4/29/02

Surface Scattering Methods

- use various types of particles to scatter off the surface and obtain ~~[illegible]~~ information about it.
  (electrons, X-rays, atoms, ions, etc.)

- for surface sensitivity, we need the scattering length (or interaction length) to be small, i.e. large interaction probability with one or a few atomic layers

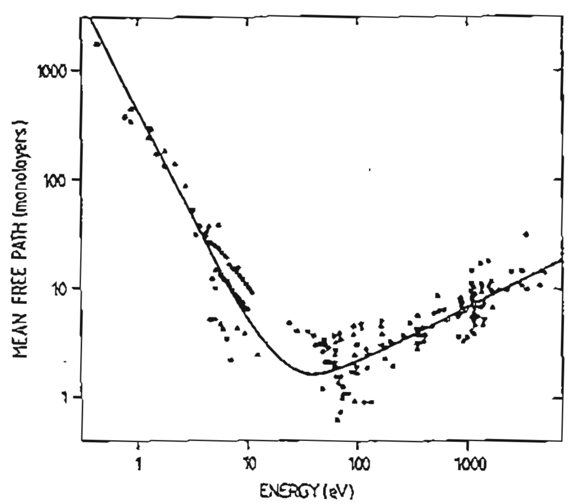


Fig. 4.1. Mean free path of electrons in solids as a function of their energy; a compilation of a variety of experimental data [4.2]. The quasi-universal dependence for a large number of different materials is due to the fact that the major interaction mechanism between the electrons and the solid is the excitation of plasmon waves whose energy is determined by the electron density in the solid

– Lüth, p. 148

Low Energy Electron Diffraction (LEED)

- incident beem usually ⊥ to sample surface
- incident electron energy typically 20 – 200 eV
- gives symmetry and structural information

Schematic Diagram of a LEED setup

(a)

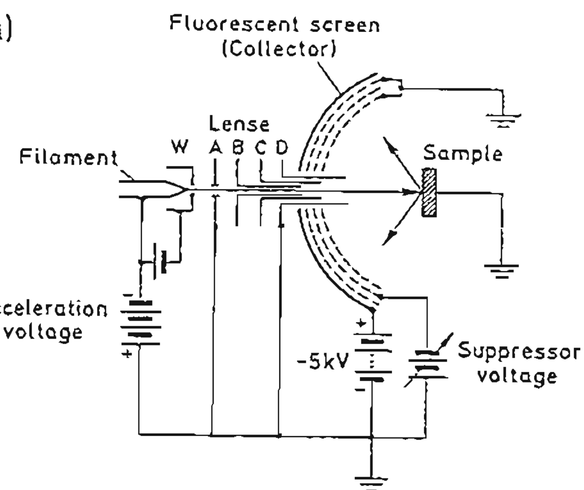


Fig. VIII.1. (a) Schematic of a three-grid LEED optics for electron diffraction experiments. The integrated electron gun consists of a heated filament, a Wehnelt cylinder (W) and the electron optics containing the apertures A–D. B and C are usually held at potentials between those of A and D.

Lüth, p.211

Acceleration voltage: ~ 20 – 200 V

In the kinematic theory of LEED, we are interested in the elastically scattered electrons.

The elastic scattering probability is derived in "Lüth" to be

$$W^{(el)}_{\vec{k}';\vec{k}} = \frac{2\pi}{\hbar} N \left| f(\vec{K}) \sum_p \exp(i K_\perp z_p) \right|^2 \delta(E'-E)\, \delta_{\vec{K}_{\parallel}, \vec{G}_{\parallel}} \quad \left(\begin{matrix}\text{Lüth}\\ 4.15\end{matrix}\right)$$

$$\vec{K}_{\parallel} = \vec{k}'_{\parallel} - \vec{k}_{\parallel} = \vec{G}_{\parallel} = \text{2-D reciprocal lattice vector}$$

N = number of surface atoms $\qquad z_p = pc$

$\vec{G}_{\parallel}$ is any surface reciprocal lattice vector (2-D)

$\vec{G}_{\parallel}$ can be calculated knowing the real space lattice

p is only a few for LEED since the electron penetration depth is only a few atomic layers

The above quantity (4.15) is also directly related to the structure factor which tells us the scattering amplitude for the scattering process.

$$W = \underset{\substack{\uparrow \\ \text{number of cells} \\ \text{or atoms}}}{N} S_{\vec{G}}$$

A convenient construction to visualize how LEED works is the Ewald Construction or Ewald sphere

