SHORT COMMUNICATIONS

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Current flow in reflection electron microscopy and RHEED.

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Abstract

Application of simple Bloch-wave theory to reflection electron microscopy and diffraction leads to inconsistent results - there are not enough boundary conditions to generate a unique solution. To overcome this problem in the past the solution for a thick slab has been used instead of that for a single surface. It is shown that a simpler method valid for a single surface is to insist that only Bloch waves with current flow into or parallel to the crystal surface are allowed. Because of the equations of continuity, this is identical to insisting that only decaying waves are excited in the crystal. An additional feature of this simpler method is that the allowed Bloch waves can be readily represented on a dispersion-surface construction.

In principle the basic analytical solutions for electron diffraction in a material can be directly solved by Bloch-wave methods. Whilst their application to transmission electron microscopy and diffraction is tried and tested, far less has been done to apply them to the important problem of reflection electron microscopy (REM) or reflection high-energy electron diffraction (RHEED). The intention of this note is to point out an important physical point which we have encountered in the process of developing a numerical Bloch-wave program for the reflection case, namely the role of current flow in determining which Bloch waves are excited in the crystal.

The basic theoretical methods for setting up the Bloch-wave solutions can be found in, for instance, the article by Metherell (1975) and will not be repeated here. In a nutshell, the problem reduces to matching from the incident wave vector to the dispersion surface along a line drawn normal to the surface of the crystal, as illustrated in Fig. 1. (We shall not discuss evanescent waves, as they do not play a role in our analysis here, although in reality they must be taken into account in any reasonable model of the diffraction.) If one assumes that the line cuts the dispersion surface, there are *two* possible Bloch waves which can be excited in the crystal for *each* branch of the dispersion surface. Assuming n different branches, we therefore have a maximum of $2n$ different Bloch waves, n different reflected waves and (after matching the wave and its derivative across the crystal surface) a total of $2n$ boundary conditions. As it stands we do not have enough boundary conditions to solve for the Bloch- and diffracted-wave amplitudes.

In the conventional transmission electron diffraction case we solve the analogous problem by insisting that the Bloch-wave vectors must be directed into the crystal. For instance, in the high-energy approximation the wave vectors occur in plus and minus pairs, and we then neglect one of the signs (which depends upon the convention used in defining an incident plane wave). It rapidly became apparent when we tried some numerical tests that this does not work in the reflection electron case. The reason is that the two possible wave vectors for each branch of the dispersion surface need not arise in pairs directed into and out of the crystal, as illustrated in Fig. 1 (see also Table 1). A method proposed by Moon (1972) and by Colella (1972) and Colella & Menadue (1972) is to solve the problem instead for a thick slab with two surfaces rather than just one. Now there are enough boundary conditions, and in the limit of a very thick slab with absorption included only n Bloch waves will be excited within the the crystal.

A simpler method of finding the additional n boundary conditions is to exploit the principle of causality. Physically, the electron beam must travel down the microscope column, reach the crystal surface and then either be reflected or enter the crystal. For any Bloch wave of general form

$$b(\mathbf{r}, \mathbf{k}) = \sum_g C_g \exp\left[2\pi i(\mathbf{k}+\mathbf{g}) \cdot \mathbf{r}\right] \quad (1)$$

the direction of current and energy flow $\mathbf{S}$ (proportional to the expectation value of the Bloch-wave momentum and the group velocity of the Bloch wave and similar to the

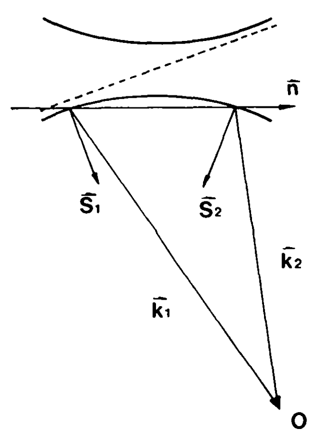

Fig. 1. Illustration of matching from the incoming wave vector to the dispersion surface in the reflection case. For the branch shown, only wave 1 is excited in the crystal, not wave 2, even though the wave vectors for both ($\mathbf{k}_1$ and $\mathbf{k}_2$) are into the crystal, as indicated by the current-flow directions $\mathbf{S}_1$ and $\mathbf{S}_2$.

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Table 1. *Values for the real and imaginary components of the wave vector and the current-flow vector for a nine-beam calculation of a real test potential*

The direction of the surface normal is along the z axis. Note that the signs of the wave vectors and the current flow are not always the same.

