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SPRING COLLEGE IN CONDENSED MATTER
ON
"THE INTERACTION OF ATOMS & MOLECULES WITH SOLID SURFACES"
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LOW ENERGY ELECTRON DIFFRACTION

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1. Low Energy Electron Diffraction Experiments

The essential elements are: an ultra high vacuum chamber to preserve surface cleanliness, an electron gun to produce a collimated beam of electrons in the energy range 0 to 500eV, a crystal holder and manipulator, and some means of observing the diffracted electrons, typically a fluorescent screen. Figure 1 shows a sketch.

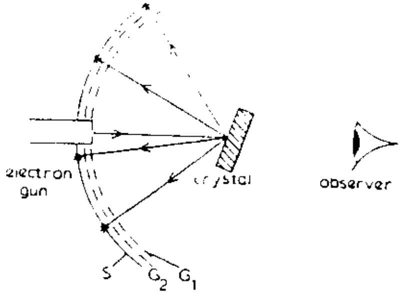

Figure 1 A schematic LEED experiment. S is a fluorescent screen, G_1, G_2, are grids.

The major difficulty is common to all surface experiments, that is to keep the surface clean. The UHV chamber will normal contain an array of techniques for cleaning the surface (provision for heating the sample, ion bombardment) as well as some means of detecting impurities at the surface, usually by detection of Auger signals from adsorbed atoms. LEED is very sensitive to the cleanliness of the surface and small amounts of contaminant can produce quite spurious results. Experiments done on clean, perfect, surfaces can produce a large amount of structural information of high precision. Obviously it is only possible to produce precise data for surfaces which are well defined in the first place.

The state of mechanical perfection of the surface can conveniently be monitored by the LEED experiment itself. Strangely enough LEED can be very tolerant of mechanical imperfections, perhaps because only perfect areas of surface contribute to the sharp diffraction features which are typically measured.

There are two sorts of observations to be made with LEED. The easiest sort is simply to take photographs of the screen. If the surface has been well prepared and is in a well ordered state, it will behave just like an optical diffraction grating. The incident beam is diffracted into a discrete set of beams. These beams can be displayed on a the fluorescent screen shown in figure 2.

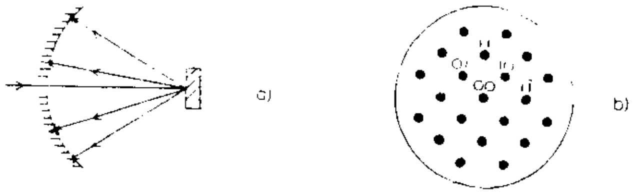

Figure 2 a) showing the diffraction pattern of an incident beam into a series of discrete beams, b) a plan view of a typical pattern made on the fluorescent screen by these beams.

The resulting pattern gives information about the unit cell of the surface structure. Sometimes in simple cases this can be inferred from the bulk structure of the crystal, in other cases the surface may form a new structure due to interactions between adsorbed atoms, or instabilities of the clean surface itself. Such observations provide important information about elemental surface processes which has enabled to greatly to expand our understanding of the surface in the past few years.

The more difficult sort of experiment to make is to observe the intensities of the diffracted beams. Whereas the spot profile on the screen tells us about the size and shape of the surface cell, the intensities are far richer in their information content: they tell us about how the contents of the cell are arranged. For example if we wish to know the positions of atoms at surfaces we must measure LEED intensities, not merely the positions of the spots.

In the early days of the subject diffracted intensities were measured by catching the electrons in a device called a Faraday cup. This was accurate, but very slow. Locating where the beam was presented difficulties that greatly taxed the patience of the experimenter and only very limited amounts of data have been acquired in this way. An easier but less accurate method is to measure the intensity of photo- luminescence of the spots on the fluorescent screen. Here one can actually see what is being measured and guide the measuring device by eye. Nevertheless even this method is time consuming when we wish to acquire the very large datasets needed for really precise work. It also lacks sensitivity requiring large currents in the incident electron beam which can cause problems when chemically delicate species are present on the surface: the molecule CO can be desorbed and decomposed by an electron beam.