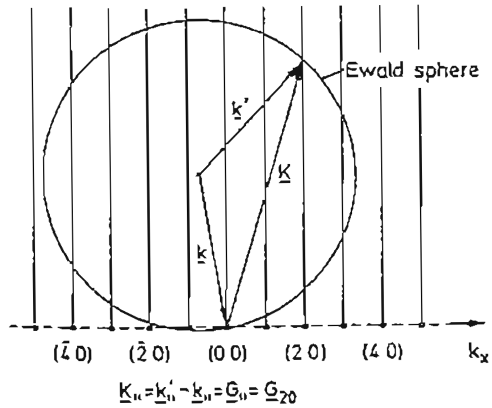


Fig. 4.3. Ewald construction for elastic scattering on a 2D surface lattice. The corresponding 2D reciprocal lattice points (hk) are plotted on a cut along k_x. The scattering condition (4.14) for the plotted beams is fulfilled for the reciprocal lattice point $(hk) = (20)$; but a number of other reflexes are also observed $(\bar{4}0)$, $(\bar{3}0)$...(30), $(\bar{2}\bar{2})$, ...(11)...

Lüth, p. 153

This geometry shows us where the diffraction maxima should occur and is consistent with:

$$\delta_{\vec{K}_{\parallel}, \vec{G}_{\parallel}}$$

$$\vec{G}_{\parallel} = \vec{k}'_{\parallel} - \vec{k}_{\parallel}$$

Fig. 4.6. LEED pattern of a clean cleaved nonpolar ZnO(10$\bar{1}$0) surface. Primary voltage $U_0 = 140$ V

Lüth, p. 156

Can we make a numerical estimate of what the electron energy should be to observe diffraction in LEED?

Imagine a real-space atomic spacing of 3 Å

$$\Rightarrow \quad |\vec{K}_{(10)}| = \frac{2\pi}{3 Å} = \frac{2\pi}{3} \times 10^{10}\ m^{-1}$$

This is on the order of the minimum necessary $\vec{K}$-vector

$$\Rightarrow \quad E_{min} \sim \frac{\hbar^2 k^2}{2m}$$

$$= \frac{(1.05 \times 10^{-34}\ J \cdot s)^2 \left(\frac{2\pi}{3} \times 10^{10}\ m^{-1}\right)^2}{2\,(9.1 \times 10^{-31}\ kg)}$$

$$= 2.65 \times 10^{-18}\ J \times \frac{1\ eV}{(1.6 \times 10^{-19}\ J)}$$

$$\underline{E_{min} = 16.6\ eV}$$

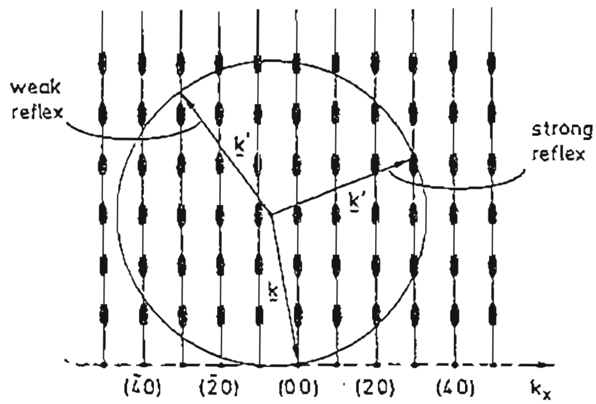


Fig. 4.4. Ewald construction for elastic scattering on a quasi-2D surface lattice, as in Fig. 4.3, but now not only scattering from the topmost lattice plane, but also from a few underlying planes, is taken into account. The "thicker" regions of the rods arise from the third Laue condition, which cannot be completely neglected. Correspondingly the (30) reflex has high intensity, whereas the $(\bar{3}0)$ spot appears weak

