PHOTOEMISSION CHARACTERIZATION OF INTERFACE DIPOLES AND ELECTRONIC DEFECT STATES FOR GATE DIELECTRICS

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In the development of Metal-Insulator-Semiconductor (MIS) devices, gate dielectric technology is of great importance and includes major scientific and technological issues to be solved for required device performance and reliability [1]. In particular, characterization of electronic defects in dielectrics and at their interfaces with semiconductor substrates as well as energy band profiles has been imperative to gain a better understanding of physics of dielectric/semiconductor heterostructures [2, 3].
In this work, our recent achievements on the characterization of gate dielectrics and their stacked interfaces by means of photoemission techniques have been reviewed. First, we have shown how valuable the cut-off energy of photoelectrons is to measure directly the potential change due to electrical dipoles at the interface in stacked dielectrics [4]. And then, we have demonstrated how powerful total photoelectron electron yield spectroscopy (PYS) [5, 6] is to quantify the energy distribution of electronic defect states in gate dielectrics and at dielectric/semiconductor interfaces.
The inner potential changes in dielectric stacks reflect in changes in the cut-off energy of secondary photoelectrons (SEs) measured in high-resolution x-ray photoelectron spectroscopy (XPS) [4]. After calibration of the kinetic energy of core-line signals from the underlying layer, an abrupt potential change due to electrical dipoles at the interface between dielectrics, resultant abrupt potential change can be measured as a change in the cut-off energy of SEs. The observation of cut-off energy provides us an advantage in simple and precise evaluation of the potential change due to electrical dipoles as compared to a discussion on dipole formation based on the energy shift of core-line signals which reflects not only the potential change due to dipoles but also the chemical shift, that is, change in the chemical bonding features. From SE spectra near the lowest limit in kinetic energy for the samples before and after the formation of various high-k dielectrics on thermally-grown thick SiO_2, we found that, with the formation of either ultrathin Al_2O_3 or HfO_2 or TiO_2 on SiO_2, the cut-off energy of SEs was shifted toward the higher kinetic energy side. On the other hand, in the cases of Y- and Sr-oxides with silicate formation at the interfaces, a slight opposite energy shift was detected. The analyses of the core line signals confirm that there is a linear correlation between the observed potential changes and the ratios in the oxygen anion density at the interfaces between SiO_2 and high-k dialectics as suggested in Ref. [8].
In the photoelectron yield measurements, the total number of photoelectrons emitting from the sample is counted considering the incident photon flux, the yield spectrum is related to an integral over the occupied density of states existing near the sample surface [5, 6]. From photoelectron yield spectra of 2nm-thick SiO_2 formed 500ºC by remote plasma enhanced CVD on n-type GaN(0001) before and after N_2 anneal at 800ºC, we found that, with the N_2 anneal at 800ºC, the yield from the defects was reduced markedly. The 1st derivative of the measured yield spectrum with respect to incident photon energy leads us to the energy distribution of occupied defect state densities in consideration of density of states of the GaN valence band, measured photoelectron yield from the GaN VB and photoelectron escape depth. As a result, occupied states are reduced down to ~$1x10^{11}cm^{-2}eV^{-1}$ at the energy corresponding to the midgap of GaN near the SiO_2/GaN interface with the N_2 anneal at 800ºC. The defect state density near the conduction band edge, which was crudely estimated in consideration of electron occupation probability based on the Fermi-Dirac distribution, is in good agreements with the result obtained from the capacitance-voltage (C-V) analysis using the Terman method [7]

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