Surface Science
Room 203 - Session SS2-FrM

Electronic Structure of Surfaces
Moderator: J.G. Tobin, Lawrence Livermore National Laboratory

8:20am **SS2-FrM1 Three-Dimensional Valence Band Structure of WTe@sub 2@**, ***T. Ohta,*** Lawrence Berkeley National Laboratory/Fritz Haber Institute*; A. Bostwick, E. Rotenberg,* Lawrence Berkeley National Laboratory

We report complete valence band structure measurement of tungsten ditelluride (WTe@sub 2@) in 3-dimensions (3D) of k-space by angle-resolved photoemission spectroscopy (ARPES). WTe@sub 2@ is comprised of Te-W-Te layers, and is known to exhibit semi-metallic conduction. Unlike most transition metal dichalcogenide compounds, WTe@sub 2@ has an orthorhombic unit cell. It was previously shown by density-function-theory calculation that WTe@sub 2@ has a metallic band in addition to a semi-metallic band, which is brought about by W 5d and Te 5p bands overlapping near the Fermi-level (E@sub F@). So far, the parallel existence of semi-metallic and metallic bands has not been clearly demonstrated in photoemission experiments due to a complex overlap of W 5d and Te 5p derived states, and because of their k@sub z@ (k perpendicular) dependence near E@sub F@. To shed light on this issue, we have conducted complete 3D band structure mapping of WTe@sub 2@ using synchrotron radiation ARPES. 3D band structure mapping is a powerful tool for investigating the entire electronic structure of a material by visualizing valence band in all three k directions. We have clearly observed the semi-metallic and the metallic bands crossing E@sub F@, and the k@sub z@ dependence of both semi-metallic and metallic bands especially close to E@sub F@. While the semi-metallic band has a slight k@sub z@ dependence, the metallic band appears only near the zone center. We compare our measured 3D band structure to the reported band structure calculation with emphasis on the Fermi surface contour. The semi-metallic conduction can be attributed to the semi-metallic band existing throughout the k@sub z@ direction, whereas the metallic band is limited to the zone center.

8:40am **SS2-FrM2 High Resolution Angle Resolved Photoemission Study of the Electronic Structure of InN(0001)**, ***L. Colakerol,*** *L. Plucinski, S. Wang, H.K. Jeong, K.E. Smith, P. Chen, T.D. Moustakas,* Boston University

We report a study of the surface and bulk electronic structure of InN(0001) thin films using high resolution synchrotron radiation excited angle-resolved photoemission (ARPES).@footnote 1@ The InN thin films were grown by plasma-assisted molecular beam epitaxy on c-plane sapphire, and transferred in air to the synchrotron. Samples were cleaned both by annealing in UHV and by cycles of nitrogen ion bombardment followed by UHV annealing. Sharp 1 x 1 hexagonal LEED patterns were observed from the films following either cleaning procedure. Aside from the expected bulk valence band states, we have observed a series of unusual states near E@sub F@, in the bulk band gap, for a narrow range of excitation energies and band momenta. These states are free electron-like, with parabolic dispersion around the surface Brillouin zone center. The number of states observed is a function of annealing temperature, and these states are likely the result of segregation of In metal to the surface. Up to four individual states are observed, and we associate them with quantum well states due to an In metal overlayer. The states are insensitive to contamination by exposure to 1000 L H@sub 2@, and are not related to intrinsic surface states. Our results are discussed in the context of both the known surface electronic structure of GaN (0001),@footnote 2@ and of charge accumulation at InAs surfaces.@footnote 3@ @FootnoteText@ @footnote 1@ Supported in part by the NSF DMR-0311792, by U.S. ARO 40126-PH, and by U.S. AFOSR. Our spectrometer system is funded by U.S. ARO DAAD19-01-1-0364. Experiments performed at the NSLS which is supported by the U.S. DOE, Divisions of Materials and Chemical Sciences.@footnote 2@ Y.C. Chao, C.B. Stagarescu, J. Downes, P. Ryan, K.E. Smith, D. Hanser, and R.F. Davis, Phys. Rev. B 59, 15586 (1998).@footnote 3@ L.O. Olsson, C.B.M. Andersson, M.C. Haakansson, J. Kanski, L. Ilver, and U.O. Karlsson, Phys. Rev. Lett. 76, 3626 (1996).

