Electron energy-loss spectroscopy and first-principles calculation studies on high-k dielectric thin films

Park, J.[1], Nam, S.[1], Chae, J.[1], Kim, M.[1] and Kim, J.[1]

[1] Materials Characterization Center, Gumi Electronics & Information Technology (GERI), Gumi, Korea, Republic of Korea

Electron energy loss spectroscopy (EELS) analysis in transmission electron microscope (TEM) has been powerful technique to study electronic structures of small volumes of materials. However, acquisition of reliable experimental EELS spectra and accurate information through interpreting them is still challenging. Recently, we established the standard process to acquire reliable EELS data by introducing uncertainty evaluation considering some parameters such as energy dispersion, energy resolution and energy drift of spectrometer. Our group was designated as the Electron Energy Loss Data Center for Standard Reference in Korea. We have produced and collected EELS reference data for materials needed by major industries such as semiconductors, displays and rechargeable batteries.

In this study, high-k dielectric thin films such as HfO_2 and ZrO_2 for semiconducting memory devices was selected as model systems. The first-principles calculation and electron energy loss spectroscopy (EELS) technique was applied to determine the crystal structure and dielectric function of the materials. We will present the comparison results between the theoretically and experimentally obtained low and high energy-loss spectra. The possibility of determining the polymorphism of HfO_2 and ZrO_2 will be discussed through interpreting reliable experimental EELS data with first-principles calculation results.

This research was supported by the MOTIE(Ministry of Trade, Industry & Energy (project number 10080654) and KSRC(Korea Semiconductor Research Consortium) support program for the development of the future semiconductor device.