Interfacial Roughness of Hf_xSi_{1-x}O₂ High-k films by TEM and AFM

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Scaling trends for semiconductor CMOS technology require the development of high dielectric constant (high-k) gate materials such as hafnium silicates to obviate problems faced by ultra-thin conventional SiO₂ such as leakage current and boron diffusion [1],[2]. Transmission electron microscopy (TEM) and electron energy loss-spectroscopy (EELS) have provided insight into high-k materials film deposition as well as the structural affects of chemical pre and post treatments on electrical properties of high-k film systems [3]. Phase separation and crystallization of high-k films have been correlated to poor electrical characteristics [4],[5].

Figure 1 shows two high-angle annular dark-field scanning transmission electron microscopy (HAADF-STEM) images from the same cross-section sample of a HfO₂/SiO₂ bilayer gate stack (this SiO₂ was grown purposefully thick). Image (a) is from a region of the TEM sample where the EELS log-ratio method thickness of the silicon substrate was 120 nm; for this sample thickness, the HfO₂ layer appears smooth and conformal so that film thickness and interfacial roughness seem deducible from the image intensity profile. Image (b) however, recorded from a 50 nm thick region on the same TEM sample, shows that the HfO₂ layer is quite rough. The HfO₂-SiO₂ interface has high contrast in HAADF-STEM images due to large difference in atomic number, but still roughness extending through the thickness of the film is difficult to interpret and quantification of the change in image intensity in the high-k layer does not necessarily lead to the correct interpretation of the extent of roughness. Also further thinning of the TEM sample can be difficult due to damage induced at surfaces while ion-polishing.

Figure 2 shows atomic force microscopy (AFM) data from the same sample in the TEM measurements. This data proves that the HfO_2 layer is considerably rough with peak to peak height changes equivalent to the thickness interpreted by "thick region" TEM data. The film is "grainy" and not a good conformal dielectric layer and a capacitor made from such a film would derive most of its dielectric capacity from the underlying SiO₂ and not the HfO₂ "layer".

In conclusion, TEM sample thickness must be carefully considered when interpretting thickness measurements of high-k films from HAADF-STEM images if interfacial or surface roughness is at lengthscales with periodicity smaller than the TEM sample thickness. Surface roughness can be determined by AFM for uncapped films. While films processed with capping electrode layers may be very different from uncapped films, the use of AFM data to aid the interpretation of TEM data from uncapped films can lead to a better understanding of TEM data from capped films.

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Figure 1. HAADF-STEM images showing (from left to right) crystalline silicon substrate (aligned to (110) axis) of a "test" HfO_2 -SiO₂ bilayer stack (a) from a 120 nm and (b) a 50 nm thick region of the TEM sample.



Figure 2. AFM data from same sample showing that the surface roughness is though the full thickness of the HfO_2 high-k layer; this is not easily appreciated by TEM cross-sections unless the sample is made nearly as thin as the roughness periodicity.