The most sophisticated solution to these problems developed so far is the "DATALEED II" apparatus developed in Erlangen, West Germany, by Müller and Heinz. The screen image is amplified by an image intensifier and digitised in real time by a TV camera working in conjunction with sophisticated electronics. Having acquired the data in electronic form it can be processed by computer so as rapidly to extract the information required.

With this apparatus very low beam currents can be used and data acquired in seconds rather than hours. It will be essential to the feasibility of the new methods for extracting structural information from diffraction data.

2. Typical Experimental Data

Figure 3 shows a typical LEED measurement of the I(E) spectrum of one of the diffracted beams from a copper surface. In principle the intensities could be measured as functions of other variables such as the angle of incidence, but this is rarely done.

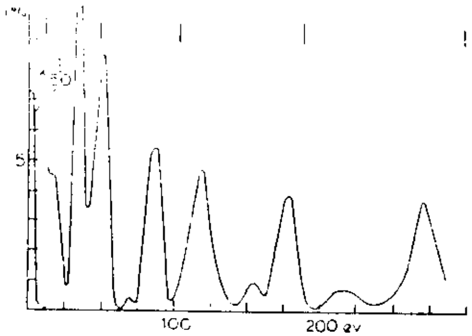

Figure 3 Intensity of the 00 beam from a copper (001) surface as a function of energy. The incident beam his the surface at 3° from the normal. Data were taken by Anderson on Göteborg. Vertical bars mark the positions where we would expect to see peaks on the basis of Bragg's law.

Several points are worth noting. First, the I(E) data are highly structured. Think of the curves from an information theory point of view: how many different numbers would you need to quote in order to describe the curves?. Well, I can identify something like 11 peaks or shoulders in the data. For each of these I would need to specify the energy and intensity, 22 numbers in all. That is a great deal of information content. Furthermore we can easily generate many more curves by looking at different beams, or by shifting the angle of incidence. This is the special power of LEED: it has an extraordinarily high information content. Even for the copper (001) surface an investigation of atomic positions will involved specifying the position of the second layer relative to the first (one atom per unit surface cell), and the third relative to the second. Sensitivity to the fourth layer is probably not great. Thus we need information on 6 independent coordinates, 3 for each displacement. Also we would expect to double check on each coordinate, hence the 11 peaks are only just enough to give a determination of the structure of this simple surface of clean copper!

3. Theoretical Problems

The experimental data contain information, but how can we extract that information? Somehow we have to relate the raw data, peak positions and intensities, to the arrangement of atoms at an atomic level.

The intensities are generated because electrons scatter from atoms in the surface. The electron wavefunction at the detector is given by a sum over all possible scattering events that the electron can make within the surface. Each scattering path will change the phase of the wavefunction by a different amount depending on the path length and the wavelength of the electron. As the energy is varied the wavelength changes and the interference conditions change: hence the succession of maxima and minima in figure 3. The problem for interpretation of the data is that the scattering paths contributing to the intensities are rather complex. In general an electron will scatter off more than one atom before it leaves the surface. This multiple scattering problem held up the development of LEED until we had developed an adequate theoretical base for calculating its effects. Today the theory is very well understood and we have access to far more sophisticated computers than was the

case only 10 years ago. The theoretical calculations needed interpret figure 3 in terms of locations of copper atoms can now easily be done on a personal computer costing less than $1000.

What ingredients control this theory? Again figure 3 proves to be a mine of information. Notice that the structure in the curves tends to be rounded: none of the peaks is very sharp. In fact the most narrow peaks seen have a width given by

$$\delta E \approx 8\text{eV}. \qquad (3.1)$$

This uncertainty in the energy of a feature we can relate by fundamental quantum mechanics to the lifetime of electrons in the surface. The uncertainty principle tells us that

$$\delta E >= \hbar/\tau. \qquad (3.2)$$

Taking the narrowest peaks we deduce that the lifetime of electrons is

$$\tau \approx \hbar/\delta E \approx 10^{-15} \text{ seconds}, \qquad (3.3)$$

during which time a 100eV electron travels about 5Å.

