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## ABSTRACT

## Defects in Crystalline and Amorphous gate oxide films

Most current electronic and electrochemical devices are stacks of thin films and interfaces operating under electrical stress. Polycrystalline and amorphous nm-thick oxide films play a crucial role in performance of these devices. Electrons and holes trapped at defect sites in these films are responsible for the mechanisms that govern the degradation and dielectric breakdown of devices, resistance switching, and the performance of photo-electrochemical and oxide fuel cells. We will compare the properties of intrinsic and extrinsic defects in crystalline and amorphous oxides. Our theoretical modelling combined with experimental observations demonstrates that structural disorder in amorphous $SiO_2$, $Al_2O_3$, and $HfO_2$ films is responsible for distribution of defect properties and creation of new H related defects. Unlike in crystalline oxides, structural precursor sites in amorphous $SiO_2$, $Al_2O_3$, $TiO_2$, ZnO and $HfO_2$ spontaneously trap up to two electrons or holes in deep states in the band gap [1-3] The electron localization in amorphous $SiO_2$ and $HfO_2$ weakens Me–O bonds, which can be broken upon thermal activation, creating an O interstitial ion and a neutral O vacancy [4]. O interstitial ions can easily diffuse through the oxide and in devices are guided to the positive electrode by the electric field [5]. Multi-scale modelling including electron injection rates, defect creation and electron hopping through created defects is used to describe leakage current and dielectric breakdown in oxide films. The results demonstrate significant differences in the behaviour of defects in crystalline and amorphous oxide films.

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## BIO

Alexander Shluger graduated from the Latvia State University, Riga, USSR in 1976. He received PhD and Doctor of Science degrees from the L. Karpov Physics and Chemistry Research Institute, Moscow in 1981 and 1988, respectively. He joined the Royal Institution of Great Britain, London in 1991 and the faculty of the University College London in 1996, where he is a Professor of Physics from 2004. He is a Fellow of the Institute of Physics and of the American Physical Society, and a Foreign Member of the Latvian Academy of Sciences. He is a Principal Investigator at the WPI-Advanced Institute of Materials Research, Tohoku University, Japan (from 2007). His current research is focused on theoretical studies of defects in oxides and at semiconductor/oxide interfaces in conjunction with microelectronics applications, the mechanisms of photo-induced processes at oxide surfaces, defects in 2D materials, as well as on modelling of imaging and manipulation of molecules on insulating surfaces using Atomic Force Microscopy.