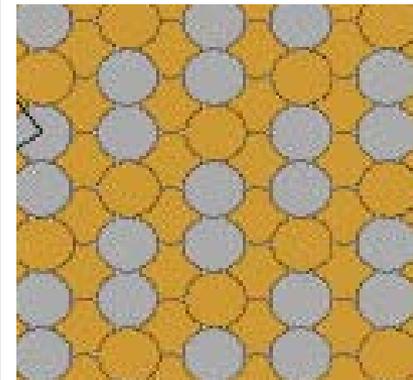
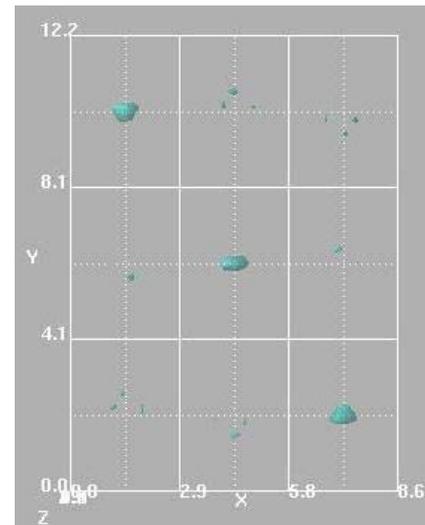
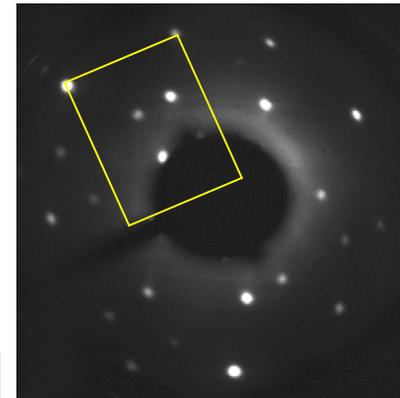


Atomic-Scale Visualization of Surface Structure

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DMR-9984442

Semiconductor surfaces and nanostructures often yield complicated atomic arrangements that hinder quantitative analysis by surface x-ray diffraction for lack of an appropriate atomic model for conventional refinement. If a starting structure could be inferred from the data, it would aid this effort significantly. We have succeeded in demonstrating that this approach is feasible on simpler systems, namely, reconstructed metal surfaces.

The new analysis allows us to assign phases to the experimental structure factors, and thereby *directly visualize* the surface atomic structure by a simple Fourier transform. We applied this method to several Sb-induced rearrangements that we discovered on the Au(110) surface. Here we show the electron diffraction pattern (and unit cell) for Sb/Au(110)-($\sqrt{3} \times \sqrt{3}$). Next, we show the direct reconstruction of the structure, revealing one diagonal row of Au alternating with two of Sb. The resultant structure is schematically shown.



In x-ray crystallography, one measures the intensity of the scattered radiation, but the phase is lost. If we had the phase, we could make a direct image of the electron density of the object under investigation by a simple Fourier transform. This well-known “phase problem” in x-ray crystallography significantly impedes determination of complicated surface reconstructions or nanostructures. The problem is that we are forced to make an intelligent guess about the likely rough atomic positions, then compare (and refine) this guess by comparison with experiment. However, if we are not able to make a roughly correct initial guess, then we will never be able to refine this model into a correct model of the surface. The method we are developing will allow a robust initial starting point that will allow quicker quantitative determination of complicated surface reconstructions on semiconductor surfaces and nanostructures.

My theoretical collaborator has developed a method to iteratively determine the phases of a set of oversampled surface x-ray diffraction data. (The oversampling is possible because the presence of a surface relaxes the stringency of the diffraction condition normal to the surface, creating the well-known “crystal truncation rods” normal to the surface.) We have demonstrated the success of this method on the well-known clean surface of Au(110)-(2x1). Next, we have begun to apply this method to heretofore unknown surface reconstructions. We discovered a series of reconstructions on the Au(110) surface, which are induced by submonolayer amounts of Sb, including a c(2x2), a rt(3)xrt(3), and a p(5x6). We are investigating these with low energy electron diffraction (LEED), x-ray photoelectron spectroscopy (XPS), and surface x-ray diffraction (SXRD), conducted at the NSLS at Brookhaven. Using the novel analysis method, we can reconstruct directly a visualization of the near-surface region. In the diagram above, the green blobs represent isosurfaces of electron density recovered by the algorithm for the Sb/Au(110)-(rt(3)xrt(3)) surface. Since Au atoms are stronger scatterers than Sb, Au atoms appear larger than Sb atoms. The structure is then seen to be composed of alternating rows of Sb and Au atoms along the diagonal. Two rows of Sb atoms are interspersed by one row of Au atoms, in agreement with the electron and x-ray diffraction pattern. With this starting point, conventional x-ray analysis is ongoing to quantitatively determine the atomic locations of the Au and Sb atoms.

This activity is an endeavor in fundamentals of a characterization method. Earlier attempts to apply these ideas first to semiconductor surfaces, yielded some success, but it became clear that there were technical difficulties with the highly strained subsurface structure common in semiconductors. Thus, a "simpler" system was chosen, which in this case meant metallic. We now think we know how to overcome the initial problems encountered on semiconductors. Having demonstrated success with the metallic systems, we have plans to pursue two directions. One is to apply this approach to oxide surfaces and nanostructured oxides (with spintronic applications in mind). Specifically, with beamtime at the ESRF to study adsorbates at the surface of the polar oxide MgO(111). the immediate goal is to examine the role of substrate reconstruction on the growth of magnetic oxides. The second direction is to pursue this diffraction technique to encompass 1D surface nanostructures and also larger (molecular) adsorbates. The goal is to be able to study "molecular wires" (in collaboration with chemists at UWM) and organic semiconductors such as pentacene (in collaboration with collaborators at UW-Madison). The "fundamental" studies that we have undertaken to date will help greatly in these efforts.

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Education:

The project involves graduate students (H. Trevor Johnson-Steigelman and Somendra Parihar), undergraduate students (most recently Rob Morien and Steven Lund), and a high-school teacher (Kristin Michalski).



The PI demonstrates selective resonant excitation to help explain to undergraduates how nuclear magnetic resonance imaging works.

Outreach:

The PI reaches a broader audience by giving lectures on medical imaging to Milwaukee-area HS students and Wisconsin Native American HS students, and by collaborating with an area HS teacher on teaching demonstrations.



The PI, RET intern Kristin Michalski and REU student Steve Lund puzzle out a problem with a circuit they are building for the Frank-Hertz experiment for Kristin's physics course.