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Theory of averaged low energy electron diffraction data

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Abstract. Recent work by Lagally, Ngoc and Webb has shown that averaged LEED spectra can be fitted with good accuracy by a curve of kinematic form. However, theoretical arguments show that a true kinematic average is impossible. The paradox is resolved by a new theory which shows that averages have a *quasi-kinematic* form with parameters different from those of the true kinematic theory. Some of the new parameters can be simply related to old ones, but others involve complicated corrections. Finally second order averaging schemes are proposed whereby more information can be extracted from experiments.

1. Introduction

Intensity/energy measurements made on electrons diffracted from a crystal surface have their form determined primarily by the scattering of ion cores immersed in a uniformly absorbing medium (the ion-core scattering model: Capart 1971, Jepsen *et al* 1971, Pendry 1969b, 1971a, Strozier and Jones 1971). Sensitivity to ion cores and their positions, especially those near the surface, makes LEED a useful tool for structural investigations.

The simplest theories of LEED took their cue from x ray work, and assumed that ioncore scattering is weak, so that the wavefield incident on an atom is determined primarily by the original beam:

where

$$K^{(0)}|^2 = 2E - 2V_{\rm P} \tag{1}$$

E is the energy of the incident electron relative to the vacuum, and V_p is the 'inner potential' correction to take account of the lower potential energy inside the crystal. In the kinematic theory it is equal to the constant potential in between the ion cores, V_0 . V_p also contains an imaginary component to reproduce effects of absorption of electrons.

We wish to set down some important results of kinematic theory. Each ion core scatters the incident beam in a manner determined by the phase shifts. The *j*th ion core in the *p*th layer scatters a wave that far from the ion core is given by

$$-T(\theta^{(s)}) \frac{\exp\left(i\left|\boldsymbol{K}^{(s)}\right|\right| \boldsymbol{r} - \boldsymbol{r}_{jp}|)}{2\pi|\boldsymbol{r} - \boldsymbol{r}_{jp}|}$$
(2)

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where

$$T(\theta^{(s)}) = -\frac{2\pi}{|\mathbf{K}^{(s)}|} \sum_{l=0}^{\infty} (2l+1) \exp(i\delta_l) \sin(\delta_l) P_l(\cos(\theta^{(s)}))$$
(3)

$$|\mathbf{K}^{(s)}|^2 = 2E - 2V_0 \tag{4}$$

 $\theta^{(s)}$ is the angle through which the electron is scattered and r_{jp} is the position of the *j*th ion core in the *p*th layer. Summing over all ion cores in a single layer parallel to the surface, and re-expressing the result in terms of diffracted beams, each differing from the incident beam in momentum parallel to the surface by a two dimensional reciprocal lattice vector of the surface, g, gives:

$$\sum_{\boldsymbol{g}} \left(-\frac{\mathrm{i}T(\theta)}{\Omega_2 \kappa_{\boldsymbol{g}}} \right) \exp\left\{ (\mathrm{i}\boldsymbol{K}^{(0)} - \boldsymbol{K}_{\boldsymbol{g}}^-) \cdot \boldsymbol{r}_p \right\} \exp\left(\mathrm{i}\boldsymbol{K}_{\boldsymbol{g}}^- \cdot \boldsymbol{r}\right)$$
(5)

$$\kappa_{\boldsymbol{g}} = (2E - 2V_0 - |\boldsymbol{K}_{\parallel}^{(0)} + \boldsymbol{g}|^2)^{1/2}$$
(6)

$$\boldsymbol{K}_{\boldsymbol{g}}^{\pm} = \left[(\boldsymbol{K}_{\parallel}^{(0)} + \boldsymbol{g})_{x}, (\boldsymbol{K}_{\parallel}^{(0)} + \boldsymbol{g})_{y}, \pm \boldsymbol{\kappa}_{\boldsymbol{g}} \right]$$
(7)

 r_p is the coordinate of the ion core at the origin in the *p*th layer; Ω_2 the area of unit cell of the layer and θ the angle between $K^{(0)}$ and K_g^- .

