

Automating Low Energy Electron Diffraction (LEED) Analysis Software for Real-Time Data Collection

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Abstract:

LEED (Low-Energy Electron Diffraction) is a diffraction technique for analyzing the surface atomic structure of thin films and substrates. The low-energy (20-400eV) electrons used in LEED penetrate the 2-3 atomic layers closest to the surface rather than the bulk of the sample, and are backscattered to form a diffraction pattern that can be analyzed to reveal quantitative characteristics of the surface [1]. Previously developed software at PARADIM is capable of this analysis, but its reliance on manual spot fitting is inefficient and incapable of providing real-time information to users. To address this problem, we developed and tested a new LEED analysis software, *P-LEED*. The key features of this new software are the automatic image processing and spot fitting algorithms, which process and update atomic lattice constants in real-time as data is collected. Not only does this new software greatly simplify the analysis process, but it also enables users to perform quantitative LEED analysis *in situ* as a direct feedback tool for thin film growths.

Summary of Research:

One of the surface characteristics from a LEED pattern that is of particular interest to us are the lattice constants. Measuring lattice constants can determine the existence of epitaxial strain. This is a property exhibited by particular film/substrate combinations that can stabilize superconductivity in materials that have not been previously shown to be superconducting [2] and control transitions between insulating and metallic ground states [3]. To handle the complexity and the tedium of the lattice constant calculations, a robust analysis software is necessary. Previously developed software prevented the user from being able to immediately extract quantitative information from the patterns. In response to this, we developed *P-LEED*, a new analysis software. The objective of the new software, which was written in Igor Pro, is to automate LEED diffraction pattern analysis so that lattice constants can be calculated in real time and refined as more images are analyzed.

Lattice constants are calculated by considering the geometry of both the electron beams and the LEED pattern, as depicted in Figure 1. The parallel components of the incident and diffracted beams, represented by wavevectors \mathbf{k}_i^{\parallel} and \mathbf{k}_f^{\parallel} respectively, satisfy the Laue condition when their difference, the scattering vector $\mathbf{G}_{\mathbf{hk}} = \mathbf{k}_f^{\parallel} - \mathbf{k}_i^{\parallel}$, matches a point on the crystal reciprocal lattice. For a rectangular surface structure, which we assume for the following calculations, $\mathbf{G}_{\mathbf{hk}}$ can be expressed in terms

of the Miller indices and lattice constants as $\mathbf{G}_{\mathbf{hk}} = 2\pi(H/a)\hat{\mathbf{a}} + 2\pi(K/b)\hat{\mathbf{b}}$. Using the known electron momentum $\frac{\sqrt{2mE}}{\hbar}$ of the diffracted beam, we can relate the diffraction angle $\theta_{\text{diffraction}}$ with the scattering vector $\mathbf{G}_{\mathbf{hk}}$, such that $\sin(\theta_{\text{diffraction}}) = \frac{\sqrt{2mE}}{\hbar |\mathbf{G}_{\mathbf{hk}}|}$. $\sin(\theta_{\text{diffraction}})$ is proportional to d , the distance between the diffraction spot and the specular reflection point on the detector, in pixels. Thus, as long as the energy, Miller indices, and pixel coordinates of the spots are known, along with a known calibration for the relationship between $\sin(\theta_{\text{diffraction}})$ and d , the lattice constants can be calculated from a LEED pattern.

The calculations implemented in the software are as follows. The first step is to manually estimate and then exactly fit the radius of the image. This screen parameter will normalize spot positions during spot fitting, ensuring accuracy when camera settings are varied. Then, the user manually provides an initial estimate of 4 symmetric spot coordinates. This initial estimate will allow us to calculate the specular position, which is also used to normalize the spot positions. Additionally, we will be able to calculate Ω , the rotation of the basis axes of the pattern with respect to the basis axes of the pixel coordinate system, which originates from the azimuthal rotation angle of the sample. As mentioned earlier, we can compute $\sin(\theta_{\text{diffraction}})$ from d using a calibration polynomial. Note that $\theta_{\text{diffraction}}$ is the angle of diffraction off of the sample surface and Ω is the angle of rotation of the spots. Using the Laue condition

from above, the magnitude of the scattering vector \mathbf{G}_{hk} can then be determined. To extract a and b , \mathbf{G}_{hk} must then be projected onto the reciprocal unit vectors $\hat{\mathbf{a}}$ and $\hat{\mathbf{b}}$, as determined from Ω . When the components of the scattering vector are expressed in this way, an initial guess for the lattice constants can be found. This information allows us to automatically guess the pixel coordinates of all other spots on the image given the spot indices, which we can easily find by iterating through different permutations of possible indices. After all spot locations have been estimated, their intensities are fitted with a 2D Gaussian fit function. By using these fitted spot locations, the lattice constants can be recalculated and continuously refined by averaging them with previously calculated values.

