PREDICTING THE PROPERTIES OF NEW OXIDES FOR NANO-DEVICES

D. Muñoz Ramo, J. Gavartin, P. Sushko and Alexander Shluger

Department of Physics and Astronomy and the London Centre for Nanotechnology,
University College London, Gower Street, London WC1E 6BT, UK

As microelectronics tends towards nanoelectronics, new materials issues affect device performance. Current transistor dimensions already fall below 40 nm and a CMOS transistor with a mere 6 nm channel length has been demonstrated. The sub 10 nm length scale creates new materials challenges for which modelling of materials, interfaces, dopants, and defects will be crucial to process design and device performance enhancement. The integrated circuit components will soon comprise tens of thousands of atoms or less, so approaching molecular scales. Therefore developing accurate and efficient theoretical tools and models is vital for defect metrology of these complex systems.

To cope with some of these issues, during the last several years the microelectronics has undergone the most significant materials revolution in 40 years by changing gate oxide from silicon oxide to a much more complex materials combination, including a stack of thin layers of oxides with a higher dielectric constant than SiO_2 (high-k oxides), e.g. HfO_2 and Hf silicates. Recent advances in film deposition techniques dramatically improved quality of hafnia films grown on silicon as well as quality of interfaces with both silicon substrate and metal gate. However, the performance of prototype high-k transistors is still affected by large concentrations of various defects. Oxygen vacancies and interstitial ions as well as other defects in HfO_2 and SiO_2 films and at $HfO_2/SiO_2/Si$ interface are often implicated in causing problems.

We will discuss challenges faced by defect detection and metrology, which are common to all nano-devices, and will present the results of calculations of the electronic structure and spectroscopic properties of oxygen vacancies in different charge states in the monoclinic phase of HfO_2, in amorphous SiO_2 and at the $HfO_2/SiO_2/Si$ interface. Our calculations predict the existence of five charge states of the vacancy and position the corresponding energy levels in the band gap. We have calculated the optical transition energies as well as optical and thermal ionization energies for all vacancy charge states and g-tensor for ESR active states. We will discuss the relation of the calculated properties to the experimental results on spectroscopic ellipsometry, ESR and electrical stress measurements.

All simple models indicate that materials with high dielectric constants are likely to show significant *polaron* effects, however, both experimental and theoretical proof of polaron self-trapping remains extremely challenging. We shall illustrate some of the wealth of such behavior in m-HfO_2 and closely-related systems. The examples will include negatively charged oxygen vacancy in m-HfO_2 and electron and hole self-trapping in the perfect m-HfO_2 lattice. We predict the existence of both hole and electron small polarons in m-HfO_2. Holes can self-trap on a single oxygen atom in HfO_2, and electrons can self-trap on three Hf ions sharing an oxygen atom. Our results suggest that both hole and electron polarons in m-HfO_2 could be observed as stable immobile defects at low temperatures and should remain localized and exhibit hopping mobility at relatively high temperatures. Therefore the hole and electron conductivity of pure m-HfO_2 samples should exhibit characteristic temperature dependence.

We will then turn to modeling $HfO_2/SiO_2/Si$ interfaces and predicting defect types at the interfaces and in thin SiO_2 layers. We will discuss the interface structure and the band alignment in this system, some effects of HfO_2 amorphization and electrical properties of defects located in various regions of the interface. Our results demonstrate the importance of interfaces in determining the properties of these nano-scale layered systems.