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) \textsuperscript{3x3} 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.


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) analyzer 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 voltm 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 HREM 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).

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.