Electronic structure of MgO thin films in external electric field

Mie Univ.[1]
○ (M1) T. Sakatani [1], and K. Nakamura[1]
E-mail: 420M608@m.mie-u.ac.jp

Intrinsic dielectric breakdown is one of very important phenomena in device applications, which abruptly reduces a resistivity in an insulator film when an electric field exceeds a dielectric strength, breakdown field. One may institutively recognize that larger energy bandgap in materials leads to larger breakdown field as seen in various semiconductors. In field of spintronics, however, the breakdown field of MgO thin films in tunnel magnetic junctions is about 6.0-8.0 MV/cm, which is very small compared to that in wide-gap semiconductors, e.g., 11.7 MV/cm of AlN, even though the energy bandgap of MgO, 7.8 eV, is larger than that of AlN, 6.2 eV. It is thus of crucial importance to understand quantitatively the mechanism of dielectric breakdown. Although several theories to the intrinsic breakdown based on the hypothesis of an electron avalanche have been qualitatively proposed, the quantum mechanical-based approach such as *ab initio* way, i.e., first principles calculations, has been just started. In the present work, for the first step, we investigated the fundamental feature in electronic structure of MgO thin films in an external electric field by using first principles calculations. A slab model of MgO (001) thin films, consisted of one to seven atomic-layers, is considered, where atomic positions along the film normal were fully optimized by atomic force calculations. Calculations were carried out by using full potential linearized augmented plane wave method [1] based on density functional theory in generalized gradient approximation. An external electric field along the film-plane normal was introduced in the vacuum regions far enough from film surfaces up to 128 MV/cm, where the internal field in the layer reduces by a factor of ten due to the dielectric screening. In a zero field, by analyzing the layer-resolved band structure, the valence top (conduction bottom) bands in the seven-layer film are found to bent upward (downward) at the surfaces so as to reduce the energy bandgap at the surfaces. When an external electric field is applied, both the valence top and conduction bottom bands at the surfaces shift in energy depending on the electric field directions while the bands in the inner layers do not alter much compared to those in the zero field. The electric-field-induced changes in the bands is emphasized in the conduction bottom band. The detail of the band structure in the electric field including the film thickness dependence will be present.

[1] K. Nakamura, R. Shimabukuro, Y. Fujiwara, T. Akiyama, T. Ito, and A. J. Freeman, Phys. Rev. Lett. 102, 187201 (2009)