Processing electron diffraction experimental data for the structural determination of crystallographic surfaces.

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Motivation

The surface of a solid can have different physical and chemical properties than the bulk of the solid due to lattice distortions of the topmost atomic layers. Low Energy Electron Diffraction (LEED) is a surface structural determination technique. The LEED experiment collects a few hundred images of diffraction patterns at different energies in the form of bitmap images. The diffraction patterns need to be analyzed to obtain experimental I(V) curves, which can be compared to theoretical ones to determine surface structure. In order to analyze the experimental raw data, the intensities of diffracted spots must be collected. Our goal is to produce a program that extracts I(V) curves from the digitized diffraction patterns.

Low Energy Electron Diffraction

During the LEED experiment an electron gun fires electrons in a low energy range at a crystal sample so that the electrons strongly interact with the top few atomic layers, which causes LEED to be a surface sensitive technique. The diffracted electrons pass through a series of grids, and a phosphorescent screen captures the diffraction pattern of the electrons with the same energy as the incident electron beam.

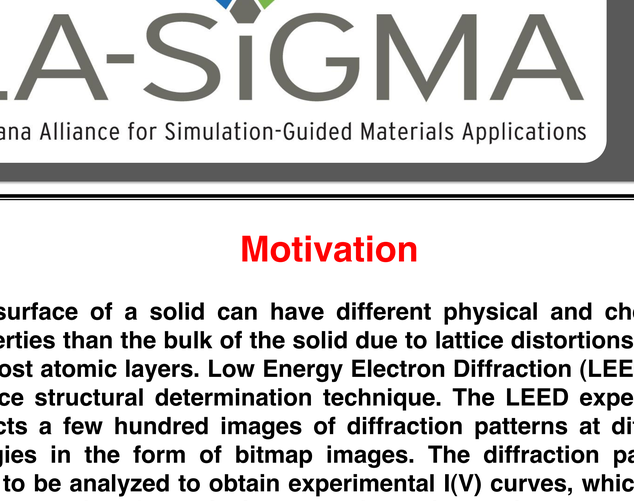
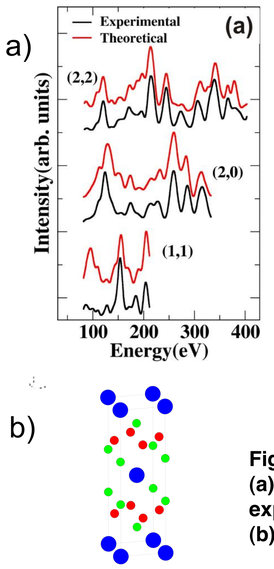


Figure 1:
(a) Schematic representation of a LEED experiment;
(b) Electron diffraction pattern for $Sr_3Ru_2O_7(001)$ surface;
(c) The intensity of the diffracted spots collected as a function of energy [I(V) curve] will contain all the surface structural information.

I(V) Curves



Experimental I(V) curves are created by plotting the intensities of diffracted electron spots as functions of energy. The set of I(V) curves for different diffracted electrons contains the surface structural, compositional, and dynamical information. Simulations provide theoretical I(V) curves in which experimental I(V) curves can be compared. The calculated R-factor, or reliability factor, quantitatively evaluates the agreement between theoretical I(V) curves and experimental I(V) curves.

Figure 2:
(a) Comparison between theoretical and experimental I(V) curves for $BaFe_2As_2(001)$;
(b) Bulk structure for $BaFe_2As_2$.

Surface Structural Determination

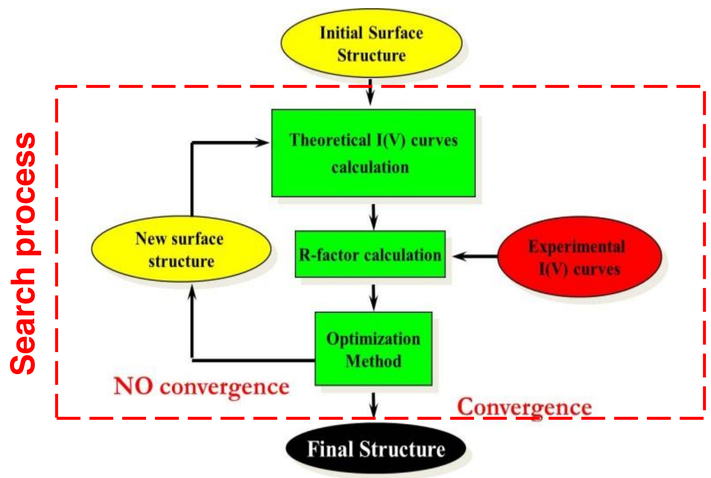


Figure 3:
Flowchart of the LEED surface structural determination process.

Running the Program

The program allows the user to select an image, draw a line for an intensity profile, create a file containing the pixel data along that line, and plot the intensity profile. An intensity profile is the plot of intensity data of the pixels along a line on a diffraction pattern. Diffracted electrons move along a trajectory towards the center of the diffraction pattern as energy increases. Intensity profiles provide intensity information for diffracted electrons, which helps plot I(V) curves. The program is written in Python and uses the Image and Pygame modules. The intensity profiles are plotted in Gnuplot.

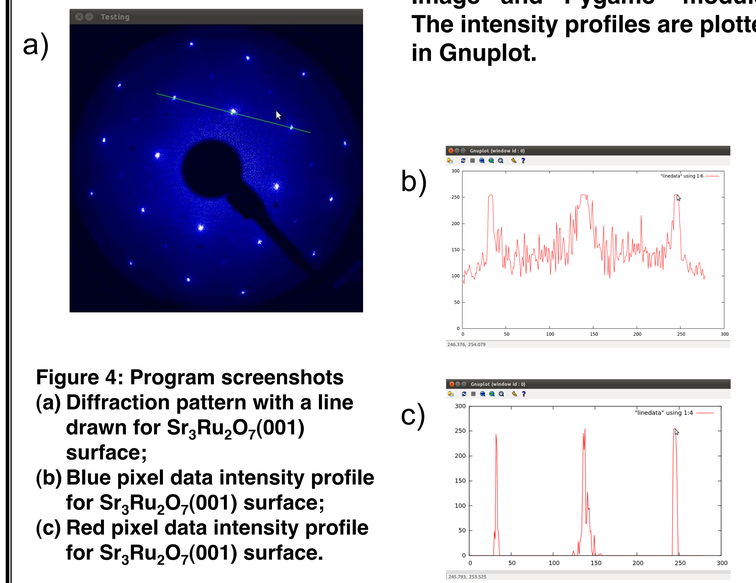


Figure 4: Program screenshots
(a) Diffraction pattern with a line drawn for $Sr_3Ru_2O_7(001)$ surface;
(b) Blue pixel data intensity profile for $Sr_3Ru_2O_7(001)$ surface;
(c) Red pixel data intensity profile for $Sr_3Ru_2O_7(001)$ surface.

This project incited the study of the LEED technique, the Linux operating system, programming concepts, and the programming language Python.

Future Work

A next step is to address background subtraction for the intensity profiles and I(V) curves. A final task is to create a script to collect intensity profiles for each energy level and plot I(V) curves. Then the experimental I(V) curves should be compared to theoretical I(V) curves.

References

[1] "Low-Energy Electron Diffraction Experiment, Theory, and Surface Structure Determination", M. A. Van Hove, W. H. Weinberg, and C.-M Chan, (Springer Verlag, Berlin, 1986).

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