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Metal- and oxide-related hydrogen-induced dipoles at the Pt/HfO_2 interface

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Abstract

Such technologically abundant agent as hydrogen has a strong effect on the metal/oxide interface energy barrier. Internal photoemission analysis of electron barrier height variations at Pt/HfO_2 interfaces caused by annealing in hydrogen reveals the formation of a significant (≥0.4 eV) electrostatic dipole layer. The orientation of the H-induced dipole appears to be sensitive to the growth conditions and treatments, e.g., Hf precursor used in the atomic layer deposition (ALD) process: In the case of the $HfCl_4$ precursor, annealing in H_2 leads to barrier lowering, whereas the barrier becomes higher in samples grown by using tetrakis(dimethylamido)hafnium. These findings indicate that hydrogen may form dipoles of opposite orientation through two different mechanisms: The positive dipole is caused by H interaction with the metal surface, which can also be found at interfaces of Pt with other oxides such as SiO_2 and Al_2O_3. By contrast, the sensitivity of the negative dipole formation to the HfO_2 ALD chemistry suggests it to be related to a negatively charged bonded state of hydrogen in the near-interface oxide. Moreover, the formation of positive dipole is also observed after high temperature anneal in nitrogen suggesting the contribution of additional mechanisms of dipole formation.

Keywords: Dipole; Internal Photoemission; Effective Work Function; Interface Barrier

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