This short penetration depth explains the surface sensitivity of electrons with energies of the order of 100eV. It is just enough to encompass the first few atomic layers of the solid in which all the interesting surface effects on atomic structure usually take place.

Now let us turn our attention to the intensities. During time τ the atoms have to scatter the electron strongly enough to give intensities of the order of 1%. Let the rate of back- scattering be given by a matrix element $|T_b|^2/\hbar$, then the scattered intensity will be given by,

$$|T_b|^2.\tau/\hbar = |T_b|^2/\delta E = 0.01 \qquad (3.4)$$

hence $$|T_b|^2 = 0.01\ \delta E \approx 0.1\ \text{eV}. \qquad (3.5)$$

One further important parameter is missing from our picture. Scattering of electrons by atoms is by now means isotropic. The atoms are much better at scattering the electrons in the forward direction. Crudely speaking we can distinguish between forward- and back- scattering by defining a separate matrix element for forward scattering, $|T_f|^2$. I have already remarked that the electron scatters from several atoms before it leaves the surface. How do I know this? If the electron only scattered from one atom, ie scattering was very weak, then we can take over the theory used to describe Xray diffraction. Here Bragg's law tells us that weak scattering waves diffract from planes of atoms. In the case of figure 3 we are observing the 00 beam from a copper (001) surface, and the relevant planes are the (001) planes. Bragg's law predicts peaks when the condition,

$$\text{wavelength} = 2d\cos(\theta), \qquad (3.6)$$

is satisfied, where d is the interplanar spacing and θ is the angle of incidence of the waves measured relative to the normal to the planes. In figure 3 I have marked where Bragg's law would predict peaks and it is evident that there are many more peaks than are predicted. The only way in which Bragg's law can break down is if the conditions for its validity are violated: the scattering cannot be weak.

We have demonstrated that the back scattering matrix element is in fact small relative to the lifetime of the electron, therefore we can expect only one back scattering event in general. Any multiple scattering must be due to forward scattering. Such this must occur in order that Bragg's law is violated, we deduce that,

$$|T_f|^2 \approx \delta E \approx 8\text{eV}. \qquad (3.7)$$

4. Kinematic Theory

So much for estimates of the nature of electron scattering at a surface. Now let us try to do a better job, first by concentrating on how a single atom scatters an electron. Later we shall discuss the multiple scattering problem.

units

to simplify the writing of equations it is usual to adopt a simplified system of units. I shall use atomic units in which,

$$\hbar = e^2 = m = 1. \qquad (4.1)$$

In this system the units work out as follows:

unit of energy = 1 Hartree = 27.2eV (4.2)

unit of length = 1 Bohr radius = 0.5292Å (4.3)

and the Schrödinger equation becomes,

$$\frac{1}{2}\nabla^2\Phi + V\Phi = E\Phi. \qquad (4.4)$$

Conventionally we divide the potential into two parts,

$$V(\underline{r}) = V_0 + V_a(r) \qquad (4.5)$$

where the constant potential,

$$V_o \quad = \quad V_{or} \ + iV_{oi}, \qquad (4.6)$$

comprises a real part which represents a shift of all electron energies in the crystal relative to the vacuum, and an imaginary part which represents the lifetime of the electron inside the solid. Typically,

$$V_{or} \ \approx \ -10\text{eV}, \qquad V_{oi} \ = \ -4\text{eV}. \qquad (4.7)$$

In fact V_o is only constant inside the surface, outside it gradually falls away to zero. However it does so very smoothly and it is usual to neglect any reflection from this step in potential at the surface. Its effects are confined solely to changing the wave vector of the electron inside the surface.

