Low Energy Electron Diffraction (LEED)

Information available from a LEED study

LEED can give two kinds of information:

1. The positions of the bright spots in the diffraction pattern give information on the symmetry of the crystal surface (i.e. on the Bravais lattice of the surface net) and on the size of the unit cell.

2. The intensities of the spots can be analysed using methods similar to those used in X-ray crystallography to determine the complete surface structure (i.e. the positions and identities of all the atoms within the unit cell)

You only need to worry about the first of these, though it is good to at least know about the existence of the second.

Notation to describe surface structures

One thing you should make sure you understand is the Woods notation used to describe surface structures. This notation takes the form

X {hkl} (pxq) Rϕ° - A.

X and A are the symbols for the substrate and adsorbate, and you can probably guess that {hkl} are the Miller indices for the surface plane. The (pxq) Rϕ° bit defines the ratio of the a and b axes of the surface to substrate meshes (i.e. the lengths of the a and b axes in the surface layer to their lengths in the bulk solid) and the angle by which these vectors are rotated in the surface relative to the bulk solid. This type of notation can be used to describe either surfaces themselves (i.e. no adsorbate layer) or the structures of adsorbed layers on the surface. Often this notation is abbreviated to simply (pxq) Rϕ°.

Another type of notation is the 'matrix notation', which is similar to the Woods notation except that instead of using (pxq)Rϕ° to describe the structure of the surface, the 2x2 transformation matrix that maps the substrate mesh onto the surface mesh is substituted e.g. a surface structure that would be written (2x2)R0° in the Woods notation would be written $\begin{pmatrix} 2 & 0 \\ 0 & 2 \end{pmatrix}$ in matrix notation; ($\sqrt{2} \times \sqrt{2}$)R45° would be written $\begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}$

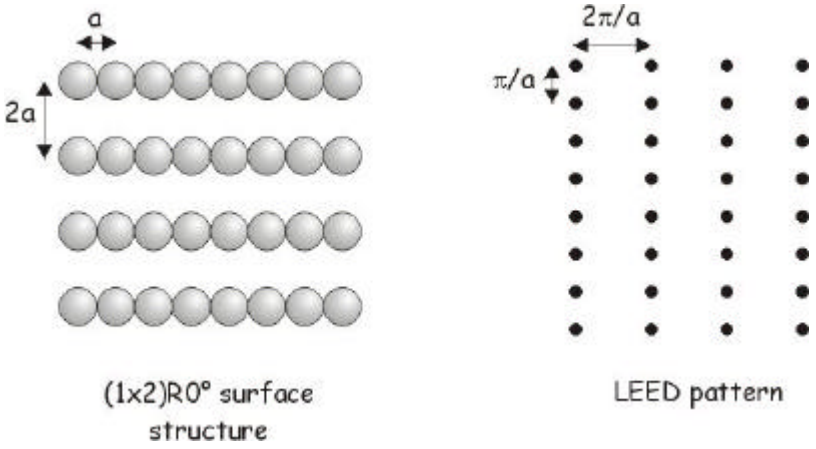
Predicting/interpreting LEED patterns

As far as LEED itself goes, the main point to take away is that the LEED pattern is the Fourier transform of the real space lattice. You will probably have come across Fourier transforms before in the context of spectroscopy. You know that if you take a signal in the time domain (units of s), such as a sine wave corresponding to electromagnetic radiation, you can perform a Fourier transform on it and get a signal in the frequency domain (units s^{-1}), which is a single spike at the frequency of the original sine wave. The idea with LEED is more or less the same, except that you take a lattice in real space (units of m) and diffraction transforms it into a 'reciprocal space lattice' or 'momentum space lattice' (units of m^{-1}). The relationship between the lattice vectors in real space (**a**,**b**) and the lattice vectors in reciprocal space (**a***,**b***) are

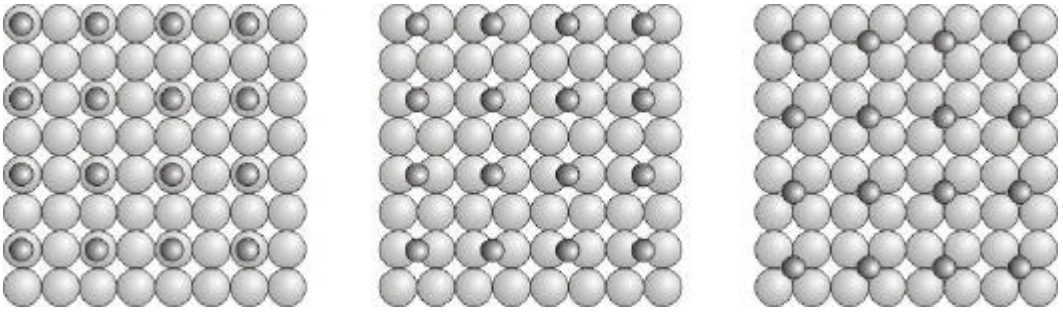
$$|\mathbf{a}^*| = 2\pi/|\mathbf{a}| \qquad |\mathbf{b}^*| = 2\pi/|\mathbf{b}| \qquad \mathbf{a} \cdot \mathbf{b}^* = \mathbf{a}^* \cdot \mathbf{b} = 0$$

This is pretty much enough to be able to predict what the LEED patterns arising from a particular kind of surface should look like. Essentially, all you need to remember is that the spacings of the spots in the LEED pattern[1] are going to be inversely proportional to the lattice point spacings in the real space lattice.

e.g.



LEED is often used (at least in exam questions!) to determine the structures of adsorbed layers on a surface. What you need to remember is that is the LEED spots are closer together in the pattern for the surface + adsorbate case than they are for the surface alone, then the adsorbate atom spacing is *greater* than that of the surface atoms (e.g. there may be one adsorbate atom every two surface atoms). Another important thing to note here is that the LEED pattern alone cannot tell you anything about the adsorption sites of the atoms on a surface, only the overall symmetry. There are generally several structures that can be drawn for an adsorbate layer for which the LEED pattern would be identical. e.g. the three surface structures below would all give the same LEED pattern.



[1] A quick explanation of why you get spots in the diffraction pattern is as follows: For diffraction from a one-dimensional array (i.e. a line of atoms), the Bragg condition, $n\lambda = a\sin\theta$, has to be satisfied. This gives a set of equally spaced lines perpendicular to the lattice. For a two dimensional array of atoms (i.e. a surface) Bragg conditions have to be satisfied in two dimensions simultaneously: $n\lambda=a\sin\theta_a$ and $m\lambda=b\sin\theta_b$. This means that diffraction is only allowed at the intersection of two perpendicular sets of 1D diffraction lines, so that the diffraction pattern consists of a series of diffraction spots corresponding to these intersection points.