at Argonne National Laboratory. Work at Argonne was supported by U. S. DOE, Office of Science under Contract No. DE-AC02-06CH11357.

Xiaoliang Zhong
Argonne Natl Lab

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