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Energy loss function and inelastic scattering cross-section of ultrathin HfO_2, Al_2O_3 and Hf-Al-O films on Si(100)

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Reflection electron energy loss spectrascopy (REELS) is surface sensitive and capable of analyzing the electronic structure of dielectric thin film since the low-energy-loss region reflects the valence and conduction structure of the solids. In development of high-k gate stacks, their electronic structures should be characterized with a nanometer scale spacial resolution because physical thickness of dielectrics is typically 2 to 3 nm. Here, quantitative analysis of REELS for ultra-thin HfO_2, Al_2O_3 and HfAlO dielectric films on Si(100) were carried out by using Tougaard QUEELS-$\varepsilon(k,\omega)$-REEL software. Inelastic scattering cross-section and energy loss function of low energy region were obtained. The theoretical inelastic scattering cross-section K_{sc} deduced from the simulated energy loss function was compared to experimental cross-section in form of λK_{sc}. The palsmon energy E_p in compounds can be theoretically determined from quantitative analysis of REELS. The energy loss function (ELF) $\mathrm{Im}(-1/\varepsilon)$ obtained with Drude-Lindhard type oscillators describes the response of material to incident electron passing through the solids. In the ELF of HfO_2, the peak appear at the vicinity of 10, 17, 27, 37 and 47 eV. In the ELF of Al_2O_3, a broad peak at 22 with a shoulder at 14 eV and weak shoulder at 32 eV was observed, while for the Al_2O_3 doped HfO_2, the peak position is similar to that of HfO_2. This indicates that when HfAlO film is used as gate dielectric in MOS transistor, its electronic structure is mainly determined by the *d* state of Hf. In addition, the inelastic mean free path (IMFP) was also calculated from the theoretical K_{sc}. The IMFP values determined are agreement with those calculated by TPP2 formula. The determining of IMFP from the ELF is convenient for compounds.