Atomic Scale Visualization of Surfaces Using X-rays

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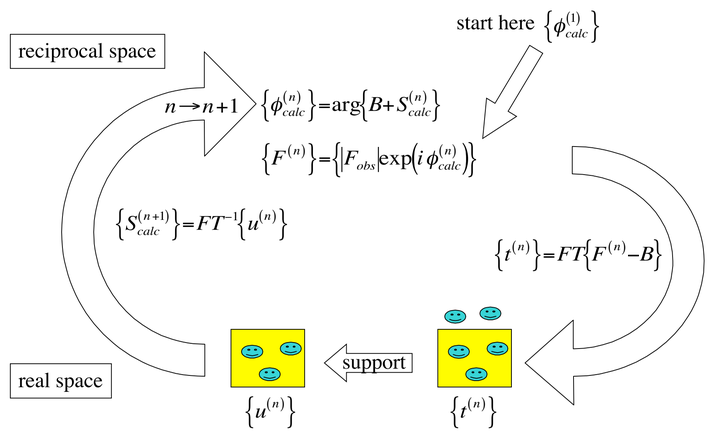
Problem:

- X-ray diffraction experiments measure only *intensity;* phase is lost ⇒ cannot simply take Fourier transform of experimental data.
- Usual approach to structure determination with SXRD is to make an educated guess of atomic positions, then compare predicted scattering intensity to experimental results. Refine by minimizing χ^2.
- However, if initial guess is incorrect, (i.e., number, identity of surface atoms), refinement procedure cannot yield correct structure.

NEED MODEL-INDEPENDENT METHOD TO IDENTIFY BASIC FEATURES OF SURFACE RECONSTRUCTION

Approach:

Use Fienup-style algorithm to iteratively assign phases ϕ to experimental structure factors F ($=\sqrt{I}$). F.T. of $F e^{i\phi}$ then directly gives real-space map of electron density $u(x,y,z)$.



J.R. Fienup, Optics Letters 3, 27 (1978)
J.R. Fienup, Applied Optics 21, 2758 (1982)

Two constraints:

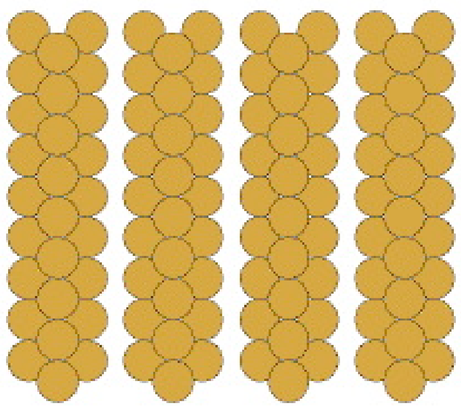
- Reciprocal space: Model $|F|$'s must match experimental ones.
- Real space: FT of $F e^{i\phi}$ must not extend unphysically far from surface region.

Notes:

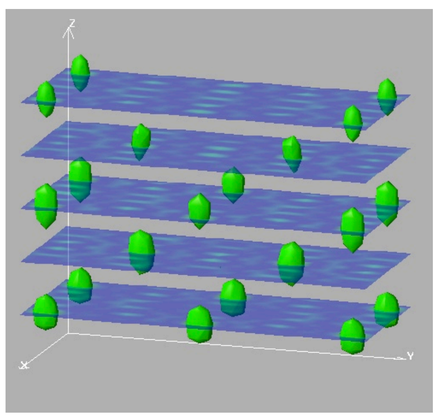
- Starting phases largely irrelevant. (Trials with random phases converge to same electron density.)
- Convergence reached in < 50 iterations (< 1 sec. on PC workstation)

D. K. Saldin, et al.,
J. Phys.: Condens. Matter 13, 10707 (2001);
J. Phys.: Condens. Matter 14, 4087 (2002).
P.F. Lyman et al.,
Phys. Rev. B Rapid Comm.71 (in press)

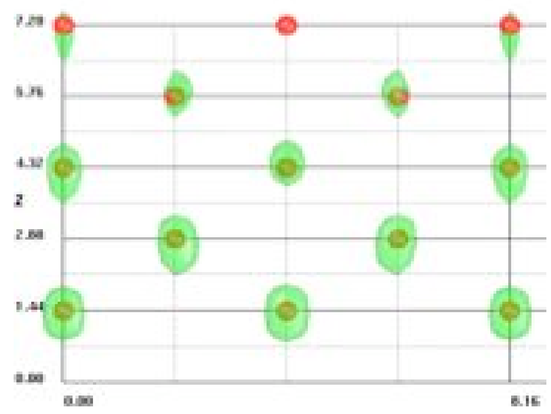
Test Case: Clean Au(110)-(2x1) (Known Structure)



Known missing row structure
(plan view)

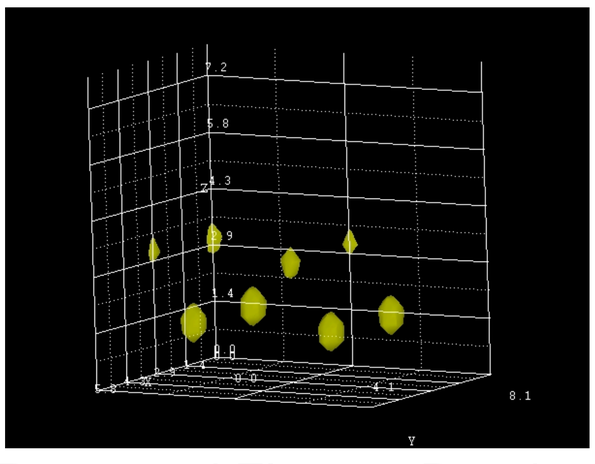


Recovered Electron Density
(perspective)

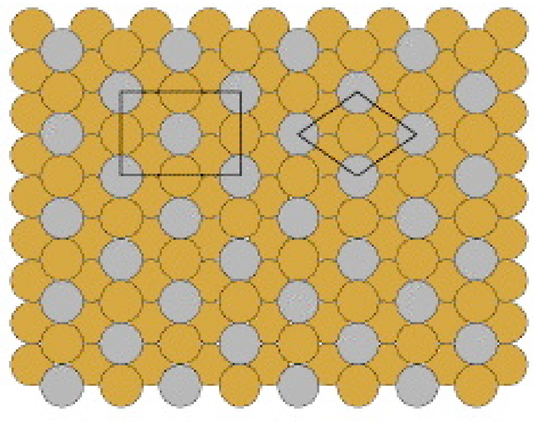


Compared to bulk termination (side view)
(relaxation, pairing, and buckling evident)

0.5 ML Sb/Au(110)-c(2x2) (Unknown Structure)



Recovered Electron Density
(perspective)



Suggested structure
(plan view)

Conventional fitting:

- Suggested structure yields $\chi^2 \approx 1.4$
- First-second layer spacing contracted 13%
- Second-third layer spacing expanded 8%
- Slight buckling in 1st and 2nd layers