Electron Transport at the Nanoscale Focus Topic
Room: 16 - Session ET+SS+GR+SP-FrM

Electron Transport at the Nanoscale: Development of Theories and Techniques
Moderator: C. Su, Bruker Nano

8:20am **ET+SS+GR+SP-FrM1 What is Missing in the Space Charge Limited Current Theory?**, ***X.-G. Zhang***, Oak Ridge National Laboratory, *S.T. Pantelides*, Vanderbilt University **INVITED**

Space-charge-limited currents are important in energy devices such as solar cells and light-emitting diodes, but the available theory from the 1950's finds it necessary to postulate defect states that are distributed in energy in order to match data. This has prevented the theory to be used in extracting reliable defect information such as energy level and trap density from measurements. Here we revisit the theory and show that this postulate is not warranted. Instead, we demonstrate that dopants and the concomitant Frenkel effect, which have been neglected, control the shape of measured current-voltage characteristics. For highly disordered material, there is a significant inter-trap tunnelling current in the Ohmic regime, which accounts for the observed peak in the noise power. The new theory can anchor efforts to develop experimental techniques to measure deep-trap levels.

This research was conducted at the Center for Nanophase Materials Sciences, sponsored at ORNL by the Division of Scientific User Facilities (XGZ), and by Division of Material Science and Engineering, Basic Energy Sciences, U.S. Department of Energy (STP), and the McMinn Endowment at Vanderbilt University (STP).

9:00am **ET+SS+GR+SP-FrM3 Mapping Solar Cell Internal Fields and Band Offsets**, ***H. Cohen***, *Y. Itzhaik, G. Hodes*, Weizmann Institute of Science, Israel

The internal fields and band offsets across device interfaces are key features in various applications and, yet, this information is generally inaccessible by standard electrical tools. A systematic approach addressing this problem is demonstrated here, based on chemically resolved electrical measurements (CREM). Studying nanoporous photovoltaic cells, we resolve the internal details layer-by-layer and, thus, extract a realistic band diagram for the multi-interfacial structure. We show the spontaneous evolution of two p-n–like junctions and quantify the associated band bending at corresponding domains. An account for the 'real' working conditions of the device is attempted by exposing the cell to optical and electrical stimuli, revealing the charge trapping at each specific layer and showing how certain sample treatments affect the trapping mechanisms. Our methodology overcomes a critical missing link in device characterization and in fundamental studies of nanoscale solid-state devices.

9:20am **ET+SS+GR+SP-FrM4 Quantum Degeneracy Revealed by the Relation between the Tunneling Current and the Chemical Force**, ***P. Jelinek***, *M. Ondracek,* Institute of Physics of ASCR, Czech Republic, *F. Flores*, Universidad Autonoma de Madrid, Spain

Recent progress has allowed merging AFM and STM into a new experimental setup where tunneling current and atomic forces are recorded simultaneously. The possibility to collect both quantities simultaneously opens new horizons not only in advanced characterization at the atomic scale but also in understanding fundamental relations between the electron transfer and formation of the chemical bond between two bodies.

Actually, there is a long-standing debate in the scientific community about the relation between the chemical force and the tunneling current (see e.g. [1]) on the atomic scale. Both the tunneling current and the short-range component of the force, induced by the formation of the chemical bond, exhibit in atomic contacts an exponential decay with increasing distance in the range of several angstroms. As the quantities depend directly on the wave-function overlap between outermost atoms of tip and surface, the corresponding exponential functions should have similar characteristic decay length. In particular, the relation between the chemical force F and the tunneling current I follows the law F^n~I, where n is an integer number. Over the last 10 years, several different scaling factors n, varying from 1 to 4, have been proposed by different groups based on both theoretical analysis and experimental measurements (see reference in [2]); still there is no consensus on the relation between the chemical force and the tunneling current.

In this contribution, we explain the relation between the tunneling current and the interaction force at the atomic scale using a simple analytical model [2]. The model unveils the existence of two characteristic scaling regimes, where the tunneling current is either proportional to the chemical force I~F or to the square of the chemical force, i.e. I~F^2. We show that the existence of a given regime is basically controlled by two parameters: (i) the electronic level degeneracy and (ii) the hopping between electronic levels involved in the interaction process. Finally, we will collate our theoretical prediction with experimental AFM/STM measurements of single-atom point contacts and complex DFT simulations [3] to confirm the existence of these two characteristic regimes.

[1] W. Hofer and A.J. Fisher, *Phys. Rev. Lett.* 91, 036803 (2003) and the reply in by C.J. Chen

[2] P. Jelinek et al, J. Cond. Mat. Phys. 24, 084001 (2012).

[3] M. Ternes et al Phys. Rev. Lett. 106, 016802 (2011).

