I-V LEED

Intensity-voltage low-energy electron diffraction, also known as quantitative LEED, is a combined experimental and computational method of crystalline surface structure analysis on the atomic scale. LEED spot intensities are recorded in dependence on the voltage, i.e., electron energy. Structure determination is indirect: I-V curves are calculated for various surface models and compared to the experimental data. Model parameters can be optimized, i.e., fitted to the experimental data.

### I-V LEED analysis using Barbieri/Van Hove packages directly:

- **Program parameters**
  - **Bulk unit cell**
  - **Slab unit cell**
  - **Atomic mufin-in constant**
  - **Bulk electronic densities**
  - **Slab electronic densities**
  - **Scattering phase shifts**

- **AQuaLEED**
  - **Crystal structure in (composite) layers**
  - **Properties of (composite) layers**
  - **Initial displacements**
  - **Program parameters**
  - **Basic results**
  - **R-plots**
  - **Properties of best fit, edited**

### Existing software

Quantitative LEED relies on computer codes capable of calculating the I-V curves and fitting them to experimental data. Apparently the most popular of them is the Barbieri/Satellite LEED package [1], which together with the phase shift calculation package [2] constitutes a complete set of programs needed for the task. First, the phase shifts of electron wave scattering on individual atoms in the crystal must be calculated. This is accomplished by the phase shift calculation package, in several steps performed by programs PhSh0 through PhSh3. The main computation, i.e., that of LEED intensities and of the tensor (Jacobian) of the tensor LEED approximation [3], is carried out by the TLEED1 program of the SATLEED package. Program TLEED2 then performs model optimization.

A number of SATLEED branches or derivatives exist, e.g., the AQuaLEED [4], SATCLEED [5], MISATLEED [1], and LD-SATLEED [5]. Independent alternatives include TenstLEED [4], CLEED [5], DL_LEED [6], and LEEDFIT [7].

### AQuaLEED

AQuaLEED (Automated Quantitative Low-Energy Electron Diffraction) is a package written in Python, which integrates the Barbieri/Van Hove programs in a compact unit with a new interface and which automates the whole procedure. LD-SATLEED is employed in place of SATLEED for its support of layer doubling. Although AQuaLEED does not perform the main computations, it implements complex features which are vital to the automation, reliability, or accuracy. The aim of AQuaLEED is to reduce the required users’ work as much as possible and thus bring the I-V LEED technique back into common use.

Features of AQuaLEED:
- uses input files in Pd file format,
- provides interactive control over the whole procedure of LEED (I-V) data analysis,
- also has an automated mode that requires no user interaction during the process,
- applies numeric filters to the experimental data if requested,
- includes necessary data for chemical elements from H to Cm,
- performs advanced analysis and transformations of the models in order to get their optimal geometrical representations and to handle their symmetries correctly,
- performs various auxiliary calculations,
- generates all the necessary input files for individual LEED programs,
- calculates program parameters (array dimensions) for the LEED programs,
- calls a Fortran compiler and linker to build the programs,
- calls the programs to carry out the main computations,
- parses outputs of the programs,
- exports intermediate and final results,
- exports 3D visualizations of the models (in order to check input correctness).

### AQuaLEED availability

An alpha version of AQuaLEED can be downloaded from [http://www.fisica.ufmg.br/~edmar/fisica/doutorado/node23.html](http://www.fisica.ufmg.br/~edmar/fisica/doutorado/node23.html). A corresponding scientific paper is being prepared.

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### References