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Effect of metallic buffer at electrode-oxide interface on current-voltage characteristics of resistive random access memories (ReRAMs): A first-principles study TAKEHIDE MIYAZAKI, HISAO NAKAMURA, KENGO NISHIO, AIST-NRI, HISASHI SHIMA, HIROYUKI AKINAGA, AIST-ICANN, YOSHIHIRO ASAI, AIST-NRI — We present the electric current (I)-voltage (V) characteristics (-1.0 eV $< V <$ +1.0 eV) for a model of ReRAM devices with metal-oxide-metal structures, based on first principles nonequilibrium Green's function (NEGF) theory [1]. We choose TiN and hafnia (HfO_2) for the electrode and oxide materials, respectively, because this combination has been widely known in literature. We investigate the I-V characteristics for two different compositions of the TiN/HfO_2 interface, (a) with and (b) without the Ta buffer layer between TiN and HfO_2. We assume cubic HfO_2 layers for simplicity. For case (a), a clear distinction between the "ON" and "OFF" states appears depending on the occurrence and absence of the oxygen vacancies (V_Os), respectively. For case (b), however, little electric current flows even when the V_Os exist in hafnia. In the latter, the O atoms abstracted from hafnia are strongly bound to N, leading to substantial separation of TiN from HfO_2. In contrast, in the former, the Ta buffer not only absorbs the O atoms but also bridges TiN and HfO_2 to secure the occurrence of the "ON" state. [1] H. Nakamura et al., J. Phys. Chem. C 115, 19931 (2011).

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