If each successive layer is displaced relative to its predecessor by a distance c, the pth layer has

$$\boldsymbol{r}_{p} = (p + \frac{1}{2})\boldsymbol{c} \tag{8}$$

Substituting for r_p into (5) and summing the diffracted amplitudes of all layers gives for the diffracted amplitude

$$A_{g} = -\frac{\mathrm{i}T(\theta_{g})}{\Omega_{2}\kappa_{g}} \frac{\exp\left\{\frac{1}{2}\mathrm{i}(\boldsymbol{K}^{(0)} - \boldsymbol{K}_{g}^{-}) \cdot \boldsymbol{c}\right\}}{1 - \exp\left\{\mathrm{i}(\boldsymbol{K}^{(0)} - \boldsymbol{K}_{g}^{-}) \cdot \boldsymbol{r}\right\}} \exp\left(\mathrm{i}\boldsymbol{K}_{g}^{-} \cdot \boldsymbol{r}\right)$$
(9)

(9) is the famous kinematic expression for diffracted amplitudes. It has maxima when the Bragg condition is satisfied,

real part
$$(S. c) = 2\pi \times \text{integer}$$
 (10)

$$S = K^{(0)} - K_{a}^{-} \tag{11}$$

Absorption gives the scattering vector, S, an imaginary component preventing equation 9 from becoming singular when the Bragg condition is satisfied.

It is unfortunate that equation 9 does not describe the process of diffraction in most real crystals with any accuracy. It has the virtue of being a relatively simple expression for the reflected amplitudes, compared with the complexities of theories taking into account multiple rather than only single scattering events: Beeby (1968) Duke and Tucker (1969), Duke *et al* (1970), Kambe (1967a, b), Jepsen *et al* (1971), McRae (1966, 1968a, b), Pendry (1969a, 1971b), Strozier and Jones (1971), Watts (1968). In consequence it is much more flexible from the point of view of computational simplicity. This is an important advantage for example in determining a complicated surface structure that can stretch the more sophisticated theories to the computational limit and beyond.

The whole objective of averaging methods (Lagally *et al* 1971, Tucker and Duke 1972) is to extract from complicated experimental curves requiring multiple scattering theory to interpret them the simple easily interpreted kinematic component.

Condition (10), for the occurrence of a maximum in the kinematic expression, depends only on $(\mathbf{K}^{(0)} - \mathbf{K}_g^-) \cdot \mathbf{c}$ not upon $\mathbf{K}^{(0)}$ and \mathbf{K}_g^- separately. This fact led Lagally *et al* to suggest that if an average of experimental results is taken over all possible values of $\mathbf{K}^{(0)}$, keeping $\mathbf{S} \cdot \mathbf{c}$ fixed, and plotted for several values of $\mathbf{S} \cdot \mathbf{c}$, then the resulting function of $\mathbf{S} \cdot \mathbf{c}$ will have a kinematic form. The assumption is that multiple scattering acts so as to increase intensities above the kinematic value, as often as to decrease them, and to displace peaks as often to higher as to lower energies. Extra peaks introduced by multiple scattering mechanisms are assumed to be as likely to occur for one value of $\mathbf{S} \cdot \mathbf{c}$ as another, and average to give a uniform background in the curves as a function of $\mathbf{S} \cdot \mathbf{c}$.



Figure 1. Full curve, experimental average at constant S.c of 00 beam intensities from a nickel 111 surface. Broken curve, calculated kinematic average using $V_{0r} = -18$ eV and $V_{0i} = -9$ eV. The intensities are normalized at $S.c/S_0.c = 5$. After Lagally *et al.*

Lagally *et al* (1972) have carried out this procedure for diffraction from a 111 nickel surface and their results are reproduced in figure 1. The theoretical curve is an average of kinematic calculations taken under the same circumstances as the experimental curves. Effectively, V_0 was used as a parameter in the kinematic curves. It is clear that the experimental averages follow the kinematic curves very closely even allowing for the fact that the theoretical curve has been adjusted in intensity.

There is one paradox that we shall come back to later: V_{0i} , the parameter representing absorptive processes has to be chosen to be -9 eV to fit the experimental curves. This value is more than twice as large as the value of $V_{0i} = -4 \text{ eV}$ deduced by comparing exact multiple scattering calculations in the same energy range with the unaveraged data (Pendry and Andersson 1972).

2. Systematic effects

We have already observed that an assumption of kinematic averaged data presupposes that features of the diffracted intensities are influenced in a random fashion by multiple scattering. There must be no systematic effects because these will not average to zero. In this section we want to draw attention to a paradox. On the one hand the experimental results of Lagally *et al* clearly indicate that a curve of kinematic form fits the averaged data. On the other hand systematic effects do occur in three separate quantities thus excluding the possibility of averaged curves being truly kinematic.

