Iterative method of calculating reflection-high-energy-electron-diffraction intensities

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A method of calculating reflection high-energy electron diffraction intensities is developed within the framework of two-dimensional Bloch-wave approach. In the course of computations only wave-field-related quantities are employed (rather than transfer or scattering matrices). The intensities of reflected beams are calculated iteratively. The very good convergence of the method is demonstrated for Pt(111). For scattering systems with a large number of diffracted beams (exceeding 100–500) this iterative method is potentially faster than traditional direct methods. More importantly, a number of possible approximations can be easily derived on the basis of the iteration sequence introduced. [S0163-1829(99)09107-9]

In recent years much interest has been generated in the use of reflection high-energy electron diffraction (RHEED) in experimental investigations of solid surfaces.[1] RHEED can be used to determine precise positions of atoms at flat surfaces. It can also be used to gain information about the surface topography arising during growth of samples by molecular beam epitaxy. However, to describe properly the movement of electrons in crystals one needs to take account of multiple scattering processes. This is especially difficult in the grazing geometry of RHEED. Consequently precise theoretical interpretations of RHEED data are rather complicated even for simple experimental situations. More importantly, such a treatment is still not available for the case of an arbitrarily rough surface. Therefore, one can conclude that fundamental theoretical research on RHEED is still needed.

In the past considerable progress in quantitative work on RHEED has been achieved due to the use of numerical methods developed in nineteen eighties within the two-dimensional Bloch-wave approach[2] (referred to hereafter as direct methods). In these methods the crystal is divided into slices parallel to the surface and transfer matrices for the slices are determined. Then a reflection matrix is computed successively from the crystal bottom to the crystal top.[3] An important feature of the direct methods is that, for both weak and strong potentials, all computation steps are executed in the same way. This is in fact in many situations a big advantage of these methods as they are universal. However, on the other hand, an implication of this feature is that the link between the direct methods and simplified kinematical approaches (which can be developed for weaker potentials) is hidden behind complicated numerical procedures, and this is why precise numerical results usually cannot be explained qualitatively. In this paper we develop a dynamical method of calculating RHEED intensities in which the exact results are obtained as a limit of an iteration sequence. In our method the full dynamical treatment of electron diffraction can be considered to be an extension of the kinematical approach. As discussed later the direct methods and our iterative method have different advantages and disadvantages and should be treated as complimentary.

There exist already in the literature important examples of RHEED dynamical calculations in which iteration sequences appear.[4] In that work authors benefit from introducing a concept of a small perturbation and a reference system. For the latter direct method calculations are carried out. We follow a different line. Our method is based on the supposition that forward scattering processes are much stronger than backward ones. In principle we do not require any earlier direct method calculations. The possibility of benefiting from the aforementioned supposition was first recognized for the case of low-energy electron diffraction (LEED). Despite the existence of important differences between RHEED and LEED, in some sense our work can be considered to be the continuation of work of Pendry and of Tong on renormalized forward scattering schemes.[5,6] From this point of view it is worth emphasising that the method presented here employs only a plane-wave representation (spherical wave expansions used in LEED cannot be applied for the case of high-energy electrons) and it works for any kind of a local potential (i.e., we do not need to limit ourselves to muffin-tin potentials). In this paper we carry out numerical tests for a flat surface of Pt(111), paying special attention to verification of the convergence.

In brief our method can be described as follows. We start from the assumption that the scattering potential is periodic in planes parallel to the crystal surface. We can then expand the crystal potential $V(\vec{r})$ in the following Fourier series:

$$V(\vec{r}) = \frac{\hbar^2}{2m_0} \sum_{\vec{\kappa}} v_{\vec{\kappa}}(z) \exp(i\vec{\kappa}\cdot\vec{\rho}), \tag{1}$$

where $\vec{\rho}$ is the parallel component of $\vec{r}$ and $\vec{\kappa}$ are vectors of the two-dimensional reciprocal lattice corresponding to the surface periodicity ($\hbar$ and m_0 are, respectively, Planck's constant and the electron rest mass). The electron wave function $\Psi(\vec{r})$ may be expressed as

$$\Psi(\vec{r}) = \exp(i\vec{k}_{\parallel}\cdot\vec{\rho}) \sum_{\vec{\kappa}} \phi_{\vec{\kappa}}(z) \exp(i\vec{\kappa}\cdot\vec{\rho}), \tag{2}$$

where $\vec{k}_{\parallel}$ is the parallel component of the incident beam wave vector $\vec{K}$. After the substitution (1) and (2) into the

