Surface Science
Room 209 - Session SS2+EL-MoA

Electronic Structure and Excitations
Moderator: R.A. Bartynski, Rutgers University

2:00pm **SS2+EL-MoA1 Recent Photoemission Studies of Quasi-1D Solids**, ***K.E. Smith***, *J. Xue, L.C. Duda,* Boston University*; A. Fedorov, P.D. Johnson,* Brookhaven National Laboratory*; W. McCarroll, M. Greenblatt,* Rutgers University **INVITED**

Much controversy surrounds the interpretation of the results of angle resolved photoemission spectroscopy (ARP) studies of the electronic structure of quasi one-dimensional (1D) solids. In principle, ARP should provide valuable information about quasi-1D solids, including the structure of the Fermi surface and possible non-Fermi liquid behavior of electrons close to the Fermi level (E@sub F@). In practice, straightforward interpretation of the spectra is often difficult. It has been reported that photoemission from states near E@sub F@ in quasi-1D conductors differs significantly from that measured from two and three dimensional solids. There are a number of possible explanations for these observations, including problems with surface defects and stoichiometry, charge density wave fluctuations leading to a pseudogap, or a Luttinger liquid state. We report here the results of a temperature dependent ARP study of the electronic structure close to E@sub F@ in the quasi-1D conductors Li@sub 0.9@Mo@sub 6@O@sub 17@ and K@sub 0.3@MoO@sub 3@.@footnote 1@ These materials are ideal for ARP studies since large high quality crystals can be grown, and surfaces suitable for ARP measurements can be prepared by cleaving in vacuum. Using very high momentum and energy resolution ARP, we clearly measured for both materials: i) quasi-1D bands dispersing across the Fermi surface; ii) substantial emission intensity at E@sub F@ in the metallic phase; and iii) a gap opening at E@sub F@ as the samples are cooled through the metal-semiconductor transition. Our results differ from many earlier ARP studies of quasi-1D solids. The differences are likely due to an order of magnitude improvement in angular resolution (and corresponding improvement in momentum resolution) for the spectrometer used here. The reported non-Fermi liquid behavior in photoemission from these solids will be discussed. @FootnoteText@ Supported in part by the DOE under DE-FG02-98ER45680 (KES) and DE-AC02-98CH10886 (PDJ).

2:40pm **SS2+EL-MoA3 Fermi Contours and Adsorbate Phonon Anomalies for Li/Mo(110) and Li/W(110)**, ***E. Rotenberg***, Lawrence Berkeley National Laboratory*; S.D. Kevan,* University of Oregon

Angle-resolved photoemission was used to measure the Fermi contours of surface-localized states on the Mo(110) and W(110) surfaces with varying amounts of adsorbed lithium up to 1 ML. In analogy with recent results for H on Mo and W(110), we find that the contours are well nested and therefore can drive a surface phonon anomaly. The nesting vector parallel to the @Sigma@ azimuth on Mo(110) at monolayer coverage is in good agreement with recent phonon measurements.@footnote 1@ We also report the variation of this nesting vector as a function of coverage, and show that a more complete understanding of the electron-phonon coupling on these surfaces might be obtained from coverage-dependent measurements of surface phonon dispersion relations. Finally, our results suggest even better nesting along the @Gamma@ --> S direction and that a more pronounced anomaly might be observed there. @FootnoteText@ @footnote 1@J. Kroger, D. Bruchmann, S. Lehwald, and H. Ibach, Surface Science 449(1-3),227 (2000).

3:00pm **SS2+EL-MoA4 Thickness Dependence of the Unoccupied Electronic States in the Pd/Ru(0001) System**, ***W.-K. Siu***, *T. Mensing, R.A. Bartynski,* Rutgers University

The unoccupied electronic structure of the Pd/Ru(0001) system has been examined using inverse photoemission spectroscopy for Pd thicknesses in the 1 - 15 monolayers range. Previous studies indicate that in the sub-monolayer coverage range, the desorption temperature of CO on Pd/Ru(0001) is less than that of CO/Pd(111) or CO/Ru(0001). Similarly, we have previously shown that the desorption temperature for CO from the Cu/fccCo/Cu(100) metallic quantum well (MQW) system is a non-monotonic function of film thickness and is correlated with MQW states crossing the Fermi level. This suggests that quantum size effects can influence the strength of the chemisorption bond. As Pd interacts more strongly with CO, our objective is to investigate the occurrence of MQW states in the Pd/Ru(0001) system and determine their influence in CO chemisorption. Metallic quantum well (MQW) states are observed at the @Gamma@ point of the Pd thin film. The energies of these states change as a function of the film thickness. A simple phase accumulation model provides a semiquantitative understanding of this behavior. There is also an unoccupied surface state at @Gamma@, which shifts to higher energy with increasing film thickness, approaching that of the single crystal Pd(111) surface state. We have also determined the energy dispersion with parallel momentum of the unoccupied Pd states along the @Gamma@K and @Gamma@M directions. Finally, the influence of MQW states on the adsorption of CO on the Pd/Ru(0001) system will be discussed.@footnote 1@ @FootnoteText@ @footnote 1@ Supported by NSF-DMR #98-01681 and ACS-PRF #33750-AC6,5.