9:00am **SS2-FrM3 Phase Diagram of Cr110 Thin Films Measured by ARPES**, ***E. Rotenberg,*** *B.K. Freelon, S.A. Morton, H. Koh, A. Bostwick,* Lawrence Berkeley National Laboratory*; K. Rossnagel,* Univ. Kiel, Germany*; A.K. Schmid,* Lawrence Berkeley National Laboratory*; S.D. Kevan,* Univ. of Oregon **INVITED**

We report the impact of dimensional confinement on physical properties associated with the spin-density wave (SDW) ground state in chromium. These properties are also of some technological importance since chromium is a common component of thin film magnetic structures. We prepared chromium (110) films of high crystalline quality on a W(110) substrate with a wedge-shaped thickness profile so that the impact of confinement can be systematically studied. We have characterized these films using a combination of low-energy electron diffraction and microscopy as well as high-resolution angle-resolved photoemission spectroscopy. By probing the Fermi surface and the nesting vectors that are relevant to the SDW ground state, we characterized the SDW incommensurability in the film directly, and we find that this incommensurability deviates markedly from the bulk value for thin films at higher temperatures: we find commensurate and incommensurate phases that are separated by nearly continuous transitions. Further changes in the SDW phase diagram arise upon hydrogen adsorbtion. Our results suggest a simple model to explain the delicate interplay between commensurate and incommensurate phases that involves a balance between SDW stabilization energy and surface and interface energetics.

9:40am **SS2-FrM5 Using Spin Resolved Resonant Photoemission to Probe Electron Correlations in Nonmagnetic Ce**, ***S.-W. Yu,*** Lawrence Livermore National Lab*; T. Komesu,* University of Missouri-Rolla*; B.W. Chung,* Lawrence Livermore National Lab*; G.D. Waddill,* University of Missouri-Rolla*; J.G. Tobin,* Lawrence Livermore National Lab

We have studied the spin-spin coupling between two f electrons of nonmagnetic Ce by means of spin resolved resonant photoemission. The two f electrons participating in the 3d5/2 to 4f resonance process are coupled in a singlet while the coupling is veiled in the 3d3/2 to 4f process due to an additional Coster-Kronig decay channel. Based on the Ce measurements, it is argued that spin resolved resonant photoemission is a unique approach to study the correlation effects, particularly in the form of spin, in the rare-earths and the actinides.

10:00am **SS2-FrM6 Localized Electronic States Around a Single Kondo Impurity from a First Principles Embedding Theory**, ***P. Huang,*** *E.A. Carter,* Princeton University

Scanning tunneling microscopy (STM) experiments of a single, magnetic adatom on non-magnetic metal surfaces reveal a sharp resonance in the immediate neighborhood around the adatom [e.g. Manoharan et al., Nature 403, 512 (2000)]. This intriguing observation has been interpreted as the presence of a "Kondo cloud", in which the localized d-electrons on the magnetic adatom hybridize with the metal band states to form an extended open-shell singlet near the Fermi level, thus effectively screening out the impurity moment. While the STM experiments have provided a first atomic-scale glimpse of this surface Kondo state, questions remain about the detailed electronic structure, and the nature of the low-lying excitations which give rise to the Kondo resonance width. We present a first-principles study of the electronic structure of a single Co adatom on Cu(111). Our approach is based on an embedding strategy [Kluner et al., PRL 86, 5954 (2001)], which views the Co adatom and nearest neighbor Cu atoms as a metal cluster embedded in a periodic slab background. The total Co/Cu(111) system is treated using density functional theory (DFT), which allows for a mean-field treatment of an extended periodic system. Using the DFT density for the total system, the effect of the background is cast into an effective embedding potential acting on the cluster. Explicitly-correlated theories (i.e. perturbation theory, configuration interaction) are subsequently applied to the embedded cluster in the presence of the embedding potential. The low-lying, many-body excited states are also treated within this same framework to yield excitation energies and wave functions.

10:20am **SS2-FrM7 Persistent Superconductivity in Ultra-Thin Pb Films: A Scanning Tunneling Spectroscopy Study**, ***D. Eom,*** *S. Qin,* The University of Texas at Austin*; M.-Y. Chou,* Georgia Tech*; C.K. Shih,* The University of Texas at Austin

We report a direct probe of the superconducting order parameter of superconducting crystalline Pb films in the ultra-thin regime (5 -18 ML) by using a home-built low temperature scanning tunneling microscopy/spectroscopy (STM/S). Surprisingly, we find that the 2D cooper pair condensates remain extremely robust down to the thinnest film (5ML)

without any signature of the transition temperature (Tc) suppression. Moreover, we find that the quantum oscillations of order parameter are also very persistent in this regime and the oscillation correlates directly with the density of states (DOS) oscillation at the Fermi level. Finally a constant value of the ratio of energy gap to Tc close to that of the bulk was found, implying the same strong coupling nature for electron-phonon interaction. More detailed analysis of the interplay of quantum size effects and superconductivity will be reported.

