

## Main factors impacting the VEELS spectra of hafnia

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Significant differences are observed among the VEELS spectra of HfO<sub>2</sub> found in the literature [1-5]. In this presentation we perform a comparative study between literature data, experimental results measured by high resolution EFTEM-VEELS and ab initio simulations by DFT and TDDFT. A device-oriented specific methodology using low energy FIB has been performed to reach the drastic requirements of a single scattering configuration with minimum sample damage. The effects of contamination, implantation and amorphization on the spectral features are detailed. After optimization of sample preparation, signal measurement and data analysis, the best agreement between experiment and simulation is finally obtained. A step towards the quantitative analysis of surfaces loss functions and energy loss functions is therefore reached. The main spectral features and sources of variability can be interpreted in details. In particular, we show that the crystalline phases and orientations may significantly impact the bulk plasmon. The possible sources of modulation of the VEELS spectra, either due to the instrumentation or to the sample geometry or crystallinity are listed and interpreted.

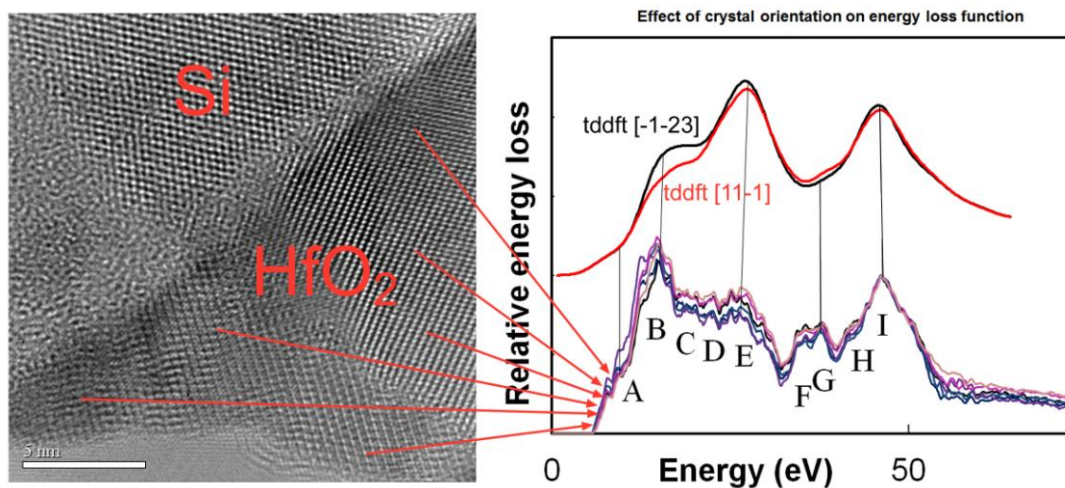


Fig. 1 Cross-sectional HRTEM image and corresponding VEELS spectra measured in monoclinic HfO<sub>2</sub> at the location marked by arrows. A significant modulation of the spectral features can be compared with tddft simulations.

### Références

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