Lüth, p. 154

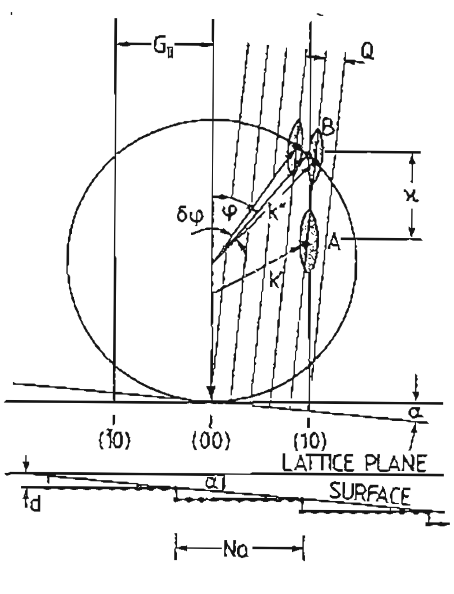
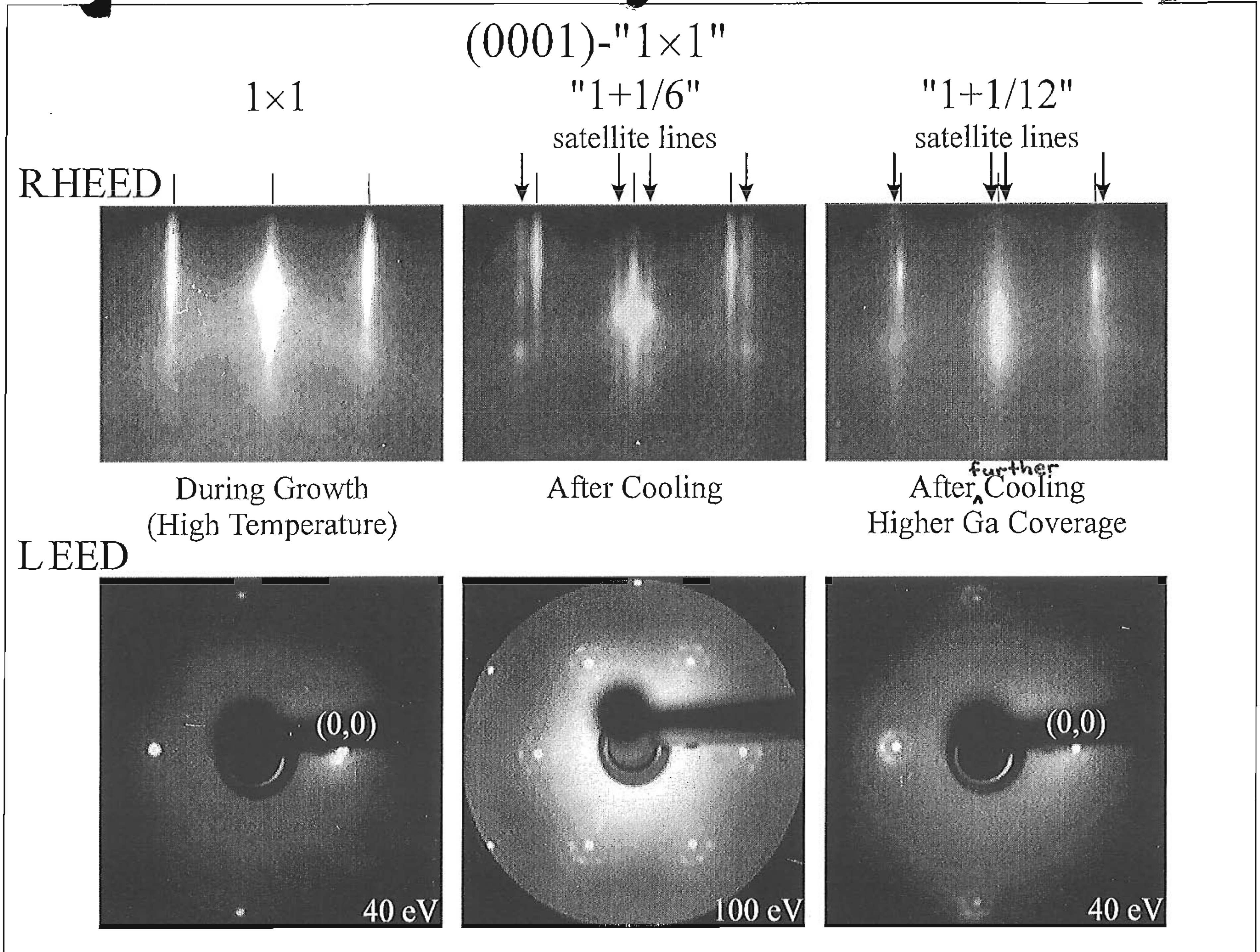


Fig. 4.9. Ewald construction for a surface with a regular step array. The steps with a height d and a terrace width aN (a is the lattice constant) cause an inclination angle α between the macroscopic surface and the main lattice plane. Corresponding to the lattice distance a, the reciprocal lattice vector is $G_\parallel$. The step array is described by a superimposed inclined reciprocal lattice of periodicity $Q = 2\pi/Na$. The primary electrons are described by the wavevector k (two different primary energies with two different lengths of k are considered) and two different scattered beams (k' and k'') are plotted ($k = k'$ and $k = k''$)

$$\delta\varphi = \frac{Q}{k'' \cos\varphi} = \frac{Q}{k \cos\varphi} = \frac{\lambda}{Na \cos\varphi} . \tag{4.19}$$

Lüth, p. 159



see A.R. Smith et al., J Vac. Sci. Technol. B 16(4), 2242 (1998).