10:40am **SS2-FrM8 Surface Electronic Transport in Ultrathin Silicon-on-Insulator**, ***P. Zhang***, *E. Tevaarwerk, B. Park, D. Savage,* University of Wisconsin-Madison*; G. Celler,* Soitec USA*; I. Knezevic, P. Evans, M.A. Eriksson, M.G. Lagally,* University of Wisconsin-Madison

Silicon-on-insulator (SOI), a thin single-crystal silicon template layer on silicon dioxide, promises to become the platform for future high-speed electronics, as well as for a range of sensor technologies. When the Si layer is very thin, unique phenomena arise. The emergence of novel electronic properties with decreasing Si template layer thickness is particularly important. In contrast to the conventional view, ultrathin SOI displays rich electronic phenomena. It is usually claimed that STM imaging of thin SOI is impossible, because a thin SOI layer is fully depleted of free carriers (and thus overly resistive), which in effect eliminates the current path from the STM electrode tip to the contact. In complete contrast to this view, we report successful STM imaging of ultrathin (10 nm) SOI, when the top native oxide is removed and a clean reconstructed Si (001) surface is exposed.@footnote 1@ We explain theoretically the low sheet resistance of ultrathin SOI that has a reconstructed-Si [(2x1)] surface. We attribute the ability to image to surface electronic transport. The presence of a high density of states in surface bands (pi and pi*) and the position of the narrow surface bandgap are the dominant mechanisms in repositioning the Fermi level in ultrathin SOI. They lead to a high density of free carriers. The bulk doping density and the density of interface states on the back Si/SiO@sub 2@ interface are largely irrelevant for electronic properties of ultrathin SOI with a clean reconstructed surface. We confirm this conclusion with sheet resistance measurements on SOI covered with thin oxide. The influence of hydrogen on conductivity in ultra-thin SOI will also be discussed. Our measurements suggest that it will be possible to follow thin-Si-membrane structure and properties continuously from bulk to the ultimate limit of a Si film one unit cell high on oxide. Research supported by NSF, AFOSR, and DOE. @FootnoteText@ @footnote 1@Pengpeng Zhang, et al., submitted.

11:00am **SS2-FrM9 Using Nano-focussed Bremstrahlung Isochromat Spectroscopy (nBIS) to Determine the Unoccupied Electronic Structure of Pu**, *M.T. Butterfield,* ***J.G. Tobin****, N.E. Teslich Jr., R.A. Bliss, M.A. Wall, A.K. McMahan, B.W. Chung, A.J. Schwartz,* Lawrence Livermore National Laboratory

The investigation of the actinides is of great interest because of their unique electronic structure. At the pivotal point of the behavior of the electronic structure of the actinide series is plutonium. Pu has the most complex phase diagram of all metals, both with regard to the intricacy of the crystal structures and the number of different phases. While there are a number of ongoing experimental efforts directed at determining the occupied electronic structure of Pu, there is essentially no experimental data on the unoccupied electronic structure of Pu. We aim to determine the conduction band (unoccupied) electronic structure of Pu and other actinides in a phase specific fashion and emphasizing bulk contributions by using Nano-focussed Bremstrahlung Isochromat Spectroscopy (nBIS). BIS is the high-energy variant of inverse photoelectron spectroscopy (IPES: electron in, photon out), which is essentially the time reversal of photoelectron spectroscopy (photon in, electron out). IPES can be used to follow the dispersion of electronic states in ordered samples. Owing to its low energies, IPES is usually very surface sensitive. However, by working at higher energies, we will sample preferentially for bulk properties, downgrading the impact of surface effects, following a philosophy similar to that of Mo et al.@footnote 1@ Thus, from BIS, we would have a direct measure of the conduction band or unoccupied electronic structure of the bulk Pu. By using a nano-focused electron source associated with a SEM, we hope to gather phase specific information from crystallites within polycrystalline Pu samples. We will discuss the experimental arrangement required to carry out such an experiment and our progress in building such a system. Acknowledgements :This work was performed under the auspices of the U.S. DOE by University of California, Lawrence Livermore National Laboratory under contract W-7405-Eng-48. @FootnoteText@@footnote 1@S.-K. Mo et al, Phys. Rev. Lett. 90, 186403.

Author Index

Bold page numbers indicate presenter