Schrödringer equation we finally get the following set of ordinary differential equations:

$$\frac{d^2}{dz^2}\phi_{\vec{\kappa}}(z)+k_{\vec{\kappa}}^2\phi_{\vec{\kappa}}(z)=\sum_{\vec{\kappa}'} v_{\vec{\kappa}-\vec{\kappa}'}(z)\phi_{\vec{\kappa}'}(z), \tag{3}$$

where $k_{\vec{\kappa}}^2=K^2-|\vec{k}_{\|}+\vec{\kappa}|^2$. Additionally, we need to specify boundary conditions. We assume that a crystal is contained between two infinite, parallel planes determined by $z=z_T$ and $z=z_B$, where $z_T>z_B$. We assume that above the crystal, for $z\geqslant z_T$, the functions $\phi_{\vec{\kappa}}(z)$ can be written in the form of $\delta_{\vec{0}\vec{\kappa}}\exp[-ik_{\vec{\kappa}}(z-z_T)]+r_{\vec{\kappa}}\exp[+ik_{\vec{\kappa}}(z-z_T)]$. Below the crystal, for $z\leqslant z_B$, we assume the functions $\phi_{\vec{\kappa}}(z)$ have the form of $t_{\vec{\kappa}}\exp[-ik_{\vec{\kappa}}(z-z_B)]$. We have two sets of unknown coefficients $r_{\vec{\kappa}}$ and $t_{\vec{\kappa}}$, and our aim is to find at least the first set. Before proceeding further we introduce some notation. In all practical work we must limit ourself to a finite number N of vectors $\vec{\kappa}$. Because of this it is useful to treat sets of coefficients, like the set of $r_{\vec{\kappa}}$, as N-dimensional vectors and to name them with corresponding capital letters. Using this convention, we may say briefly that we are interested in finding the vector $\mathbf{R}$. In our method we get a sequence of vectors $(\mathbf{R})_k$ that converges to the exact solution $\mathbf{R}$. We have two combined iteration schemes in our method. The first scheme, called by us a multislice scheme, is formally the main one, and completing its k iterations gives us $(\mathbf{R})_k$. We employ also another iteration scheme which we call a single-slice scheme. Formally it appears as an auxiliary scheme, but nevertheless it is a very relevant component of our method.

1. A multislice iteration scheme taking account of the local average potential

We divide the crystal slab into J slices and count them in the increasing order from the bottom to the top. The jth slice has boundaries at z_j and z_{j+1}, and moreover $z_1=z_B$ and $z_{J+1}=z_T$. For the jth slice we introduce vector quantities $\hat{\mathbf{P}}_j^+(z)$ and $\hat{\mathbf{P}}_j^-(z)$ [which have components $\hat{p}^+_{\vec{\kappa}j}(z)$ and $\hat{p}^-_{\vec{\kappa}j}(z)$] using the following relations:

$$\frac{d\phi_{\vec{\kappa}}(z)}{dz}=i\hat{k}_{\vec{\kappa}j}\hat{p}^+_{\vec{\kappa}j}(z)-i\hat{k}_{\vec{\kappa}j}\hat{p}^-_{\vec{\kappa}j}(z), \tag{4}$$

$$\phi_{\vec{\kappa}}(z)=\hat{p}^+_{\vec{\kappa}j}(z)+\hat{p}^-_{\vec{\kappa}j}(z), \tag{5}$$

where

$$\hat{k}_{\vec{\kappa}j}=\sqrt{K^2-\hat{v}_{\vec{0}j}-|\vec{k}_{\|}+\vec{\kappa}|^2}, \tag{6}$$

