

ROLE OF CARRIER INJECTION IN DEGRADATION OF OXIDE FILMS

Alexander Shluger, University College London, UK
a.shluger@ucl.ac.uk

David Gao, University College London, UK

Jack Strand, University College London, UK

Oliver Dicks, University College London, UK

Moloud Kaviani, WPI-Advanced Institute of Materials Research, Japan

Key Words: amorphous oxide films, DFT calculations, carrier injection, defect creation.

Most current electronic and electrochemical devices are stacks of thin films and interfaces operating under electrical stress. Nanometre-thick oxide films play crucial role in performance of these devices. In particular, injection of excess electrons and holes into oxide films and the nature of electron trapping sites are important for our understanding of the mechanisms that govern the formation of conductive filaments in resistance switching memory devices, the dielectric breakdown in microelectronic devices, and the performance of photo-electrochemical and oxide fuel cells. It is usually assumed that excess electrons and holes induced into crystalline oxides as a result of irradiation, doping or electron injection from electrodes contribute to conductivity or become trapped at shallow or deep states. Our theoretical modelling combined with experimental observations demonstrates that structural disorder in *amorphous* SiO₂, Al₂O₃ and HfO₂ films creates precursor sites which can spontaneously trap up to two electrons or holes in deep states in the band gap [1,2]. This results in weakening of Me–O bonds, which can be broken upon thermal activation, creating an O²⁻ interstitial ion and a neutral O vacancy. O²⁻ interstitial ions can easily diffuse through the oxide and in devices are guided to the positive electrode by the electric field [3,4]. Hole injection in amorphous HfO₂ films facilitates the formation of stable V²⁺ oxygen vacancies and interstitial O atoms, both of which can diffuse relatively fast. Thus electron and hole injection can lead to the formation of new defects and significantly alter the structure of oxide films at large injection densities. I will discuss the implications of this effect for the mechanisms of electrical breakdown and resistance switching in electronic and memory devices. The creation and field-driven movement of oxygen ions causes changes in oxide structure on a much larger scale than previously thought. I will discuss the mechanisms of oxygen release from stressed oxide films [5] and we show that these changes are apparent at electric fields comparable to those routinely used in microelectronic and photonic devices.

[1] A.-M. El-Sayed, M. B. Watkins, V. V. Afanas'ev, and A. L. Shluger, Phys. Rev. B89, 125201 (2014).

[2] M. Kaviani, J. Strand, V. V. Afanas'ev, A. L. Shluger, Phys. Rev. B94, 020103 (2016).

[3] S. R. Bradley, A. L. Shluger and G. Bersuker, Phys. Rev. Appl. 4, 064008 (2015)

[4] D. Z. Gao, A.-M. El-Sayed and A. L. Shluger, Nanotechnology 27, 505207 (2016)

[5] A. Mehonic, M. Buckwell, L. Montesi et al. Adv. Mater. 28, 7486 (2016)