2.1. Intensities of peaks

It is not the case that multiple scattering acts to increase intensities as many times as to decrease them. There are several processes which work systematically to decrease intensities.

When multiple scattering is strong the electron pursues a much more tortuous path than in the kinematic case. Because electrons making up a multiple scattering spectrum have travelled a much longer path length in the crystal the effect of absorption is greatly increased. Figure 2 shows the decay of electron density in a beam incident on a crystal surface, for a multiple scattering and for a kinematic calculation at 300 K. It is clear that much more absorption is taking place in the multiple scattering calculation. Thus spectra are systematically reduced in intensity by multiple scattering effects.



Figure 2. Density of incident electrons: normal incidence on a copper 100 surface. E = 150 eV, $V_{0r} = -15 \text{ eV}$, $V_{0i} = -4 \text{ eV}$. Full curve, kinematic theory; broken curve, multiple scattering theory. T = 300 K.

Suppose that a Bragg peak is formed in the 00 beam. As the intense back reflected 00 beam travels out of the crystal into the vacuum some of its intensity can be transferred by multiple scattering to other beams, a phenomenon known as beam sharing.

There is a third effect, related to the last one: again suppose that the incident beam is being Bragg reflected into the 00 beam. Flux is multiply scattered out of the incident beam into other beams not necessarily in a Bragg reflecting condition, and flux is lost to the intensity of the peak in the 00 beam.

So there are three effects which combine to reduce multiple scattering curves (ie the experimental ones) below the kinematic ones. Therefore the experimental average will have considerably less intensity than the kinematic result.

2.2. Peak positions

Multiple scattering peaks do not coincide with Bragg peaks in general. Multiple scattering pushes peaks away from the Bragg condition and we must assume that there is no systematic displacement of peaks to retrieve the proper average. In fact multiple scattering by the ion cores can shift peak positions systematically. For example in high energy electron diffraction (Hirsch *et al* 1965) the ion cores behave as attractive potentials and in scattering the electrons lower their potential energy. The effect varies with incident energy and makes a contribution to the 'energy dependent inner potential'.

2.3. Widths of peaks

It has been shown (Pendry 1969b, 1972, Andersson 1970) that peak widths in LEED spectra are limited by the amount of absorption taking place inside the crystal.

The inequality is

$$\Delta E \geqslant 2V_{\rm 0i} \tag{12}$$

and is valid for both multiple scattering and kinematic theories. In the case of kinematic spectra the limiting width is achieved as can be shown from equation 9. No peaks are narrower than kinematic peaks.

Averaging a series of peaks, some displaced up in energy and some displaced down, must give an averaged peak that is wider than the original peaks by something like the average displacement of the peaks. Since it is known as an experimental fact that peaks are often displaced from the kinematic positions by large amounts, it follows that widths of averaged peaks will be much broader than those of true kinematic peaks. This result is reflected in the fact that Lagally *et al* needed to use a much larger value of V_{0i} to reproduce widths of averaged peaks ($V_{0i} = -9$ eV) than the true value of $V_{0i} = -4$ eV.

Thus several systematic effects can be pinpointed, spoiling the validity of the kinematic averaging postulate. Nevertheless it is true that averaged peaks do have a kinematic form as figure 1 makes clear. The only conclusion open to us is that parameters used in a kinematic-like fit to averaged data do not correspond directly with those of the true kinematic theory. Averaged intensities are said to be quasi-kinematic.

3. Quasi-kinematic intensities

In several theories of LEED it is usual to divide up the crystal into layers of ion cores parallel to the surface. Then multiple scattering events fall into two classes: those taking place consecutively within a single layer, and those that scatter between layers. Let us neglect for the moment multiple scattering within a single layer.

In §1 we saw how to calculate single scattering events. The incident wave propagates to the *p*th layer (factor of exp (i $\mathbf{K}^{(0)} \cdot \mathbf{r}_p$)) is back-scattered there through an angle θ into another beam $(-iT(\theta)/\Omega_2\kappa_g)$ and propagates to point \mathbf{r} (exp { $i\mathbf{K}_g(\mathbf{r} - \mathbf{r}_p)$ }), the total being given in equation 9. Representing propagation by lines and scattering by dots we draw the kinematic process schematically in figure 3.

