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Controlling Interface Properties for Advanced Energy Applications

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Controlling Interface Properties for Advanced Energy Applications

Abstract

Internal interfaces in materials play an important role in the performance of many devices used in energy applications including solar cells, LEDs, passive electronics, and fuel cells. Efficiencies in energy and power consumption may be realized by optimizing and often miniaturizing these devices. Our studies show that internal boundaries and biomaterial interfaces cause local property variations. These effects will dominate device performance as the systems become smaller. A fundamental understanding of the effect of atomic structure on local properties is a prerequisite to device optimization. Developing this understanding requires new probes that access local properties, controlled interface structure, atomic resolution electron microscopy and first principles calculations of geometric and electronic structure.

Comments

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Controlling Interface Properties for Advanced Energy Applications

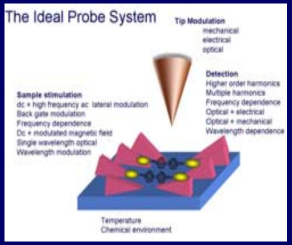
R. Shao, D. Li, R. Kraya, D. Bonnell, Department of Materials Science

Introduction

Internal interfaces in materials play an important role in the performance of many devices used in energy applications including solar cells, LEDs, passive electronics, and fuel cells. Efficiencies in energy and power consumption may be realized by optimizing and often miniaturizing these devices. Our studies show that internal boundaries and biomaterial interfaces cause local property variations. These effects will dominate device performance as the systems become smaller. A fundamental understanding of the effect of atomic structure on local properties is a prerequisite to device optimization. Developing this understanding requires new probes that access local properties, controlled interface structure, atomic resolution electron microscopy and first principles calculations of geometric and electronic structure.

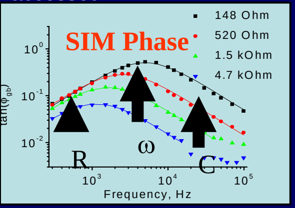
New Probes of Local Properties

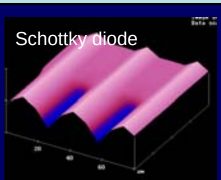
The two new multiple modulation techniques, developed at Penn, have been shown to successfully overcome barriers to quantifying local electrical behavior.



Scanning Impedance Microscopy SIM

The modulating electric signal is applied *laterally* across the surface rather than to the tip, allowing R, C, and trap state time constants to be accessed.

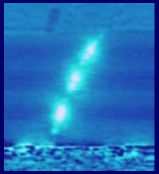


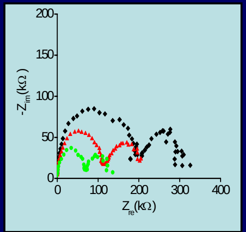


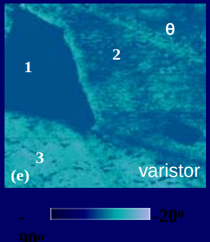
Nanoimpedance Microscopy NIM

Monitoring the frequency dependence over 6 orders of magnitude yields the real and imaginary contributions to impedance.

Defects in a Carbon Nanotube

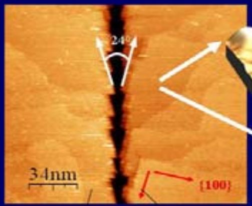


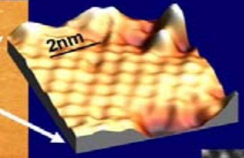


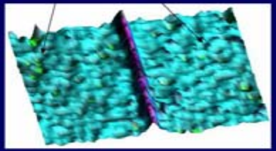


Structure and Properties of Internal Interfaces

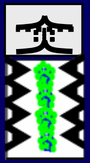
The charge at SrTiO3 grain boundaries is due to periodic under coordinated Ti in the boundary so the amount at any boundary depends on the atomic structure, i.e. there is one electron associated with each Ti polyhedron. This interface charge causes local dielectric constant suppression adjacent to the interface. In addition the charge induces ferroelectric dipole formation and alignment at a mid temperature phase transition in SrTiO3.

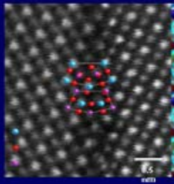




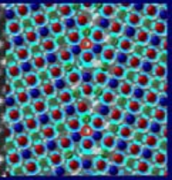


Direct imaging of charge at a $SrTiO_3$ bicrystal boundary by SSPM

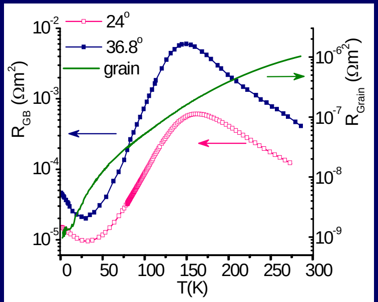




Aberration corrected Z-contrast TEM image of a SrTiO3 bicrystal grain boundary



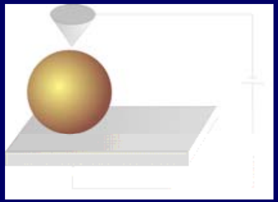
Calculated charge density distribution at the grain boundary



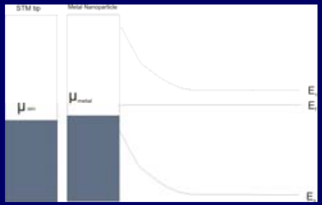
Extension to Interfaces of Nanocontacts

Characterizing the properties of a metal-semiconductor nano-contact is crucial to the emergence of nano-electronic devices. We have shown that contact potential can be size dependent. Discovering the mode of conduction through the contact and the effects of surface states on the interface barrier are two of the most important aspects of understanding the nature of the contact. By combining SIM with STM and spectroscopy, the fundamental properties governing the interaction of metals and semiconductors can be determined.

A metal nanoparticle on a semiconductor substrate.



Band-level diagram of a 2-step electron transfer process. In this diagram electrons flow from the semiconductor to the metal nanoparticle and finally to the tip.



References:

D. Carroll, M. Wagner, M. Ruehle, D. Bonnell, *Phys. Rev. B* 55 (1997).

R. Shao, MF Chisholm, G. Duscher, D. Bonnell, *Phys. Rev. Lett.* 95 (2005).

R. Shao, S. Kalinin, D. Bonnell, *Appl. Phys. Lett.* 82 (2003).

S. Kalinin, D. Bonnell, *J. Applied Physics.* 91 (2002).

M. Freitag, S. Kalinin, D. Bonnell, A.T. Johnson. *Phys Rev Lett.* 89 (2002)