Properties of ultrathin high-k dielectrics on Si probed by electron spin resonance-active defects: interfaces and interlayers

A. Stesmans
Department of Physics, University of Leuven
Celestijnenlaan 200 D, 3001 Leuven, Belgium

It appears the semiconductor integrated circuit (IC) industry is rapidly nearing a crucial turning point in its hectic history in the near future. In a bold perspective brought about by the dazzling miniaturization strive, the relentless scaling of metal-oxide-silicon (MOS) devices in current IC technology will require the replacement of the superb, still unexcelled, conventional SiO_2 and SiO_xN_y gate insulators by alternative dielectrics of significantly higher dielectric constant κ. Hence, semiconductor industry is facing a most challenging problem to be solved in order to keep on track with projected future progress. Naturally, this has instigated intense research in appropriate alternative high-κ materials for future deep sub-µm MOS generations.

On the material aspect side, multiple high sensitivity analyzing techniques[1] are combined to explore microstructural, compositional, and bonding chemistry aspects of ultrathin high-κ layers on Si. Inserted in MOS arrangements and devices, their electrical performance is scrutinized with the most advanced electrical tools as has been carried out previously for the SiO_2 case. Not unexpectedly, an aspect that comes to the fore is the occurrence of defects and charge traps[2] which incisively affect the electrical quality of the new high-κ layers. Interface traps appear to play a prominent role. With regard to the Si/SiO_2 entity, the crucial information as to the atomic nature of point defects, interface defects in particular, has predominantly come from electron spin resonance (ESR) analysis. So, interesting information may be expected from subjecting the newly advanced Si/alternative insulator structures to similar ESR perusal.

This is addressed in the present work, dealing with ZrO_2, Al_2O_3, and HfO_2 layers. The latter is currently considered as a most promising high-κ gate oxide, in view of encouraging properties such as its high κ (=20-25) value and remarkable thermal stability, enabling minimization of intermixing at interfaces upon post deposition anneal treatments, and allowing the growth of smooth and abrupt interfaces.

On overview will be presented of results of ESR observations on high-κ films, with particular emphasis on the interface defects. Results will be discussed of stacks of ultrathin SiO_x and Al_2O_3 films sandwiched between (100)Si and thin ZrO_2 layers, with the aim to provide atomic identification and quantification of occurring defects. The known characteristics of the amply studied Si/SiO_2 structure are used as backdrop. Among others, it is revealed that the ruling paramagnetic inherent interface defects in Si/SiO_2, i.e., P_b-type centers, also appear dominant defects at the interface of (100)Si with ultrathin Al_2O_3 and SiO_x layers. It is outlined that their salient ESR features may serve as a unique probe –a criterion– of the (electrical) quality of the interface and its behavior during subsequent thermal treatments.

Through the probed interface defects, particular attention is paid to the interface nature and the role if ultrathin interlayers, either inserted during manufacturing of the Si/high-κ film stacks or developed during postdeposition thermal treatments. As it appears from numerous researches, thermally induced interlayers, such as SiO_x and silicates, may readily form, the control of which is crucial. Among others, interesting information is obtained regarding the stress state of the interface region.

In a particular case, the influence of the manufacturing method on interface nature and quality is studied in a comparative ESR analysis of Si/HfO_2 entities fabricated using three variants of the chemical vapor deposition method. In terms of revealed interface defects, a distinct variation is observed, which, when combined with post deposition thermal steps, has enabled us to study interface quality evolution in relation with interlayer formation. ESR measurements in conjunction with electrical capacitance-voltage and conductance-voltage analysis have enabled to trace the atomic nature of the dominant part of fast interface states.

[1] *D. Wilk, R. M. Wallace, and J. M. Anthony, J. Appl. Phys. 5243 (2001)*
[2] *M. Houssa et al. J. Appl. Phys. 87, 8615 (2000)*