$$\hat{v}_{\vec{0}j}=v_{\vec{0}}\left(\frac{z_j+z_{j+1}}{2}\right), \tag{7}$$

and in Eq. (6) we assume that $\mathrm{Re}\,\hat{k}_{\vec{\kappa}j}\geqslant 0$ and $\mathrm{Im}\,\hat{k}_{\vec{\kappa}j}\geqslant 0$. We also define $\hat{\mathbf{P}}_j^+(z)$ and $\hat{\mathbf{P}}_j^-(z)$ below and above the crystal (then formally $j=0$ and $j=J+1$) taking $\hat{v}_{\vec{0}j}=0$. Next, for $j=0,\ldots,J$ we define vectors ${}^H\hat{\mathbf{P}}_j^+$ and ${}^H\hat{\mathbf{P}}_j^-$

$${}^H\hat{\mathbf{P}}_j^+\equiv\hat{\mathbf{P}}_j^+(z_{j+1}), \tag{8}$$

$${}^H\hat{\mathbf{P}}_j^-\equiv\hat{\mathbf{P}}_j^-(z_{j+1}), \tag{9}$$

and for $j=1,\ldots,J+1$ we define vectors ${}^L\hat{\mathbf{P}}_j^+$ and ${}^L\hat{\mathbf{P}}_j^-$

$${}^L\hat{\mathbf{P}}_j^+\equiv\hat{\mathbf{P}}_j^+(z_j), \tag{10}$$

$${}^L\hat{\mathbf{P}}_j^-\equiv\hat{\mathbf{P}}_j^-(z_j). \tag{11}$$

The vectors ${}^H\hat{\mathbf{P}}_j^+$, ${}^H\hat{\mathbf{P}}_j^-$, ${}^L\hat{\mathbf{P}}_j^+$, and ${}^L\hat{\mathbf{P}}_j^-$ contain all basic information about the electron wave field in the crystal and just below and above its boundaries. The aim of our multislice scheme is to find all these vectors iteratively. We have four vectors for each crystal slice, additional two for the crystal top and additional two for the crystal bottom. The vectors marked with ''$-$'' describe the wave propagating from the top to the bottom, similarly the vectors marked with ''$+$'' are for the wave moving in the opposite direction.

Computations are carried out in the following way. Initially all the vectors defined by Eqs. (8)–(11) are taken to be equal to the N-dimensional zero vector (this constitutes our 0th iteration). In the kth iteration, first we assume that we know all vectors marked with ''$+$'' and we calculate only vectors marked with ''$-$'' starting with $j=J+1$ and ending with $j=0$. Namely, we start with $({}^L\hat{p}^-_{\vec{\kappa}J+1})_k$ equal to 1 for $\vec{\kappa}=0$ and to 0 for all others values of $\vec{\kappa}$. We then use the formula [developed from Eqs. (4) and (5)]

$$({}^H\hat{p}^-_{\vec{\kappa}j})_k=\frac{2\hat{k}_{\vec{\kappa}j+1}}{\hat{k}_{\vec{\kappa}j}+\hat{k}_{\vec{\kappa}j+1}}({}^L\hat{p}^-_{\vec{\kappa}j+1})_k+\frac{\hat{k}_{\vec{\kappa}j}-\hat{k}_{\vec{\kappa}j+1}}{\hat{k}_{\vec{\kappa}j}+\hat{k}_{\vec{\kappa}j+1}}({}^H\hat{p}^+_{\vec{\kappa}j})_{k-1} \tag{12}$$

