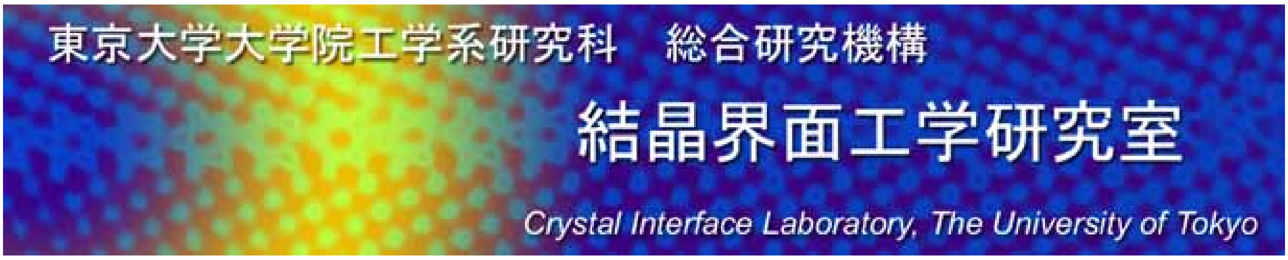

Crystal Interface Lab. Seminar Series

Institute of Engineering Innovation
The University of Tokyo

Electron trapping by grain boundaries in positive and negative electron affinity materials

by

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There is growing evidence that boundaries between grains in polycrystalline oxide films p favorable paths through which electrons can conduct or tunnel. This has important implicatio MOSFETs employing polycrystalline gate dielectrics and also for other nanoscale electronic d such as magnetic tunnel junctions. In this presentation we will show, by first principles calcula how the preferential trapping of electrons at defects which are known to segregate to bounc such as oxygen vacancies, can open up conducting channels through the oxide. We compai important materials, MgO and HfO_2, and show that, although they have similar band gaps electron trapping properties are quite different. One of the reasons for this is that MgO has a ne affinity while HfO_2 has a positive affinity to electrons[1,2]. To investigate the structure and proper grain boundaries we developed a multi-scale approach linking atomistic calculations, periodi and an embedded cluster method. We have studied several models of MgO and HfO_2 grain bou structures, calculated their electronic properties and investigated the segregation and diffus vacancies and relevant impurities. Dislocations forming as a part of the interface between Mg HfO_2 grains lead to trapping of electrons and holes in one-dimensional states. Electrons and may then subsequently trap at defects and impurities that segregate to grain boundarie demonstrate that the flexibility of the HfO_2 lattice and its higher dielectric constant encourag formation of polarons in the bulk[3] and inside the dislocation cores.

[1] K. P. McKenna and A. L. Shluger, Nature Mat. **7**, 859-862 (2008)

[2] K. McKenna et al., J. Am. Chem. Soc. **129**, 8600 (2007)

[3] D. Muñoz Ramo, et al. Phys. Rev. Lett. **99**, 155504 (2007)

February 19 (Thursday), 2009　15:00 -17:00

Main meeting room at Institute of Engineering Innovation, UT
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