9:40am **ET+SS+GR+SP-FrM5 Understanding the Influence of the Tunneling Current and the Chemical Force on the Contrast Formation in KPFM**, ***Z. Majzik***, *M. Ondráček, M. Švec, J. Berger, P. Jelínek*, Institute of Physics of ASCR, Czech Republic

Kelvin Probe Force Microscopy (KPFM) [1] senses the variation in the electrostatic force. The electrostatic force is *Fel=-dCTS/dz(Vbias-Vlcpd)2*, where *Vlcpd* denotes to the local contact potential difference (LCPD). Atomic scale resolution was achieved by KPFM on the prototypical Si(111)–7×7 surface [2]. It was shown that the formation of a chemical bond between the closest tip-surface atoms induces significant variation in the LCPD [2]. Lately it was observed that the tunneling current leads to the raise of an additional electrostatic (phantom) force [3]. Consequently, the total electrostatic force must be the combination of several components where the contribution of each component is defined by the tip-sample separation.

Recent progress in Scanning Probe Microscopy opens the possibility of simultaneous acquisition of the tunneling current, atomic forces and local potential difference with atomic resolution [4]. The aim of this contribution is to discuss the origin of electrostatic force contribution at different tip-sample separations. In particular, we performed simultaneous site-specific AFM/STM measurements on Si(111)–7×7 using a modified Omicron qPlus (tuning fork based) system [5]. We found that along the tip approach three characteristic regions can be well distinguished. At large tip-sample separations, the capacitance is a function of tip geometry and the tip-sample distance. Approaching the tip closer towards the surface, quantum effects become to play important role. The overlap between the tip and sample wave functions produces electron tunneling, which induces additional electrostatic force. Formation of the chemical interaction between the tip apex atom and the adatoms of the 7x7 surface induces changes in the electron charge distribution reflected in variation of the LCPD [2] and the permittivity in the tunneling gap. Hence the capacitance is modified accordingly. In order to have better understanding of the impact of the chemical interaction, atomic hydrogen was deposited to saturate the dangling bonds of adatoms. Over the hydrogenated adatoms, nor strong shift in the LCPD or sudden change in the capacitance was observed. Further to gain more insight into ongoing processes we carried out DFT calculations for tip-sample interaction to understand affect of the formation of covalent bond between tip apex and surface adatoms on the Si 7x7 surface.

References

[1] M. Nonnenmacher et. al, App. Phys. Lett. 58, 2921 (1991)

[2] S. Sadewasser et. al, Phys. Rev. Lett. 103, 266103 (2009)

[3] A. J. Weymouth et. al, Phys. Rev. Lett. 106, 226801 (2011)

[4] F.J. Giessibl, Appl. Phys. Lett. 73, 3956 (1998)

[5] Z. Majzik et. al. B. J. Nano 249, 3 (2012)

10:00am **ET+SS+GR+SP-FrM6 An *In Situ* Technique for Using Ballistic Electron Emission Microscopy to Measure Hot Electron Transport at Metal Semiconductor Interfaces**, ***R. Ralsano***, *V.P. LaBella*, University at Albany-SUNY

Ballistic electron emission microscopy (BEEM) is a scanning tunneling microscopy (STM) technique that can measure transport of hot electrons through materials and interfaces with high spatial and energetic resolution. BEEM requires an additional contact to ground the metal base layer of a metal semiconductor junction. Performing BEEM *in situ* with the sample fabrication requires a custom built STM or modifying a commercial one to facilitate the extra contact, which leaves the technique to highly trained experts. This presentation will describe our work to develop a special silicon substrate that has the extra contact and oxide hard mask built in to enable *in situ* BEEM without modifications to the STM. Electrically

isolated contact traces are lithographically patterned *ex situ* onto the silicon substrate. Then a hard mask is grown and lithographically patterned and connected to the BEEM sample plate which is then inserted into the ultra-high vacuum chamber. The metal is then deposited on top of the hard mask and then mounted *in situ* onto the STM for BEEM measurements. BEEM measurements comparing both *in situ* and *ex situ* deposited films will be presented.

10:20am **ET+SS+GR+SP-FrM7 Electronic Transport on the Nanoscale**, ***R. Moeller***, University of Duisburg-Essen, Germany **INVITED**

To study the transport through objects at the nanoscale a scanning tunneling microscope with several tips is used. Two different configurations will be discussed. The lateral transport of electrons may be studied by using two tips to drive a current parallel to the surface. A third tip enables to map the corresponding electrochemical potential. Measurements for a 2D conducting layer will be discussed. To analyze the transport perpendicular to the surface, a thin metallic layer is placed on a semiconducting surface. At the interface a Schottky barrier is formed, which can only be overcome by electrons of sufficient energy. This may be used to split the current of electrons coming from the tip of the microscope into two parts, the ballistic electrons and the electrons which have been scattered. This technique has been applied to study the ballistic transport of electrons through individual molecules. On the other hand inelastic processes may be revealed by analyzing the fluctuations in the tunneling current observed at different positions of the tunneling tip above an adsorbed molecule.

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