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LEED Peak Widths: a Fabry–Perot Etalon Analogue

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Abstract

An analogy is drawn between the theory of the Fabry–Perot etalon for multiple reflections between two mirrors and that of the reflections between atomic layers with absorption in LEED. The analogy leads to an estimate of the LEED 'finesse', which in turn explains the widths and low intensities of LEED intensity versus voltage features. It is also shown that this explanation is consistent with the widely accepted Uncertainty Principle explanation.

Introduction

The intensity I of a spot in an electron diffraction pattern changes as the primary electron beam energy E_p (or voltage V) is altered. The spot intensities are observed to alternate through peaks and troughs, the peaks often being closely related to single- or multiple-scattering Bragg reflection conditions. Several theories have been presented to account for the extraordinary widths and low intensities of LEED $I(V)$ peaks. Slater (1937) correctly proposed that strong electron absorption and consequently short penetration were the cause of the $I(V)$ behaviour, and suggested the use of a complex potential. Harding (1937; also Marcus *et al.* 1969) preferred adsorption of gases and layer-spacing changes at the surface to electron absorption as the dominant mechanism. McRae (1966) included an imaginary term in the atomic scattering phase shifts (similar to the modern temperature dependence) to account for the $I(V)$ behaviour by means of inelastic losses through atomic excitation. He also included a depth dependence 'correction factor'. Heine and Pendry (1969) proposed strain field fluctuations due to lattice phonons. Their model predicted a $T^{1/2} E_p^{3/4}$ peak width dependence, which has not been observed (Trueba 1972), for peak widths are usually nearly independent of the temperature T and vary roughly as $E_p^{1/2}$ (Andersson 1969; Demuth *et al.* 1975). Multiple scattering (Gersten 1969) was presented as a possible cause, since single-scattering (kinematic) theory alone did not predict peak widths of (typically) 5–20 eV. Band structure calculations suggested that the observed peaks were merely envelopes of many band-like peaks, so that limited experimental resolution was suggested as a possible answer (Hoffstein and Bourdreaux 1970).

Pendry (1969) proposed that the peak widths ΔE were the direct result (Whelan 1965; Stern and Taub 1970) of the Uncertainty Principle:

$$\Delta E \gtrsim 2 V_{oi}. \qquad (1)$$

Here V_{oi} is the imaginary part of the complex optical potential

$$V_{op} \equiv V_{or} + iV_{oi}, \tag{2}$$

in which V_{or} represents the inner potential and V_{oi} represents absorption due to inelastic scattering. The inequality (1) has been supported by a number of authors (Andersson and Kasemo 1971; Demuth and Rhodin 1974).

Recently, Van Hove (1975) stated that the basic mechanism which determined peak widths was electron penetration 'regardless of the magnitude of the electron absorption'. Finite penetration of the electron beam limits the number of scatterers contributing to the diffraction and, just as for an optical diffraction grating, the fewer the scatterers (or grating slits) there are the wider the diffraction maxima. Elastic electron beam penetration would be limited by both elastic reflection (via the elastic mean free path λ_e) and inelastic scattering (via the inelastic mean free path λ_i). If N layers scatter, with each layer spaced a distance a apart, then from the grating equation (note that our definition of ΔE differs from that of Van Hove (1975)) we have

$$\Delta E \approx \tfrac{1}{2}\pi k/Na. \tag{3}$$

The present authors were puzzled as to how, from seemingly different approaches, the relations (1) and (3) could be related to each other in the limit that penetration was determined by λ_i. In attempting a solution to this problem, we have ignored the effects of multiple scattering. Though multiple scattering is extremely important at LEED energies, we have adopted the kinematic limit for two reasons: (i) so that the physics may be seen more clearly through the mathematical complexities of modern LEED theory; (ii) because the kinematic limit provides the minimum estimate of LEED peak widths. Multiple scattering broadens the peaks beyond this minimum by two means: (i) through the near coexistence of a number of peaks which are merged by strong absorption; (ii) by reduced penetration of the LEED beam into the surface. As a first approximation, multiple scattering could be included in the following model by replacing λ_i with $\lambda = \lambda_i \lambda_e/(\lambda_i + \lambda_e)$.

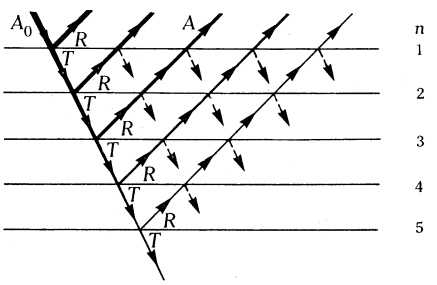

Fig. 1. Schematic representation of LEED scattering from plane layers.