That an imaginary potential reproduces the effect of finite lifetime can be seen as follows: neglect V_a in the Schrödinger equation. Then we can solve for Φ in a constant complex potential,

$$\Phi \quad = \quad \exp(i\underline{K}.\underline{r})\exp(-iEt) \qquad (4.8)$$

so that,

$$|\underline{K}|^2 \ + \ V_{or} \ + \ iV_{oi} \ = \ E. \qquad (4.9)$$

Evidently if we choose $\underline{K}$ to be a real vector, then E becomes complex, so that

$$|\Phi(t)|^2 \quad = \quad \exp(2\text{Im}(E)) \quad = \quad \exp(2V_{oi}), \ (4.10)$$

and since V_{oi} is negative, this represents decay of Φ with time. Alternatively we may require E to be real (it may be fixed by voltages in the electron gun, for example) in which case we are free to choose the components of $\underline{K}$ to be complex. If we define x, y axes to lie in the surface plane, and the positive z axis to point into the surface, then we can only choose the z component of $\underline{K}$ to be complex: complex $\underline{K}_x$ would result in the wavefunction growing unphysically to ∞ at $+/-x = \infty$, and similarly for $\underline{K}_y$. On the other hand we are free to choose $\underline{K}_z$ to have a positive imaginary part so that Φ decays away into the surface. Thus absorption can result in a wavefunction that decays in time, or in space depending on the experimental circumstances. In a LEED experiment the energy is fixed to be real in the electron gun, therefore from (4.4),

$$\underline{K}_z \quad = \quad +\sqrt{[2E - 2V_{or} - 2iV_{oi} - \underline{K}_x^2 - \underline{K}_y^2]}. \qquad (4.11)$$

The x and y components of $\underline{K}$ are fixed by the direction of the incident beam.

Next consider the atomic part of the potential. It is usually a good approximation in a LEED calculation to take this to be spherically symmetric. Its effect is to scatter the wavefunction Φ into a different state so that far outside the range of V_a itself we have to add corrections to our wavefunction to take account of the scattering by an atom located at R_j,

$$\Phi' = \exp(i\underline{K}.\underline{r}) + f(\Theta)\exp(i\underline{K}.\underline{R}_j + i|\underline{K}||\underline{r}-\underline{R}_j|)/(|\underline{K}||\underline{r}-\underline{R}_j|), \qquad (4.12)$$

where Θ is the angle between $\underline{K}$ and $\underline{r}$. The scattered wave is an outgoing spherical wave centred on the atom, and whose amplitude depends on the direction in which it is scattered. $f(\Theta)$ will be large for forward scattering, and small for backward scattering, as we have discussed. It is usual to express the scattering factor in terms of entities, δ_l, called phase shifts:

$$f(\Theta) = 4\pi|\underline{K}|^{-1} \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} \exp(i\delta_l)\sin(\delta_l)\ (-1)^m Y_{lm}(\hat{\underline{K}}) Y_{l-m}(\hat{\underline{r}}) \quad (4.13)$$

where Y_{lm} is a spherical harmonic, and $\hat{\underline{r}}$ denotes the angular coordinates of $\underline{r}$.

In LEED theory we usually think of a surface in terms of layers of atoms, each layer parallel to the surface, and the scattering from the surface as a whole is built up in step wise fashion: first considering the individual atoms, next the layers of atoms, and finally the combined effect of the layers is calculated.

Suppose that we have a complete layer of atoms, all of the same type, spaced on a Bravais lattice defined by,

$$\underline{R}_j = m_j\underline{a} + n_j\underline{b}. \quad (4.14)$$

Then the wavefield corrected for the effect of the layer scattering can be written:

$$\Phi'' = \exp(i\underline{K}.\underline{r}) + \sum_{\underline{g}} M(\underline{K}_{\underline{g}}^{+/-},\underline{K}) \exp(i\underline{K}.\underline{R}_n + i\underline{K}_{\underline{g}}^{+/-}.(\underline{r}-\underline{R}_n)), \quad (4.15)$$

where $M(\underline{K}_{\underline{g}}^{+/-},\underline{K}) = 2\pi i\ f(\theta_{\underline{g}})/[A|\underline{K}||\underline{K}_{\underline{g}z}|]$, (4.16)