	$k_r z$	$k_i z$	S_z
1	1·21079200	0·00000000	0·64091170
2	−1·21079200	0·00000000	−0·64091770
3	0·79729930	0·00000000	0·35488550
4	0·76076230	0·00000000	0·31050750
5	−0·79729790	0·00000000	−0·35502030
6	−0·76076210	0·00000000	−0·31294940
7	0·54941490	0·00000000	0·27685250
8	−0·54941450	0·00000000	−0·27872131
9	0·23151970	0·11244540	0·00000000
10	0·27873130	0·00000000	0·16785510
11	0·23151990	−0·11244520	0·00000000
12	0·19733600	0·00000000	−1·16209000
13	−0·23151930	0·11244520	0·00000000
14	−0·27873170	0·00000000	−0·26795830
15	−0·23151930	−0·11244500	0·00000000
16	0·07455112	0·00000000	0·47119920
17	−0·19335300	0·00000000	2·04193400
18	−0·07455094	0·00000000	−1·21555400

Poynting vector in X-ray diffraction) is given by

$$\mathbf{S} = \text{real part of}\left[(he/m)\sum_g |C_g|^2(\mathbf{k}+\mathbf{g})\right]. \qquad (2)$$

($\mathbf{S}$ is proportional to the mean value of the probability-current density averaged over a unit cell if $\mathbf{k}$ is real.)

The vector $\mathbf{S}$ defined by (2) determines the true path of the electron wave, and geometrically is normal to the dispersion surface, *not* in general along the direction of the wave vector. (Note that it is *wrong* to use the wave vector to describe the electron path.) Clearly, if the current flow of a Bloch wave is not into the crystal, it is unphysical to consider that this Bloch wave is excited even if the wave vector is directed into the crystal. For the two possible Bloch waves corresponding to each branch of the dispersion surface, geometrically (see Fig. 2) the current-flow vectors must correspond to one of three cases: (a) pairs directed into and out of the surface; (b) for the special case when the cut is tangential to the dispersion surface, the two solutions are equivalent and the current flow is parallel to the surface; or (c) for an evanescent wave again only one solution exists with current flow parallel to the surface. Therefore we have only n possible Bloch waves (travelling or evanescent) within the crystal after we have applied this boundary condition. As a hard example, Table 1 lists the wave vectors and current flow perpendicular to the crystal surface from a numerically calculated example (with an arbitrary real potential). It should be noted that the signs of the wave vectors and the current-flow vectors do not correlate in general.

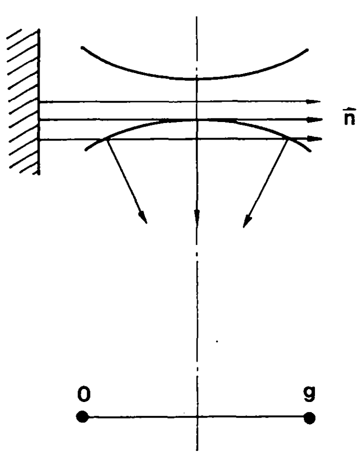

Fig. 2. Illustration of the three possible cases described in the text.

An additional and important point is that this condition also guarantees that all the Bloch waves of interest decay into the crystal. This we can prove with the continuity equation (*e.g.* Schiff, 1968)

$$\mathrm{d}P(\mathbf{r}, t)/\mathrm{d}t + \nabla \cdot \mathbf{j} = -2V_i(\mathbf{r})P(\mathbf{r}, t), \qquad (3)$$

where $P(\mathbf{r}, t)$ is the probability density as a function of space and time, $V_i(\mathbf{r})$ is the imaginary component of the potential and $\mathbf{j}$ is the probability-current density, given by

$$\mathbf{j} = h/4\pi \, \mathrm{Im}\,[\psi^*(\mathbf{r})\nabla\psi(\mathbf{r}) - \psi(\mathbf{r})\nabla\psi^*(\mathbf{r})]. \qquad (4)$$

For any Bloch wave in (3) which is time independent, after cancelling the common term $\exp(-4\pi\mathbf{k}_i \cdot \mathbf{r})$, where $\mathbf{k}_i$ is the imaginary component of the wave vector, and integrating over a unit cell we obtain

$$(2\pi/e)\mathbf{S} \cdot \mathbf{k}_i = \int |b(\mathbf{r}, \mathbf{k})|^2 V_i(\mathbf{r})\,\mathrm{d}\mathbf{r}. \qquad (5)$$

Since the right-hand side is necessarily positive, it follows that

$$\mathbf{S} \cdot \mathbf{k}_i > 0. \qquad (6)$$

As the imaginary component for the reflection case can only exist normal to the plane of the surface, all the waves are decaying into the crystal.

For completeness, it should be mentioned that Kohra, Moliere, Nakano & Ariyama (1962) also appear to have used the concept of energy flow to reduce the boundary conditions for a four-beam Bloch-wave solution in the reflection case, although these authors did not extend the argument to the general n-beam case, point out that this approach will always reduce the number of possible waves to n or less or show that this condition forces all the waves to be decaying.

As a final point, it should be noted that the same arguments hold for the transmission case, and are more rigorous than the normal arguments based solely on the sign of the Bloch-wave vector. Here the Bloch wave with a current flow out of the crystal also has a wave vector oriented out of the crystal, so that one can exclude one of the two wave vectors just by its sign.

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