Interferometer Analogue

The amplitude of an electron beam will decay into a crystal (assuming normal incidence) according to

$$A \approx \exp(-an\delta), \tag{4}$$

where n is the number of the layer from the surface and δ is defined by

$$\delta \equiv 1/2\lambda_i \approx V_{oi}/\{2(E_p + V_{or})\}^{\frac{1}{2}}. \tag{5}$$

Let us consider the schematic diagram of LEED scattering given in Fig. 1. Here T and R are the amplitude fractions transmitted and reflected respectively due to scattering at each layer. Assuming strong absorption and $R^2+T^2 = 1$, we let $T \approx 1$, which is equivalent to allowing $\lambda_e \gg \lambda_i$. Hence only single-scattering events need be considered. Thus, if the incident amplitude at a distance of an atomic radius above the centre of the first layer is A_0 (intensity I_0) then the kinematic specularly reflected amplitude A at this distance is (from equation 4) given by

$$\begin{aligned} A &= A_0 R\{\exp(-a\delta) + T\exp(-3a\delta) + T^2\exp(-5a\delta) + \ldots\}, \\ &= A_0 R[\exp(-a\delta)/\{1 - T\exp(-2a\delta)\}], \\ &\approx A_0 R[\exp(-a\delta)/\{1 - \exp(-2a\delta)\}]. \end{aligned} \tag{6}$$

In travelling from layer to layer, the complex beam amplitude will change in phase due to the 'optical' path length between the layers and to electron–atom interactions. In simple terms, if a phase difference ϕ is introduced between each layer, both for beams travelling into and out of the crystal, then equation (6) becomes

$$A = A_0 R\exp\big(-(a\delta + i\phi)\big)/\big\{1 - \exp\big(-2(a\delta + i\phi)\big)\big\}. \tag{7}$$

Thus the reflected intensity I is given by

$$\begin{aligned} I/I_0 &= A^*A/A_0^2, \\ &= R^2\exp(-2a\delta)/\{1 + \exp(-4a\delta) - 2\exp(-2a\delta)\cos(2\phi)\}. \end{aligned} \tag{8}$$

Equation (8) then reduces to

$$I/I_0 = \tfrac{1}{4}R^2F/(1 + F\sin^2\phi), \tag{9}$$

where

$$F = 4\exp(-2a\delta)/\{1 - \exp(-2a\delta)\}^2. \tag{10}$$

Equation (9) is formally similar to the governing transmission equation for the Fabry–Perot etalon (Hecht and Zajac 1974). Therefore $\mathscr{F} = \frac{1}{2}\pi\sqrt{F}$ may be identified as the LEED 'finesse' of the crystal. Typically $\mathscr{F} \approx 30$ for Fabry–Perot interferometers (Hecht and Zajac 1974) but, in the LEED case, for $E_p = 100$ eV, $\lambda_i \approx 4$ Å ($= 4\times10^{-10}$ m) and $a \approx 2$ Å (that is, $a\delta = 0{\cdot}25$), we have $\mathscr{F} \approx 4$ only. The objective in the Fabry–Perot etalon is to obtain a high number of reflections between two mirrored surfaces. This is achieved, excluding mechanical problems, by the use of mirror coatings of high reflectivity. In LEED, high finesse would be achieved by reflection from a large number of layers; strong absorption prevents this, while ensuring high surface sensitivity. Also, from equation (9), when R is low, the reflected intensities will be low. For LEED, we have $R \approx 0{\cdot}1$ (typically), so that $I(\text{peak}) \approx 0{\cdot}2\%\, I_0$.

From interferometry theory (Hecht and Zajac 1974; but note their different definition of ϕ), the phase width $2\Delta\phi$ of a peak is given by

$$2\Delta\phi = 2/\sqrt{F}. \tag{11}$$

But from the Bragg relation (at normal incidence), we have

$$2\Delta\phi = 2a\Delta k, \tag{12}$$

so that

$$\Delta E = 2k\Delta k = k\{1-\exp(-2a\delta)\}/a\exp(-a\delta). \tag{13}$$

For $\exp(-2a\delta) \approx 1-2a\delta$ and $\exp(-a\delta) \approx 1$, we therefore have

$$\Delta E \approx 2\delta k, \tag{14}$$

or

$$\Delta E \approx 2V_{oi}. \tag{15}$$

Equation (15) is just what is expected from the Uncertainty Principle (see inequality 1).

The interferometry theory presented above differs from the diffraction grating approach of Van Hove (1975). The intensity on each slit of a grating is normally assumed to be constant whereas, for LEED and the Fabry–Perot etalon, successive layers (or reflections) have proportionately lower intensities. In LEED, deeper layers are not equivalent. Ideally, penetration is infinite, while the intensity drops rapidly. Thus an effective number N_{eff} of scattering layers may, alternatively, be derived from the diffraction grating approach of Van Hove. Combining equations (3) and (14) we find that

$$N_{eff}\, a \approx \tfrac{1}{2}\pi\lambda_i. \tag{16}$$

For $a \approx 2$ Å and $\lambda_i \approx 4$ Å, we have $N_{eff} \approx 3$ layers. LEED peaks would thus be equivalent in width to the peaks from a grating of only three slits. The observed LEED widths of 5–20 eV would therefore, in retrospect, be no surprise. High surface sensitivity has been achieved at the cost of low peak resolution, and good structural determinations can therefore only be achieved from intensity studies made over a wide energy range.

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