A is the area occupied by each atom in the layer, $\theta_{\underline{g}}$ is the angle through which the gth beam is scattered, and the superscript +/- refers to whether the relevant beam has been scattered to the +z or -z side of the layer. Note that, now we are scattering from a periodic object, the scattered amplitude has the form of a discrete set of beams defined by the reciprocal lattice vectors, $\underline{g}$. These in turn are defined in terms of the unit cell:

$$\underline{g} = h\underline{A} + k\underline{B}, \quad (4.17)$$

where $$\underline{A} = \frac{2\pi}{(a_x b_y - b_x a_y)} (b_y, -b_x), \quad (4.18)$$

and $$\underline{B} = \frac{2\pi}{(a_x b_y - b_x a_y)} (-a_y, a_x). \quad (4.19)$$

The wave vectors of the scattered waves are given by,

$$[\underline{K}_{\underline{g}}^{+/-}]_x = \underline{K}_x + \underline{g}_x, \quad (4.20)$$

$$[\underline{K}_{\underline{g}}^{+/-}]_y = \underline{K}_y + \underline{g}_y, \quad (4.21)$$

$$[\underline{K}_{\underline{g}}^{+/-}]_z = +/-\sqrt{[2E - 2V_o - (\underline{K}_y + \underline{g}_y)^2 - (\underline{K}_x + \underline{g}_x)^2]}. \quad (4.22)$$

Equation (4.16) is an approximation to the exact expression for the layer scattering. We have omitted to take account of the multiple scattering terms. However they enter as corrections to M, and the general form of the scattered wave is retained even in the multiple scattering regime.

Equations (4.15) and (4.16) can be simply interpreted as follows: in the single scattering approximation, an ordered array of atoms results in the scattering directions being quantised; the amplitude of waves in each quantised direction being given by the atomic scattering factor for that direction.

Next we add together scattering from several layers to calculate the scattered wavefield just outside the surface.

We assume that layers are equally spaced and that no multiple scattering occurs between layers:

$$\underline{R}_n = n\,\underline{c}, \tag{4.23}$$

and

$$\Phi''' = \exp(i\underline{K}.\underline{r}) + \sum_{n=0}^{\infty}\sum_{\underline{g}} M(\underline{K}_{\underline{g}}^{-},\underline{K})\exp(i\underline{K}.\underline{R}_n + i\underline{K}_{\underline{g}}^{-}.(\underline{r}-\underline{R}_n)),$$

$$= \exp(i\underline{K}.\underline{r}) + \sum_{\underline{g}}\Phi_{\underline{g}}\exp(i\underline{K}_{\underline{g}}^{-}.\underline{r}), \tag{4.24}$$

where

$$\Phi_{\underline{g}} = \frac{M(\underline{K}_{\underline{g}}^{-},\underline{K})}{1-\exp[i(\underline{K}-\underline{K}_{\underline{g}}^{-}).\underline{c}]}. \tag{4.25}$$

Expressions (4.24) and (4.25) constitute the so called kinematic formula for diffracted amplitudes. It contains no multiple scattering at all and therefore rarely represents an accurate account of a realistic situation. It does illustrate some interesting aspects of LEED which do not depend on multiple scattering. Figure 4 shows the kinematic formula evaluated for the (100) surface of a simple cubic crystal using typical values of the parameters:

$$V_{or} = -0.5 \text{ Hartrees}, \tag{4.26}$$

$$V_{oi} = -0.15 \text{ Hartrees}, \tag{4.27}$$

$$\underline{c} = (0,0,\pi) \text{ Bohr radii}, \tag{4.28}$$

$$\underline{K}_x = 0, \quad \underline{K}_y = 0, \tag{4.29}$$

$$\underline{g}_x = 0, \quad \underline{g}_y = 0, \tag{4.30}$$

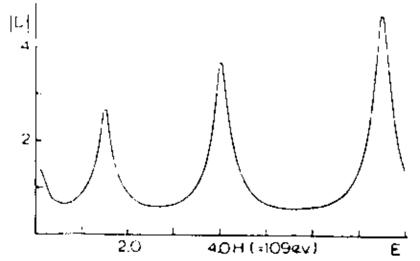

Figure 4. Diffracted intensity, $|\Phi_{\underline{g}=\underline{0}}|^2$, calculated in the kinematic approximation assuming constant atomic scattering amplitude and plotted against incident energy for a simple cubic crystal. Note the strong peaks near the Bragg diffraction conditions.