to change the local representation of the wave field. Furthermore, with the help of the single-slice iteration scheme, we find the wave transmitted through a slice or more precisely we determine $({}^L\hat{\mathbf{P}}_j^-)_k$ using $({}^H\hat{\mathbf{P}}_j^-)_k$,$({}^L\hat{\mathbf{P}}_j^+)_{k-1}$, and $({}^H\hat{\mathbf{P}}_j^+)_{k-1}$. In the second part of the kth multislice scheme iteration we assume that we know all the vectors marked with ''$-$'' and we calculate vectors marked with ''$+$'' starting with $j=0$ and ending with $j=J+1$. We begin with $({}^H\hat{p}^+_{\vec{\kappa}0})_k$ equal to 0 for all $\vec{\kappa}=0$. Correspondingly to Eq. (12) we use the formula

$$({}^L\hat{p}^+_{\vec{\kappa}j})_k=\frac{2\hat{k}_{\vec{\kappa}j-1}}{\hat{k}_{\vec{\kappa}j}+\hat{k}_{\vec{\kappa}j-1}}({}^H\hat{p}^+_{\vec{\kappa}j-1})_k+\frac{\hat{k}_{\vec{\kappa}j}-\hat{k}_{\vec{\kappa}j-1}}{\hat{k}_{\vec{\kappa}j}+\hat{k}_{\vec{\kappa}j-1}}({}^L\hat{p}^-_{\vec{\kappa}j})_k \tag{13}$$

to change representations, and with the help of the single-slice iteration scheme we determine $({}^H\hat{\mathbf{P}}_j^+)_k$ using $({}^H\hat{\mathbf{P}}_j^-)_k$,$({}^L\hat{\mathbf{P}}_j^+)_k$, and $({}^L\hat{\mathbf{P}}_j^-)_k$.

Finally, in the kth iteration we get from this scheme $({}^L\hat{\mathbf{P}}_{J+1}^+)_k$, which is equal to $(\hat{\mathbf{R}})_k$. It is essential for convergence to use local wave field representations [see Eqs. (6) and (7)].

2. A single slice inner iteration scheme with successive correction of starting values

For each slice we have the following set of ordinary differential equations for $\hat{\mathbf{P}}_j^+(z)$ and $\hat{\mathbf{P}}_j^-(z)$:

$$\frac{d\hat{p}^{+}_{\vec{\kappa}j}(z)}{dz} = +i\hat{k}_{\vec{\kappa}j}\hat{p}^{+}_{\vec{\kappa}j}(z) + \frac{1}{2i\hat{k}_{\vec{\kappa}j}}\sum_{\vec{\kappa}'}\left[v_{\vec{\kappa}-\vec{\kappa}'}(z) - \delta_{\vec{\kappa}\vec{\kappa}'}\hat{v}_{\vec{0}j}\right] \times\left[\hat{p}^{+}_{\vec{\kappa}'j}(z) + \hat{p}^{-}_{\vec{\kappa}'j}(z)\right], \tag{14}$$

$$\frac{d\hat{p}^{-}_{\vec{\kappa}j}(z)}{dz} = -i\hat{k}_{\vec{\kappa}j}\hat{p}^{-}_{\vec{\kappa}j}(z) - \frac{1}{2i\hat{k}_{\vec{\kappa}j}}\sum_{\vec{\kappa}'}\left[v_{\vec{\kappa}-\vec{\kappa}'}(z) - \delta_{\vec{\kappa}\vec{\kappa}'}\hat{v}_{\vec{0}j}\right] \times\left[\hat{p}^{+}_{\vec{\kappa}'j}(z) + \hat{p}^{-}_{\vec{\kappa}'j}(z)\right]. \tag{15}$$

