MS01.08.04 NEW TECHNIQUE FOR SURFACE CRYSTALLOGRAPHY: DIRECT INVERSION OF KIKUCHI ELECTRON PATTERNS. C. M. Wei, Institute of Physics, Academia Sinica, NanKang, Taipei, Taiwan 11529, Republic of China

Direct inversion of the diffraction patterns of low-energy Kikuchi electrons named Kikuchi electron holography, using integral-energy phase-summing method [1], is found to yield the three-dimensional Patterson function of the near-surface structure. The results on the Ag(100), Ag(111), Si(001) (2x1), and Si(111) $\sqrt{3}$x$\sqrt{3}$ R30°-Au surfaces will be present. High-fidelity, artifact-free three-dimensional images of nearby atoms measured from the emitters on surfaces are obtained with a high-resolution (~1Å) in all direction [2]. These works have demonstrated high surface sensitivity of Kikuchi electrons and thus led to direct surface structural determination by inverting Kikuchi electron patterns. Finally, the future of this new surface technique will be discussed.

[1] C. M. Wei and S. Y. Tong, *Surf. Sci. Lett.* **274,** L577 (1992).
[2] C. M. Wei, I. H. Hong, and Y. C. Chou, *Surface Review Letters* **1**, p335 (1994)

MS01.08.05 THE SCANNING TUNNELING ATOM PROBE. POINT REFLECTION MICROSCOPY. J. C.H. Spence, J. Zuo, U. Weierstall, X. Zhang, Physics, Arizona State Univ., Tempe, AZ 85287 USA, SPENCE@phyast.la.asu.edu

We describe two new surface science instruments. The first aims to identify atom types at individual defect sites on extended crystal surfaces. The need for such a capability arises in areas as diverse as catalyst poisoning, impurity atmospheres around emerging line defects, composition gradients at interfaces and the identification of foreign atoms at kinks and surface steps, which may influence rates of crystal growth. An STM has therefore been constructed which allows atomic clusters of interest to be transferred into a time-of-flight spectrometer for species identification. Atoms are first transferred onto the STM tip, using a small voltage pulse. The sample is then removed, and these atoms ejected into a time-of-flight (TOF) analyser for mass identification. A channel plate above the tip is used for both time-of-flight detection, and field-ion and field emission imaging of the tip. The output is led to a digital oscilloscope, whose trace is triggered by the tip pulse. Scope, triggering and H.V. are all under Labview control. Examples of Si atoms identified by their TOF spectra and corresponding STM images will be shown. (More details in J. Vac Sci., 1996, in press).

The low voltage point reflection microscope consists of a nanotip field emission source (at about 200 volts) above a grounded clean crystalline surface. The specular reflected cone of rays forms an in-line reflection electron hologram on a distant channel plate, with resolution equal to source size and magnification equal to the ratio of sample-detector / source - sample distances. The hologram is a shadow image projected from the virtual source image inside the crystal, and is out-of focus by the source to sample distance. Examples of the reconstruction of 100 volt experimental in-line electron holograms will be shown, in which they are brought back into focus. The apparatus uses a stick-slip piezo goniometer for the tip, and inch-worm motions for the stage. Experimental Bragg lines in reflection patterns (similar to HOLZ lines in CBED or CBIM patterns) and reflection images will be shown. Theoretical computations of these spherical-wave RHEED patterns from surface steps will be shown and discussed. A method of computing RHEED patterns of steps from a point source will be outlined, based on a phase-grating perturbation of the Bloch-wave solutions (NSF award DMR9412146. More details in Proc. MSA 1995).

PS01.08.06 SURFACE STRUCTURE DATABASE (SSD): VERSION 2. M. A. Van Hove[1], K. Hermann[2], P. R. Watson[3]. [1]Materials Sciences Division, Lawrence Berkeley National Laboratory, University of California, Berkeley, CA 94720, USA; 2 Abteilung Theorie, Fritz-Haber-Institut, Faradayweg 4-6, D-14195 Berlin, Germany; [3]Department of Chemistry, Oregon State University, Corvallis, OR 97331, USA

The second version of SSD (Surface Structure Database) appeared in early 1996, updating the first version of SSD, published in 1993. SSD-2 includes nearly 1000 structures (an increase of over 50%) published through mid-1995, as well as numerous software extensions and improvements.

SSD is an interactive PC-based database of experimentally determined surface structures. For maximum reliability and usefulness, the structures are critically selected to be completely solved, by any established technique. The database includes extensive information not only about atomic positions and bond lengths and angles, but also about experimental preparation, measurement and analysis methods.

The main features of SSD will be exhibited. They include an advanced search and display system, as well as an interactive 3D color visualization that has great flexibility. It is also possible to generate publication-ready color or gray-scale prints of any structure.

Neutron Scattering II Instrumentation & Techniques

MS01.09.01 NEUTRON REFLECTION FROM MOLECULAR FILMS. R.K. Thomas, Physical and Theoretical Chemistry Laboratory, Oxford University, UK

Neutron reflection has become a very effective technique for studying molecular layers at soft interfaces, particularly those involving liquids. The effective resolution can be greatly enhanced by using isotopic labelling as a means of determining intralayer distances and it is now possible to determine molecular conformations, especially of hydrocarbon chains, at disordered interfaces.

The method of using isotopic substitution in conjunction with neutron reflection will be illustrated by examples of structure determination at air/liquid and solid/liquid interfaces.

MS01.09.02 END-GRAFTED POLYSTYRENE BRUSHES IN A CRITICAL BINARY MIXTURES. S. K. Satija, P.D. Gallagher, A. Karim, NIST, Gaithersburg, MD and L. Fetters, Exxon Corporate Research Laboratories, Annandale, NJ

We report neutron reflectivity measurement on end-grafted polystyrene brushes in contact with binary mixtures of cyclohexane and methanol. End-grafting was done by adsorbing trichlorosilane terminated perdeuterated polystyrene on silicon substrates. Neutron reflectivity measurements were done with mixtures of cyclohexane and methanol of various proportions (including the critical composition) and at different temperature. On the methanol rich side the brush is quite collapsed, however, the brush height increases on decreasing the temperature indicating that the proportion of cyclohexane next to the brush increases upon lowering the temperature. As we lower the temperature through the phase transition, the brush streches suddenly and further decrease of temperature brings about a normal decrease in brushheight. On the cyclohexane rich side, a small amount of addition of methanol (5%) gives rise to a very large change in the reflectivity. Our preliminary results in this regime indicate that with the addition of methanol the brush has streched considerably compared to the pure cyclohexane case. Results of all these composition and temperature scans will be described.