This simple model reproduces peaks of the correct sort of shape and width. Including the proper atomic scattering factor would give roughly the right intensities, provided we correct them for thermal vibrations, a topic which we shall not have time to treat here. We can also see from (4.25) that the peak positions are determined by the energy and the interplanar spacing. This give the structural sensitivity we seek. Increasing the spacing between planes moves the peaks to lower energies. The shape of the peaks is modified if each pair of planes has a different spacing: in this way it is possible to resolve all relevant inter planar spacings.

5. Multiple Scattering

This subject is a technical one and those interested in making detailed calculations should read one of the relevant texts on LEED theory. The underlying principles can be demonstrated by a one dimensional model. Take a 1D array of atoms: figure 5 shows a schematic picture of the potential.

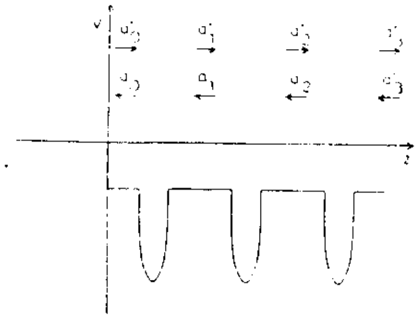

Figure 5. A one dimensional potential in which an electron may move. Amplitudes of forward and backward travelling waves between scatterers are indicated.

We shall assume that if a wave,

$$\exp(+ik(z-nc)),\quad z < nc, \tag{5.1}$$

is incident on a layer located at $z=nc$, then the transmitted and reflected waves are respectively:

$$t\exp(+ik(z-nc)),\quad z > nc, \tag{5.2}$$

$$r\exp(-ik(z-nc)),\quad z < nc. \tag{5.3}$$

Correspondingly if a wave,

$$\exp(-ik(z-nc)),\quad z > nc, \tag{5.4}$$

is incident on a layer located at $z=nc$, then the transmitted and reflected waves are respectively:

$$t\exp(-ik(z-nc)),\quad z < nc, \tag{5.5}$$

$$r\exp(-ik(z-nc)),\quad z > nc. \tag{5.6}$$

For simplicity we have assumed that for each of the two different incident waves, the relevant transmission and reflection coefficients are equal. In general this is not true.

Transfer Matrices

We are now in a position to show how to calculate the band structure of the system. Bloch's theorem tells us that if the system consists of a set of identical objects, equally spaced, then the electron wavefunctions can be classified by a wave vector, K. In this instance, between layers n-1 and n we have forward and backward waves of amplitudes $a_n^{+/-}$, and between layers n and n+1 waves of amplitudes $a_{n+1}^{+/-}$. Bloch's theorem says that we can find solutions of the Schrödinger equation which satisfy

$$a_{n+1}^{+} = \exp(iKc)\ a_n^{+}, \tag{5.7}$$

$$a_{n+1}^{-} = \exp(iKc)\ a_n^{-}. \tag{5.8}$$

We can calculate the wave vector K from the scattering properties of the layers. Using equations (5.1)-(5.6) we find the following relationships:

$$a_{n+1}^{+} = \exp(+ikc)\ t\ a_n^{+} + r\ a_{n+1}^{-} \tag{5.9}$$

$$a_n^{-} = \exp(+ikc)\ t\ a_{n+1}^{-} + r\ a_n^{+}. \tag{5.10}$$

Defining,

$$t' = \exp(ikc)\ t \tag{5.11}$$

and we can rearrange these equations, writing them in matrix form to give:

$$\begin{bmatrix} 1, & -r \\ 0, & t' \end{bmatrix}\begin{bmatrix} a_{n+1}^{+} \\ a_{n+1}^{-} \end{bmatrix} = \begin{bmatrix} t', & 0 \\ -r, & 1 \end{bmatrix}\begin{bmatrix} a_n^{+} \\ a_n^{-} \end{bmatrix} \tag{5.12}$$

and matrix inversion leads to,

$$\begin{bmatrix} a^+_{n+1} \\ a^-_{n+1} \end{bmatrix} = \begin{bmatrix} 1-r^2/t'^2, & r/t' \\ -r/t' & , 1/t' \end{bmatrix} \begin{bmatrix} a^+_n \\ a^-_n \end{bmatrix} \qquad (5.13)$$

Substituting for the left hand side using the Bloch condition from (5.6) and (5.7),

$$\exp(iKc) \begin{bmatrix} a^+_n \\ a^-_n \end{bmatrix} = \begin{bmatrix} 1-r^2/t'^2, & r/t' \\ -r/t' & , 1/t' \end{bmatrix} \begin{bmatrix} a^+_n \\ a^-_n \end{bmatrix}, \qquad (5.14)$$

we see that the band structure, that is to say exp(iKc), can be found from the eigenvalues of the <u>transfer matrix</u>,

$$T = \begin{bmatrix} 1-r^2/t'^2, & r/t' \\ -r/t' & , 1/t' \end{bmatrix}. \qquad (5.15)$$

The most general way of solving the problem of reflection from surfaces involves using the eigenvectors of the transfer matrix, ie the Bloch waves. Here are the rules by which the calculation is made:

i) solve for the eigenvectors of the transfer matrix: there will be two of them: $[b^+_1, b^-_1]$, and $[b^+_2, b^-_2]$.

ii) choose the eigenvector with net current flowing <u>into</u> the the surface, let us say $\underline{b}_1$:

$$k\ (b^{+2}_1 - b^{-2}_1) > 0.$$

iii) the reflection coefficient is then given by,

$$R = b^-_1/b^+_1.$$

Rule i) simply states that the wavefunction inside the surface must solve Schrödinger's equation. Rule ii) means that the wavefunction must not correspond to any sources of current buried inside the surface. This leaves a wavfunction corresponding to an externally incident wave plus a reflected wave.

This general method is rarely used in practice and simpler methods are used. the most popular of which is the "layer doubling method". It works like this: a single layer has reflection and transmission coefficients,

$$t(1) = t', \quad r(1) = r. \qquad (5.16)$$

Taking two layers and calculating the scattering from the pair gives for the combined transmission coefficient,

$$t(2) = t(1).t(1) + t(1).r^2(1).t(1) + t(1).r^4(1).t(1) + t(1).r^6(1).t(1) + \dots \qquad (5.17)$$

The terms in this series can be interpreted as follows: the first term describes transmission through both the layers; the second term corresponds to transmission through the first layer, reflection from the second, another reflection from the first and finally transmission through the second layer at the second attempt. This is what we mean by multiple scattering. The series is a simple geometric series which can be summed to give,

$$t(2) = t^2(1)/(1 - r^2(1)). \qquad (5.19)$$

Similarly the combined reflection coefficient of the pair of layers is given by,

$$\begin{aligned} r(2) &= r(1) + t(1).r(1).t(1) + t(1).r^3(1).t(1) \\ &\quad + t(1).r^3(1).t(1) + \dots. \\ &= r(1) + t^2(1).r(1)/(1 - r^2(1)). \qquad (5.20) \end{aligned}$$

We can repeat the process to calculate t(4) and r(4) from t(2) and r(2), doubling the number of layers each time. In this way we can easily find the reflection coefficient of an effectively infinitely thick pile of layers representing the surface. In practice 8 layers are usually enough, though 16 may sometimes be needed.

These methods have been described for a simple one-dimensional example, but they can be generalised to real surfaces using the same principles, the only difference being that t and r are matrices.