There are other contributions to the scattered amplitude, for example by propagation to the *p*th plane (factor of $\exp(iK^{(0)}, r_p)$) scattering there through angle θ into another forward travelling beam $(-iT(\theta)/\Omega_2\kappa_g)$ propagation to the *q*th layer $(\exp[iK_g^+, (r_q - r_p)])$



Figure 3. Contributions to kinematic amplitudes.

and scattering through angle θ' into a backward travelling beam $(-iT(\theta')/\Omega_2\kappa_{g'})$ and finally propagation to point r (exp $\{iK_{g'}^-, (r, r_q)\}$) giving a total

$$-\frac{T(\theta)T(\theta')}{\Omega_2^2 \kappa_{\boldsymbol{g}} \kappa_{\boldsymbol{g}'}} \exp\left\{\mathrm{i}(\boldsymbol{K}^{(0)} - \boldsymbol{K}_{\boldsymbol{g}}^+) \cdot \boldsymbol{r}_p + \mathrm{i}(\boldsymbol{K}_{\boldsymbol{g}}^+ - \boldsymbol{K}_{\boldsymbol{g}'}^-) \cdot \boldsymbol{r}_q + \mathrm{i}\boldsymbol{K}_{\boldsymbol{g}'}^- \cdot \boldsymbol{r}\right\}$$
(13)

Several processes of this nature are shown in figure 4.



Figure 4. Some contributions to multiple scattering.

Spectra taken at a given direction of incidence will contain contributions to diffracted intensities from both processes mentioned, and from others as well. Applying the expression (13) and equation 8 for r_q it will be seen that processes shown in figure 4 sum to give maxima when

$$(\mathbf{K}_{\boldsymbol{a}}^{+} - \mathbf{K}_{\boldsymbol{a}}^{-}) \cdot \mathbf{c} = \mathbf{S}' \cdot \mathbf{c} = 2\pi \times \text{integer}$$
(14)

in contrast with the kinematic condition

$$(\mathbf{K}^{(0)} - \mathbf{K}_{\mathbf{a}'}) \cdot \mathbf{c} = \mathbf{S} \cdot \mathbf{c} = 2\pi \times \text{integer}$$

When angles of incidence are changed, keeping S.c constant, S'.c will not be constant and secondary peaks caused by the processes of figure 4 will change their positions, and any interference terms between kinematic and secondary processes are changed too. Averaging over many angles of incidence and plotting the results as a function of S.c gives a uniform background from secondary contributions plus the kinematic peak that always occurs at the same value of S.c. Interference terms will average to zero.

The whole argument hinges on conditions for peaks caused by higher order scattering processes depending on variables other than S.c so that after averaging, multiple scattering peaks contribute only to the uniform background. Any higher order diagrams producing peaks at the kinematic condition spoil the kinematic nature of the average.



Figure 5. Zero angle scattering contributions to quasi-kinematic amplitudes.

There are several sets of diagrams that do just this. In figure 5 are shown a series of processes in which at all scattering events except one the electron is scattered through zero angle. Therefore it follows the same path through the crystal as the kinematic beam and therefore peaks depend on $S \cdot c$, and will make a contribution to structure in the averaged data. When making a theory of averaged data the diagrams of figure 5 must be included.

Fortunately zero angle scattering can be taken account of in a simple manner. First we observe that potentials constant over the entire unit cell are the only ones that produce zero angle, but no other, scattering. If a constant potential $V_{\rm f}$ exists in each unit cell, the scattering produced per unit cell is

 $\Omega V_{\rm f}$ (15)

where Ω is the volume of the unit cell. On the other hand each ion in the unit cell contributes t(0) to zero angle scattering. Taking the case of one ion per unit cell we have

$$V_{\rm f} = t(0)/\Omega \tag{16}$$

If more than one ion were present in the unit cell, t(0) would be replaced by a sum over the t(0) for each separate ion.

Thus our prescription for taking account of zero angle scattering contributions to the average is to add to the self energy of the electron, V_0 , the term, V_f , and then calculate the kinematic average using this modified self energy in place of V_0 . Equations 6 and 7 must then be rewritten

$$\kappa'_{\boldsymbol{g}} = + (2E - 2V_0 - 2V_f - |\boldsymbol{K}_{\parallel}^{(0)'} + \boldsymbol{g}|^2)^{1/2}$$
(17)

$$K_{g}^{\pm'} = \left[(K_{\parallel}^{(0)'} + g)_{x}, (K_{\parallel}^{(0)'} + g)_{y}, \pm \kappa_{g}' \right]$$
(18)

and $\mathbf{K}^{(0)'}$ itself satisfies

$$|\mathbf{K}^{(0)'}|^2 = 2E - 2V_0 - 2V_f \tag{19}$$

The new average, using kinematic theory with modified parameters, is referred to as a quasi-kinematic average.