Below we give a prescription for finding two scattered waves if we know two incident ones for the case of an arbitrary thin slice. More formally, let us assume that we know $\hat{\mathbf{P}}^{-}_{j}(z_{j+1}) = \mathbf{A}$ and $\hat{\mathbf{P}}^{+}_{j}(z_j) = \mathbf{B}$ and that we want to determine $\hat{\mathbf{P}}^{-}_{j}(z_j)$ and $\hat{\mathbf{P}}^{+}_{j}(z_{j+1})$. From the basic theory of RHEED it is known that this problem has a unique solution (it can be proved using the concept of scattering matrices). We solve it iteratively. Let us start by recalling basic information on how a set of ordinary differential equations may be solved with the help of a computer (for more details see, for example, Ref. 7). Numerical techniques are best developed for so called *initial value problems*, i.e., for cases where for a certain value of the independent variable, all values of the dependent variables are given. In our case the values of the dependent variables are specified at two values of the independent variable and subsequently our problem belongs to a class of *two-boundary problems* that generally may be very complicated. However, we can benefit from the assumption of small thickness of the slice. Let us define the following iteration procedure. We put at the slice top $[\hat{\mathbf{P}}^{-}_{j}(z_{j+1})]_0 = \mathbf{A}$ and $[\hat{\mathbf{P}}^{+}_{j}(z_{j+1})]_0 = \mathbf{0}$. The first relation follows from our boundary conditions, the second one constitutes our starting approximation of the scattered wave. Having now determined all values of the dependent variables at the top of the slice we can find the solution of the set (14) and (15) for the whole slice proceeding consecutively from the top to the bottom, and by employing for example the Runge-Kutta method (the standard method for solving initial value problems). After reaching the bottom of the slice we can define another initial value problem. Let us preserve at the bottom the part ''$-$,'' from the the solution just found, as $[\hat{\mathbf{P}}^{-}_{j}(z_j)]_1$ (the part ''$+$'' of the solution may be discarded), and according to our original boundary condition let us put $[\hat{\mathbf{P}}^{+}_{j}(z_j)]_1 = \mathbf{B}$. We now find the full solution of this new initial value problem by proceeding from the bottom to the top. At the top we preserve the part ''$+$'' of the solution as $[\hat{\mathbf{P}}^{+}_{j}(z_{j+1})]_1$. By putting $[\hat{\mathbf{P}}^{-}_{j}(z_{j+1})]_1 = \mathbf{A}$ we form another initial value problem and we can proceed again to the bottom. We can repeat this procedure and in this way we get an iteration sequence of vectors $[\hat{\mathbf{P}}^{-}_{j}(z_j)]_l$ and $[\hat{\mathbf{P}}^{+}_{j}(z_{j+1})]_l$ for $l \geqslant 1$. If the slice is very thin iterations always converge (this can be show using the concept of transfer matrices) and in the limit we obtain the solution to our problem.

Let us now come back to the multislice scheme and consider the case of determining ''$-$'' vectors in the kth iteration (in fact exactly the same concepts are valid for finding ''$+$'' vectors and only a change of the notation is required for this case). We want to find $({}^{L}\mathbf{P}^{-}_{j})_k$ if we know $({}^{H}\hat{\mathbf{P}}^{-}_{j})_k$ and $({}^{L}\mathbf{P}^{+}_{j})_{k-1}$. Taking $\mathbf{A} = ({}^{H}\hat{\mathbf{P}}^{-}_{j})_k$ and $\mathbf{B} = ({}^{L}\hat{\mathbf{P}}^{+}_{j})_{k-1}$ we can in principle apply the algorithm just described. However, in practice we need to terminate single slice iterations after L steps. If we proceed straightaway, always taking zero vectors as starting approximations for scattered waves, we cannot avoid the appearance of some truncation error. However, if we employ in the zeroth approximation, the vector $({}^{H}\hat{\mathbf{P}}^{+}_{j})_{k-1}$ (this constitute a correction of the initial guess) then the truncation error is successively reduced.

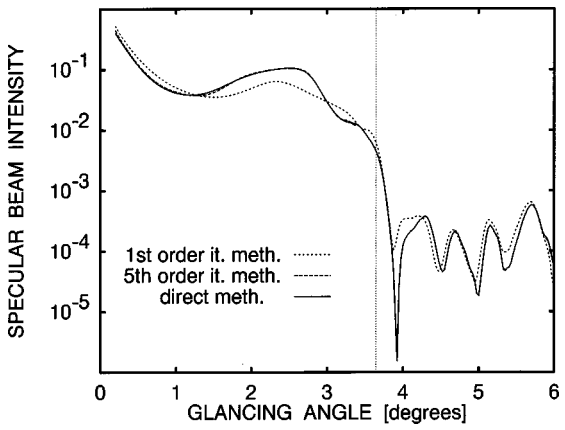

FIG. 1. The rocking curves for Pt(111) calculated using the iterative and direct methods. The dotted vertical line near 3.6° shows the side beam emergence condition.