P-LEED features a front panel with interactive elements (buttons, dropboxes, etc) that allow users to control the calculations during the initialization stage, as shown in Figure 2. By selecting the AutoFit box, the spot fitting process is automatically executed for the rest of the images. Important values, such as Ω , the specular position, and the lattice constants are displayed in the main panel for quick user reference. The active image is displayed with the spot guesses and fits. The user can also display histograms of the continuously updated lattice constants. Figure 3 depicts the lattice constant histograms of SrTiO₃ (STO) and FeSe thin films grown on STO.

Results & Future Work: To test the efficacy of the software, we measured the lattice constants of STO and 1, 5, and 20 unit cells of FeSe grown on STO. The bulk lattice constants of STO and FeSe are 3.905 Å and 3.765 Å, respectively. Thus, we would expect to see much more strain in 1 unit cell of FeSe growth than in 5 or 20 unit cells. This strain gradient can be observed in the lattice constant histograms in Figure 3, indicating that the software is calculating the values correctly. There are a few small improvements that can be made to further refine the software. The initial spot fitting process should be expanded to be compatible with any 4 symmetric spots. Additionally, the 2D Gaussian fitting function used to fit the guesses should also be refined to reject false positives caused by noise in the image, which we observed on occasion during testing.

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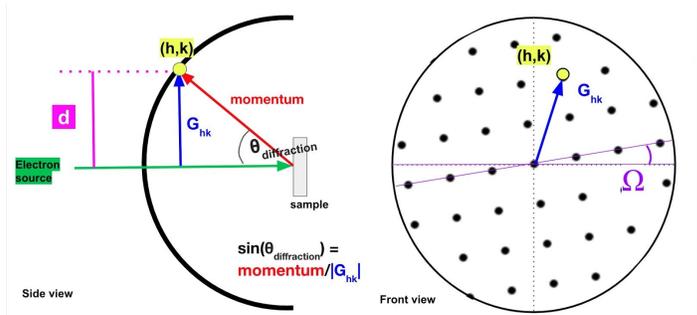


Figure 1. LEED Geometry.

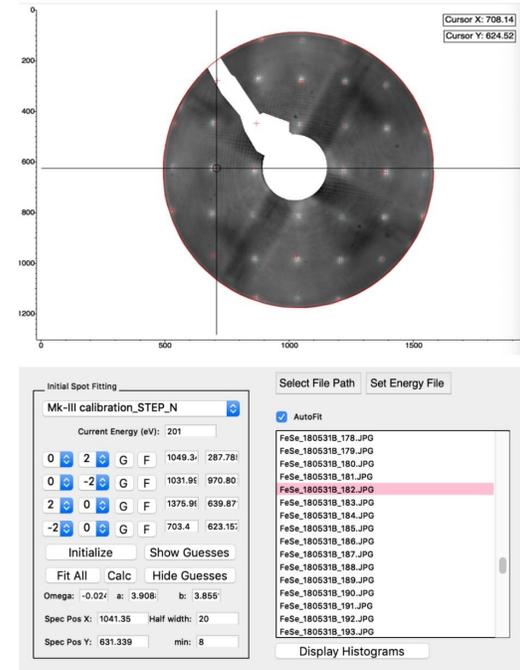


Figure 2: *P*_LEED Control Panel.

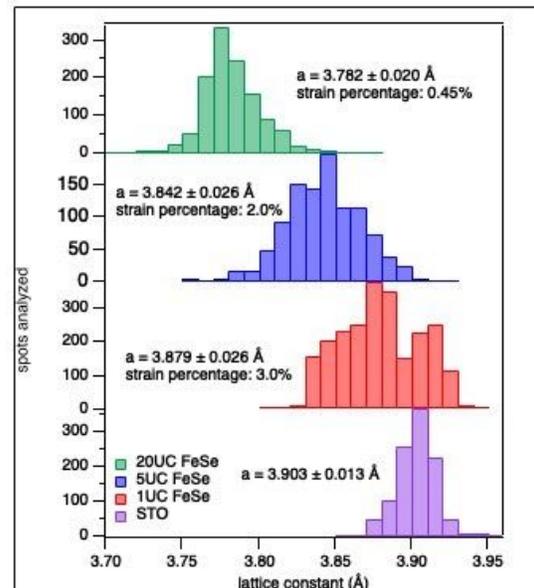


Figure 3: Lattice constant histograms.

