Optical Properties and Electron Inelastic Mean Free Path of HfO_2

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Hafnium dioxide is a high-*k* dielectric material frequently used in semiconductor devices. HfO_2 also plays a key role in optical coating materials field for its high transmittance in the ultraviolet to near-infrared band, and high laser damage threshold. Therefore, hafnium dioxide becomes nowadays an important material for fabricating different multilayer optical devices, such as optical coatings for astronomical CCDs and anti-reflection multilayer coatings for night vision equipment and infrared optical equipment [1-3]. Hence, hafnium oxide is likely to play an increasingly important role in shaping the future of electronics, energy and materials science. Accurate knowledge of the optical and electrical properties of HfO_2 is the key factors to develop the corresponding applications. In recent years, reflection electron energy loss spectroscopy (REELS) has played an important role to explore the dielectric response of the material to the external charged particles. However, the analysis of REELS spectrum faced difficulty because of the strong surface excitation effect in the measured spectrum. To extract the bulk optical property of the sample one must have an advanced spectrum analysis technique. The aim of our work is, therefore, to present an accurate energy loss function (ELF) and optical constants of HfO_2 from the measured REELS spectrum by using our unique reverse Monte Carlo (RMC) method [4]. This RMC method can remove the surface excitation effect, elastic scattering effect and multiple scattering effect as well as the instrumental effect from the measured REELS spectrum and, hence, lead to the derivation of accurate bulk optical property. The accuracy of the obtained data can be checked by the sum-rules.

The sum-rule results indicate that the derived ELF, n, k, ε_1 and ε_2 indeed have high accuracy. The highly accurate electron inelastic mean free path (IMFP) and stopping power have also been presented by applying the relativistic dielectric response theory. The full Penn algorithm (FPA) is used to expand the

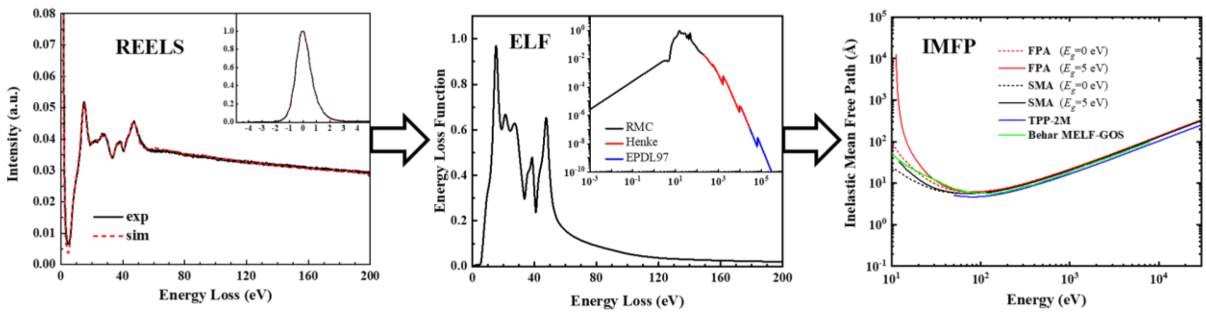

Figure 1. The REELS, ELF and IMFP of hafnium-dioxide determined in this work with high accuracy.

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optical energy loss function, Im{-1/$\varepsilon(\omega)$} into the (q, ω)-plane [5]. Furthermore, we also applied the super-extended Mermin algorithm model to calculate the IMFP and stopping power for comparison with the FPA model [6]. We show that the bandgap has a significant influence to the IMFP and the stopping power.

Keywords: Hafnium-dioxide; REELS; ELF; IMFP.

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BIOGRAPHY

Jiamin Gong has obtained PhD degree at USTC in 2023 and now she is a postdoctor at the School of Materials Science and Engineering, ZJU. Her research interests include surface analysis and Monte Carlo simulation of REELS, AES and XPS spectra.