Modification of V_0 by V_f meets many of the objections raised in §2. The real part of V_f shifts the kinematic peaks in energy thus correcting for the general lowering (or raising) of inner potential caused by ion core scattering, and meeting the objection of §2.2. The imaginary part of V_f produces more absorption thus reducing intensities (objection of §2.1) and, through equation 12, increasing peak widths (objection of §2.3).

The physical interpretation of this term is that V_{fi} is given from (16) by the imaginary part of the zero angle scattering, which from the optical theorem gives the total elastic scattering by the ion core. This term takes account of all flux removed from the kinematic beam by multiple scattering, and therefore effectively lost to the kinematic process.



Figure 6. Corrections to the self energy in nickel from zero angle scattering. \oplus real part. \Rightarrow -imaginary part.

Using equations 3 and 16 it is easy to calculate $V_{\rm f}$ directly from the phase shifts. In figure 6 we show $V_{\rm f}$ evaluated in this way for nickel-ion cores, as a function of incident energy. Corrections to the real part of the self energy are of the order of 2–3 eV, and those to the imaginary part, fairly constant at 4–5 eV. Lagally *et al* found that their best value for the inner potential was -18 eV. From comparison of band structure calculations for nickel with work function data (Pendry and Andersson 1972) $V_{\rm 0r}$ is found to be -18eV for incident energies below 100 eV. There is some evidence from multiple scattering LEED calculations for a reduction in magnitude of $V_{\rm 0r}$ above 100 eV. Thus $V_{\rm 0r} + V_{\rm fr}$ varies from -17 to -21 eV over the range of averaging of the experimental data of Lagally *et al*, in reasonable agreement with their inner potential. In fitting the averaged data with a kinematic curve Lagally *et al* found it necessary to use an extinction distance inside the crystal corresponding to an imaginary part of the self energy of -9 eV. This value is to be compared with a value of $V_{\rm 0i}$ of -4 eV, found by fitting exact calculations



Figure 7. Calculations of the 00 beam for normal incidence on a nickel 100 surface at T = 0 K : \bigoplus kinematic theory using $V_{0r} = -18$ eV, $V_{0i} = -4$ eV; \star quasi-kinematic theory using $V_0 + V_f$.

to experiment, plus $V_{fi} = -5$ eV giving -9 eV in good agreement with Lagally's value. Note the importance of including V_{fi} in this last expression.

In figure 7 we present calculations of kinematic and quasi-kinematic intensities to point to the differences that $V_{\rm f}$ produces in spectra. Intensities are much lower and peak widths broader.

4. Extracting more information from averaging

One of the disadvantages of averaging is that it throws away a lot of structure in spectra, containing information that may be of use. For example the processes shown in figure 4 averaged for constant $S \cdot c$ give a uniform background as a function of $S \cdot c$ from which no structural information is available.

The expression (13) gives the amplitude of one of the processes in figure 4. The sum over all processes has a peak in intensity when S'. c not S. c satisfies a Bragg condition (equation 14). That is why averaging at constant S. c gives a uniform background. If instead a new sort of average is taken keeping S'. c constant, the processes of figure 4 will give rise to structure in the new average. Such an average could be called a 'second order average'. It corresponds to averaging one reflected beam whilst keeping the scattering vector for some other beam constant.

In this way much more useful information could be extracted from the beams than by the simple first order averaging procedures. Of course, the theoretical second order average is a little more difficult to calculate than the kinematic average, but not so much so as to lose all advantages of simplicity over a full multiple scattering theory.

It remains to be seen whether averaging procedures are sensitive enough to detect structure in second and even in higher order averages. Such averages would be useful in treating structure in extra beams introduced by an overlayer on the surface. Most of the detailed structure in these beams is caused by second order processes involving scattering by both the overlayer and the substrate. Only second order averaging can pick out such structure.

5. Further corrections

Zero angle scattering is not the only process that modifies the kinematic nature of averaged peaks. There are some contributions from multiple scattering within a layer.