To test our method we carried out iterative and direct calculations of rocking curves for Pt (111), for the azimuth $\langle 11\bar{2} \rangle$ and the electron energy of 19 keV. The real part of the potential was determined using electron scattering coefficients tabulated by Jiang and Li,[8] assuming thermal vibrations typical for 300 K. The imaginary part of the potential was taken in the form of the real part multiplied by factor of 0.2. The calculations were carried out for 37 beams from 5 Laue zones. In iterative calculations we considered slices with the thickness of about 0.07 Å and we fixed the number L of a single-slice iterations to be equal to 4. The time required to complete each multislice scheme iteration turned out to be about equal to a quarter of the time required for the direct method.

We computed the curves for glancing angles between 0.025° and 6.0° at steps of 0.025°. For the angles of 0.025° and 0.050° the iteration sequence does not converge. For angles between 0.075° and 0.175° the convergence occurs but is very slow (for example, for 0.1° after completing 10 multislice scheme iterations, we still observe variations in the specular beam intensity exceeding 20% of the precise value). However, for angular points from the range of 0.2° to 6.0° the convergence is fast. Respectively, for the range of 0.2° to 6.0° we show in Fig. 1 two curves obtained after completing 1 and 5 multislice scheme iterations, together with a curve calculated by the direct method. We can see that the curve obtained for 1 iteration constitutes only a qualitative approximation of the exact results. However, the curve for 5 iterations can hardly be distinguished from the direct method curve. If the number of iterations exceeds 10 then the respective curves are in excellent agreement and on the scale

of Fig. 1 we could not see any differences. We can add that the same situation happens for other beams.

Let us discuss now the most important features of our method more generally. It is clear from the results presented in this paper that apart from the region of very small glancing angles the iteration sequence may converge very quickly. Nevertheless, one should also admit that the lack of a good convergence may occur in principle for any angle. We have found that the convergence improves if the magnitude of the real part of the potential is made smaller and/or of the imaginary part larger. Subsequently if we use the proportional model of the potential (i.e., the imaginary part is proportional to the real part) then for lighter elements than Pt a number of situations may happen. Usually for light elements the convergence is very rapid; however, sometimes the method may fail to work at all. The latter situations seem to be related to resonance scattering. Taking a larger imaginary part of the potential may lead to convergence in such situations. Concerning the computer time needed, we can say that in the course of computations only operations, which scale in time like N^2 occur. However, if the number of beams is less than 100, our method cannot be practically faster than the traditional direct methods if precise results are required. For example, for the direct method used by the author[3] most of the computation time is spent in finding transfer matrices by the integration of differential equations. We can estimate that the time required is about equal to $2cN^3$, where c is some factor depending on thickness of the crystal. For the same conditions using the iterative method, to complete k multislice scheme iterations we require the time about equal to $4ckLN^2$, where c is the same constant and L is the number of iterations executed in the single-slice scheme. We have omitted possible benefits from considering crystal symmetries, but actually they may be slightly larger for the direct method. Thus, if we require precise results (for $L=4$ we should take $k\simeq 10$) iterative computations are potentially faster than traditional ones if the number of beams N exceeds 100–500. Finally, it seems that the biggest advantage of our iterative method is that it is especially convenient for developing approximate approaches. Namely, we can limit the number of iterations executed in both schemes, ignore coupling between certain beams (or groups of beams) and additionally combine iterative computations with direct ones for crystal-bulk layers. For example if we limit ourselves to executing only one iteration in both schemes ($L=1$ and $k=1$) then we get an approximation, which is very similar to the kinematical approaches used by Knibb[9] and by Mitura, Dudarev, and Whelan.[10]

In summary, a dynamical method of calculating RHEED intensity has been proposed.

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