Band alignment at Me/$BaTiO_3$ (Me=Fe, Pt) interfaces

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The non-volatile memory concept of ferroelectric tunnel junctions (FTJ) consisting of metal-insulator-metal (MIM) structures takes advantage of an ultrathin ferroelectric (FE) layer as the barrier material between two metal electrodes, where the resistance switching is realized via an electronic mechanism involving FE polarization reversal [1]. The tunneling electroresistance is controlled by flipping the polarization of the FE barrier and hence the electronic potential profile across the FTJ [2,3]. In order to clarify the electronic properties of metal/FE interfaces and to verify the theoretical models predicting the functional properties of MIM structures with FE barriers, the experimental determination of the band alignment at the the metal/FE interface is of major importance. In this work, the electronic band alignment at Fe/BTO and Pt/BTO interfaces has been experimentally determined using REELS and HAXPES analyses. In addition, the chemical state of the metal (Fe, Pt) in contact with the FE has been investigated.

The Me/BTO bilayered structures were grown by PLD on a MgO(100) substrate. Epitaxial ~10 nm thick Fe (Pt) layers were grown at T=250°C (450°C). The BTO layer (2-7 nm) was grown from the stoichiometric BTO target at T=450°C and further annealed at T=600°C either in residual vacuum ($\sim 5 \cdot 10^{-8}$ mbar, indexed V) or in O_2 atmosphere ($P_{O2}=10^{-4}$ mbar, indexed O). Both Me/BTO and BTO/Me types of interfaces were formed. The band gap of BTO depending on the growth conditions was measured using REELS. The Me/BTO band alignment experiments using standard Kraut methodology [4] were performed utilizing the HAXPES instruments at the DORIS III and PETRA III storage rings at E=6 keV, both enabling to probe deep (10-20 nm) layers and thus providing an opportunity to directly establish the electronic conditions at the metal/FE interfaces, including a continuous capping metal layer. Photoemission spectra at variable glancing take-off angles were used to analyze the chemical state of the metal underlayer in contact with BTO.

The band gaps derived from REELS spectra (not shown) taken from BTO layers grown in vacuum and in O_2 are E_g = 4.1 eV and 4.3 eV, respectively. The Fe (10 nm) underlayer in contact with a 3 nm thick BTO_V grown on top in the same vacuum cycle was found unoxidized up to a monolayer scale judging from the photoemission spectra taken both at normal (0º) and glancing (70º) take-off angles (spectra not shown). The same conclusion is made for an Pt underlayer in contact with BTO on top. The core level and valence band photoemission spectra for individual BTO, metal (Fe, Pt) and Me/BTO bilayers with the opposite types of interfaces were taken to determine the respective Me/BTO electronic band alignment. Selected valence band spectra of Fe_{under}/BTO_V and Pt_{top}/BTO_V with respect to that of the individual BTO_V layer are presented in Fig. 1. The band alignment diagrams for both types of Fe/BTO_V interfaces and for the Pt/BTO_V interface are summarized in Fig. 2.

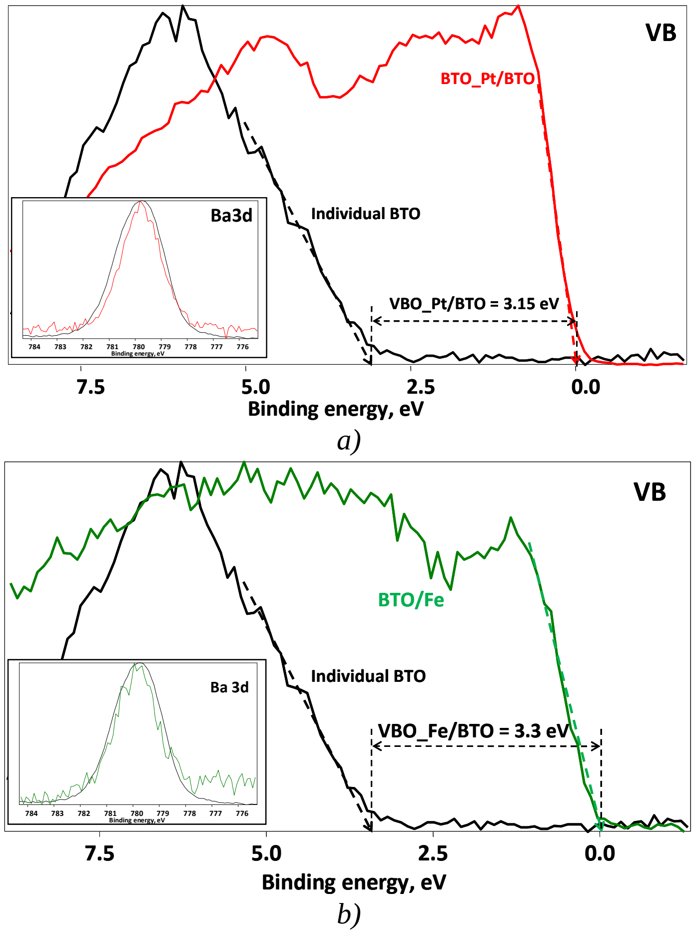

Figure 1: Valence band offsets (VBO) derived from HAXPES spectra for Pt/BTO and Fe/BTO bilayers are VBO(Pt_{under}/BTO_V)=3.15 eV (a) and VBO(Fe_{under}/BTO_V)=3.3 eV (b), respectively.

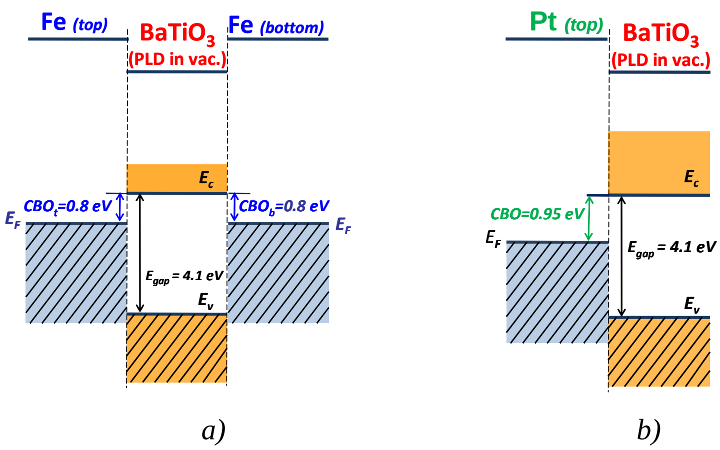

Figure 2: Electronic band alignment diagrams reconstructed from REELS and HAXPES data for both types of Fe/BTO_V interfaces (a) and Pt/BTO_V interface (b).

References

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