The kinematic expression (5) for scattering through angle θ from beam $K^{(0)}$ to beam K_{a}^{-} is

$$T(\theta) = -\frac{2\pi}{|\mathbf{K}^{(0)}|} \sum_{l=0}^{\infty} (2l+1) \exp(i\delta_l) \sin(\delta_l) P_l(\cos(\theta))$$
$$= -\frac{2\pi}{|\mathbf{K}^{(0)}|} \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} 4\pi \exp(i\delta_l) \sin(\delta_l) Y_{lm}(\Omega(\mathbf{K}_{\mathbf{g}}^-))$$
$$\times Y_{l-m}(\Omega(\mathbf{K}^{(0)}))(-)^m$$
(20)

where $\Omega(K_g^-)$ is the angular direction of K_g^- . Beeby (1968) has shown how to take account of multiple scattering within a layer to give $T_{\rm ms}(\theta)$. Using Pendry's (1971a) notation

$$T_{\rm ms}(\theta) = -\frac{2\pi}{|\mathbf{K}^{(0)}|} \sum_{lm} \sum_{l'm'} \{(\mathbf{i})^{-l} Y_{lm}[\mathbf{\Omega}(\mathbf{K}_{g}^{-})] \exp(\mathbf{i}\delta_{l}) \sin(\delta_{l})\} \times \{1 + X + X^{2} + \ldots\}_{lm, l'm'} \{(\mathbf{i})^{l'}(-)^{m'} Y_{l'-m'}(\mathbf{\Omega}(\mathbf{K}^{(0)}))\}$$
(21)

If only the zeroth power of X is included, (21) reduces to (20). The *n*th power of X includes *n*th order scattering processes within the layer.

Once more we must beware of terms producing peaks in intensity at the kinematic condition. Many multiple scattering events within a layer do average away to a constant background but terms which do not can be identified. Figure 8 shows a series of such



Figure 8. Corrections to amplitudes of quasi-kinematic peaks (a) from intralayer, (b) from interlayer, multiple scattering.

terms. Scattering from one atom to another in the layer is shown by a loop beginning and ending in the layer. After being scattered twice in the first layer, the beam emerges to be diffracted kinematically subsequently. The loop provides a factor that is the same for all terms in figure 8a. On changing angles of incidence and energy but keeping only the scattering vector S.c constant, the factor for the loops will change and in this way interference effects with other processes average to zero. But the intensity peaks from this set of terms do not average to a uniform background. Each term differs from the others in the same manner as a kinematic term and therefore the terms add coherently at the kinematic condition.

In addition the averages of these terms must be corrected for zero angle scattering. They add to the intensities of peaks in the averaged spectra, but since their contributions have the same widths (determined by $V_{0i} + V_{fi}$) and shape as kinematic peaks, do not distort the shape or change the positions of the averaged peaks.

Multiple scattering within a layer is not the only process that can add to strengths of averaged peaks. The processes in figure 8b involving multiple scattering between layers make contributions similar to those of 8a. It is not hard to think of many more diagrams that produce averaged peaks at the kinematic condition.

It is possible to make corrections for these terms but since this involves taking detailed account of certain multiple scattering processes, the simplicity of kinematic theory is lost and the whole point of averaging removed.

Under certain circumstances there is some hope that corrections other than those from zero angle scattering (these are always large) will be small. Contributions of the type shown in figure 8a will be small if the electron scatters into the layer only weakly. At normal incidence when the temperature is high it is reasonable to suppose that the two scatterings through 90° involved will have small amplitudes and can be neglected to a first approximation. It can also be argued that contributions shown in figure 8b are relatively weak because two layers have to be penetrated before any back-reflection takes place.

Consequently to eliminate these processes so far as possible we would recommend that experiments are performed at high temperatures and averages made over angles of incidence not too far from the normal.

Nevertheless there must still remain some doubt about these additional contributions to averaged data. It seems that the corrections for zero angle scattering enable us to find the parameters for inner potential $(V_{0r} + V_{fr})$ and absorption $(V_{0i} + V_{fi})$ in quasi-kinematic calculations, but the effective scattering factors, giving intensities of the averaged peaks, involve complicated contributions from processes outlined above.

It is clear that some extension of this theory must be made to find a simple way of calculating effective scattering factors in order that the averaging technique can be applied with confidence to structural determinations.

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