Formation of Interface Dipole Layers between Two Dielectrics: Considerations on Physical Origins and Opportunities to Manipulate Its Strength

Koji Kita, Associate Professor, Department of Materials Engineering, The University of Tokyo

The interface dipole layer formation in a gate stack is one of the dominant sources of anomalous threshold voltage of high-k MOSFETs. The interface dipole layer is the concept that considers pairs of identical amount of effective sheet charges with opposite signs emerged at the interface. When those positive and negative sheet charges locate on the different sides of an interface in a distance of atomic scale, this pair of charges induces a steep electrical potential drop in the stack to induce a significant flatband voltage (V_{FB}) shift. Even though such charge pair formation was at first an unexpected phenomenon in the system consisting only of insulating materials, now the concept of interface dipole layers at various high-k/SiO_2 interface is widely accepted based on experimental verifications and theoretical modeling.

One of the unique features of this phenomenon is that not only the strength of dipoles, but also the direction of dipoles often varies for different high-k materials. For high-k/SiO_2 systems this phenomenon was found to be well described by the model considering net displacement of oxygen ions due to the mechanical strain relaxation at the interface by reducing the inconsistency of oxygen atom densities in two oxides. The transfer of other ions driven by interface reactions across the interface also seems to contribute to the dipole layer formation. Such models tell us that the formation of the dipole layer would be a natural consequence of the modification of ionic arrangement in near-interface region to reduce the mechanical or chemical disadvantage emerged when two different dielectric materials make the interface.

Recently we also demonstrated an anomalously huge (>1V) dipole effect in $(Al_2O_3/SiO_2)_n$ laminated dielectric stack, where the dipole layer formations at SiO_2-on-Al_2O_3 interfaces were suppressed by tuning the growth conditions of deposited-SiO_2 whereas those at Al_2O_3-on-SiO_2 interfaces were clearly observed. Such a technique enables us to introduce a positive remarkable shift of threshold voltage, which is expected to be useful in various applications including high-voltage power device applications.