3:20pm **SS2+EL-MoA5 High Resolution Photoelectron Spectroscopy of Pu at the Advanced Light Source**, ***D.A. Arena***, *J.G. Tobin,* Lawrence Livermore National Laboratory*; D. Shuh, E. Rotenberg,* Lawrence Berkeley National Laboratory*; J. Terry, R.K. Schulze, J. Lashley, T. Zocco, D. Farr,* Los Alamos National Laboratory

High resolution photoelectron spectroscopy of Pu has been performed at the Spectromicroscopy Facility (Beamline 7.0) at the Advanced Light Source in Berkeley. Based upon an initial analysis of the data, two key results are immediately obvious. (1) The 5d-5f Resonant Photoemission of the Pu 5f levels exhibits a dependence upon the Pu phase and structure. For example, the results from alpha and delta Pu differ significantly. This strongly suggests that electronic behavior is linked to atomic ordering and structure in Pu. (2) Contamination with oxygen and carbon may be more insidious and subtle than initially believed. Photoemission measurements at a photon energy of 800eV exhibit oxygen and carbon core level peaks, while the same sample shows no contamination utilizing a photon energy of 1253eV, a typical laboratory source energy used in ECSA machines (i.e., Mg k-alpha). In other words, what was thought to be "clean" may not have been. Furthermore, contamination issues like these have a crucial impact upon interpretation of Pu core level spectra, e.g. localized and delocalized screening by 5f electrons. Additionally, 5f-6p Resonant Photoemission, core level spectra (particularly the Pu 4f's) and X-Ray absorption data, all from the Pu will be presented and discussed. Future plans, including ideas about studying magnetic effects in Pu, will also be described. UCRL-JC-133518 Abs.

3:40pm **SS2+EL-MoA6 Plasmon Resonance Spectroscopy of Plutonium Metal Allotropes**, ***R.K. Schulze***, *J.D. Farr,* Los Alamos National Laboratory

We have measured the plasmon resonance response of the cleaned and well characterized surfaces of the six plutonium thermal allotropes (@alpha@, @beta@, @gamma@, @delta@, @delta@', @epsilon@) using backscatter electron energy loss spectroscopy (EELS). The energy of the plasmon resonance is highly dependent upon the electronic structure of the solid surface, and in particular, the density of electrons available for conduction. Using this method we probe directly, for the first time, the number of free elec trons, and the changes in the electronic structure of the plutonium. EELS spectra were acquired on a high purity sample of plutonium with primary electron beam energies of 150, 200, 500, 700, and 1000 eV, and with the sample at seven different temperatur es: -125 (@alpha@), 45 (@alpha@), 156 (@beta@), 250 (@gamma@), 410 (@delta@), 465 (@delta@'), and 525°C (@epsilon@). Changes in the plasmon resonance spectra over the 150 to 500 eV primary beam energy range indicate that a surface reconstruction e xists for each of the Pu allotropes. The 700 and 1000 eV EELS measurements are alike, indicating that bulk characteristics are being probed at these energies. The bulk plasmon resonance energies for the allotropic series (@alpha@, @beta@, @gamma@, @delta@, @delta@', @epsilon@) are 12.23, 11.18, 11.16, 10.81, 10.94, and 10.92 eV. From these measurements, we extract the volume density of free electrons in each allotrope. In electrons per nm@super 3@ these are, for the series, 108.5, 90.7, 90.3, 84.8, 86.8, and 86.5. These results correlate directly with measurements of resistivity and magnetic susceptibility for the series of allotropes, indicating that the changes in free electron density are identically responsible for the changes in these physical properties. The implications of these results in terms of the electronic properties of Pu and in the changes of electronic structure between the allotropes will be discussed.

4:00pm **SS2+EL-MoA7 Lifetimes of Conduction Band States at Semiconductor Surfaces**, ***Th. Fauster***, *M. Kutschera, C. Kentsch, M. Wiets, I.L. Shumay, M. Weinelt,* University Erlangen, Germany

In time-resolved two-photon photoemission electrons are emitted after absorption of two photons. By a suitable delay between the two photons the lifetimes of conduction band states can be directly measured in pump-

probe experiments. Using time-resolved two-photon photoemission we have studied several semiconductor surfaces. On the Si(100)-(2x1) surface several bulk and surface transitions with unoccupied intermediate states between the conduction band minimum and the vacuum energy are observed. Below the conduction band minimum we find a lifetime in the ps range, which we attribute to the unoccupied surface state. This unoccupied as well as the occupied surface state which originate from the silicon dangling bonds are clearly resolved within the same experiment. On epitaxial, metallic CoSi@sub 2@(111) films on a Si(111)-substrate three unoccupied states could be identified. Their lifetimes lie in the 10 fs range. Neither the lifetimes nor the energetic positions of those unoccupied states depend on the film thickness. On the SiC(0001)-(@sr@3x@sr@3)R30° surface the occupied and unoccupied Mott-Hubbard surface bands are observed. An asymmetric splitting relative to the Fermi level is found in agreement with recent theoretical calculations.

4:20pm **SS2+EL-MoA8 Oscillating Band-bending at the Initial Stage of Sb Growth on Si(100) held at 60K***, **J.M. Seo,*** Chonbuk National University, Korea

Using the synchrotron photoemission spectroscopy, the band-bending, the work-function and the valence band edge were simultaneously monitored at the initial stages of Sb growth on Si(100) held at 60 K. By the intensity attenuation of Si 2p with increasing Sb coverage, it can be deduced that Sb forms a relatively uniform overlayer on Si(100) at 60 K. The band-bending, determined by the bulk Si 2p position, oscillates within 0.15 eV up to about 4 ML of Sb, while the corresponding work-function, monitored by the secondary-cutoff position of biased substrate, negligibly changes. The metallicity, monitored by the valence band edge, indicates that the surface becomes semiconductor-like up to about 1.5 ML but recovers its metallic character with additional Sb coverage. These results implicate that the oscillating band-bending is due to the local charge exchange between the dimer row and Sb at the interface, while the corresponding metallicity of Sb film is determined by the amount of confined and available charges within the film.

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