SIMULATION OF LOW ENERGY ELECTRON DIFFRACTION PATTERNS IN KINEMATICAL APPROXIMATION

Ivan Yakovkin
Faculty of Physics, Taras Shevchenko National University of Kyiv, 64/13, Volodymyrska Str., Kyiv, Ukraine

The work is devoted to the development of the software that calculates low energy electron diffraction (LEED) patterns for adsorbed layers on single crystal surfaces. The calculations are performed in kinematical approximation. The program is written in the C++/Win32 code using the Code::Blocks programming environment. The Win32 API is used to create a user-friendly interface of the program and to provide the visualization of simulated diffraction patterns. This program substantially facilitates the interpretation of diffraction patterns for adsorbed layers which are observed in real LEED experiments and therefore can be useful for a wide community of investigators working in the field of surface science.

Low energy electron diffraction (LEED) is a powerful method for investigations of structures of layers adsorbed on crystalline surfaces. However, in some cases, the interpretation of obtained LEED patterns can be very complicated, so the development of a program that could facilitate the structural determination is of a primary importance. The most straightforward and simple approach here is the calculations of LEED patterns, for a number of the most probable film structures, within so-called kinematical approximation [1]. This task was performed by K.E. Hermann and M.A. Van Hove [2], but the program proposed in [2] has certain restrictions and is inapplicable for complex surface structures, in particular, does not allow for modeling the film structures forming with occupation of different type of adsorption sites. In contrast, the program, developed in the present study, can be used to calculate the LEED patterns for various layers adsorbed on crystal surfaces having either rectangular or hexagonal structure and therefore has a much wider field of applications for interpretation of experimental diffraction patterns.

The work with the program is illustrated by Fig. 1, which shows the snapshots of the screen for modeling rectangular (a) and hexagonal (b) unit cells. The control panel located at the top of the screen allows for setting the symmetry and size of the unit cell, which is represented by a ball model on the right in the working field. The adsorbed atoms are positioned with the help of the mouse. Then the program calculates the corresponding LEED pattern.

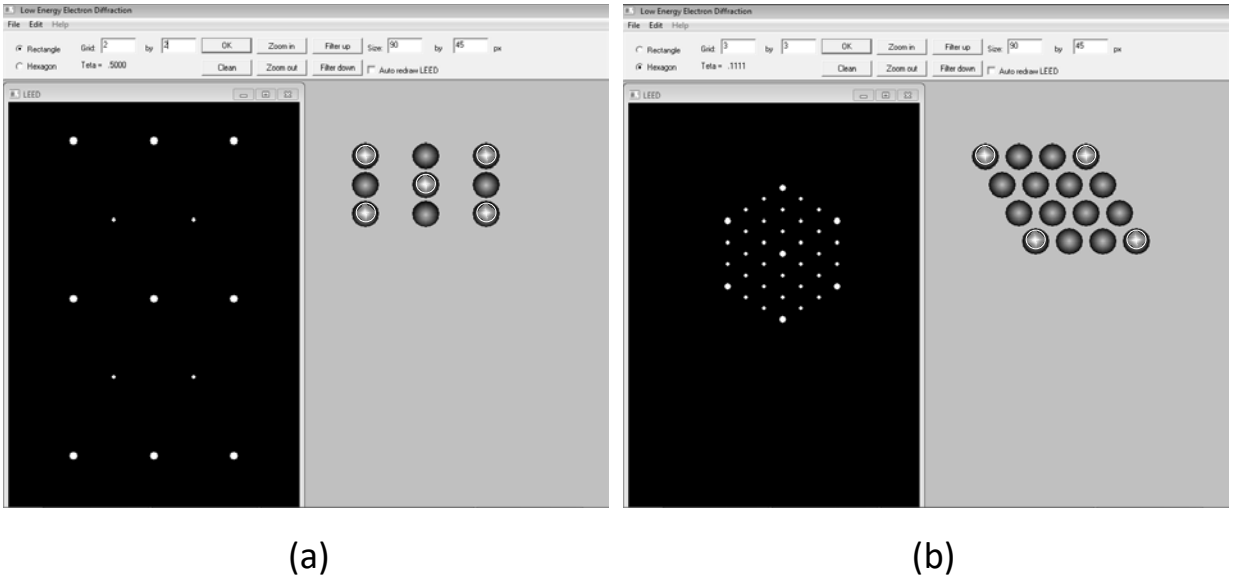
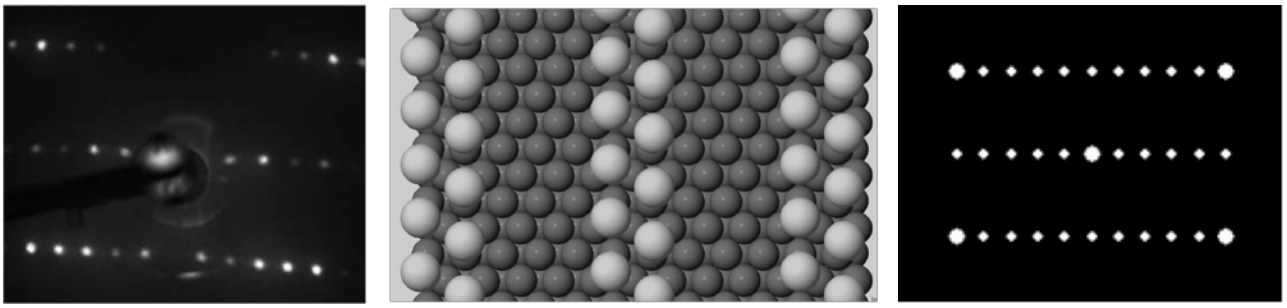


Fig. 1. The snapshots of the program for rectangular (a) and hexagonal (b) unit cells.

The program was tested for a number of different structures, specifically, for rectangular, rectangular centered and hexagonal unit cells. In most cases, the LEED patterns calculated for suggested model structures were found to be in a perfect agreement with experimentally obtained.

An example of the application of the program for interpretation of real LEED patterns is shown in Fig. 2. The experimental diffraction pattern for the Nd/Mo(110) [3] is shown in Fig. 2a, and the corresponding suggested model structure, in which adsorbed Nd atoms are arranged in zigzag chains, is shown in Fig. 2b. The LEED pattern, calculated for the model structure in Fig. 2b using the program developed in the present study is shown in Fig. 2c. It is evident that the LEED pattern, calculated for the suggested zigzag chain structure agree well with the pattern obtained in experiment. Thus, this example convincingly illustrates a usefulness of the developed program in interpretation of complex LEED patterns.



(a) (b) (c)

Fig. 2. The experimental diffraction pattern (a) for the Nd/Mo(110) [3], the corresponding model structure with adsorbed atoms arranged in zigzag chains (b), and the calculated LEED pattern for the zigzag structure (c).

Conclusion

The program, presented in this study, can be used for calculations of diffraction patterns for various adsorbed layers having either rectangular or hexagonal structure and therefore provides a convenient utility for interpretation of LEED patterns of adsorption systems. I hope that this program will be useful for researchers working in the field of surface science.

References

[1] A. Zangwill, *Physics at surfaces*. Cambridge, United Kingdom: Cambridge University Press, 1988.

[2] LEEDpat, Version 4.1, utility by K.E. Hermann (FHI) and M.A. Van Hove (HKBU), Berlin / Hong Kong, 2014; see also http://www.fhi-berlin.mpg.de/KHsoftware/LEEDpat/index.html.

[3] M. Wiejak et al., “Adsorption of Nd on the Mo(1 1 0) surface”, Applied Surface Science, vol. 256, no. 15, pp. 4834–4838, 2010.