Theory of reflection high-energy electron diffraction

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We present a new scheme to calculate reflection high-energy electron-diffraction rocking curves based on the technique to solve coupled second-order differential equations developed by Magnus and others. Furthermore, a layer-doubling method, which was originally developed for the low-energy electron diffraction, is incorporated into this scheme very naturally.

I. INTRODUCTION

Reflection high-energy electron diffraction (RHEED) (Ref. 1) is a structural analysis technique that is routinely adopted for use in molecular-beam-epitaxy (MBE) systems. In RHEED, the electron energy is in the range 10–40 keV. Therefore, ordinary techniques utilized in low-energy electron diffraction (LEED) (Refs. 2–4) are no longer practical. Since LEED theories are constructed based on the electron-scattering partial waves in angular momentum space, many partial waves are needed in order to obtain a reliable answer. Usually, LEED is used in the energy range 20–200 eV. Thus, in the very-high-energy range for RHEED analysis, only the plane-wave method can become a feasible technique. Nonetheless, constructing a practical RHEED theory is a very difficult task because so many plane waves participate in the scattering process, and some of the transmitted waves can penetrate deep into the solid.

Until now, several theories to calculate RHEED rocking curves have been proposed. For example, Maksym and Beeby[5] proposed a theory based on the Sams-Kouri method.[6] Their method is fast, but the evanescent waves bring about the numerical instability problem. So Maksym[7] has used the layer-doubling technique originally introduced in LEED (Ref. 2) to stabilize the numerical calculation. However, since Maksym and Beeby have chosen to separate the coefficients and exponential parts of the plane waves, phase matching becomes a sensitive part as with the LEED analysis. Peng and Cowley[8] proposed a method to slice a slab normal to the surface. Their method has an advantage in handling a step, but considerable computing time may be required. On the other hand, Zao, Poon, and Tong[9] proposed a theory to use the R matrix, recursively. They have adopted a technique to solve the coupled second-order differential equations developed by Stechel *et al.*;[10] furthermore, a temperature correction was also discussed. Since the R-matrix method handles plane waves without separating the coefficients and exponential part, numerical instability does not appear. However, the R-matrix method requires us to choose the position to start the recursion process. Thus, until we get the converged reflectivity, by choosing a new starting point, we have to repeat the recursion process for the R matrix. In this paper, we propose a new scheme to calculate a RHEED rocking curve without separating the plane wave into two parts, as was done by Zao *et al.*, and illustrate how the layer-doubling method can be incorporated into the new scheme.

In Sec. II, we derive the scattering matrices for a slab using the technique for solving coupled second-order differential equations developed by Magnus and others[11,12] rather than that by Stechet *et al.* In Sec. III, those scattering matrices will be combined with the layer-doubling method very naturally. Furthermore, we will explain how flexible and efficient the new method is. Finally, a brief summary is given in Sec. IV.

II. ELECTRON SCATTERING BY A SLAB

In the presence of the periodicity in x-y plane, the electron-ion interaction potential can be expanded in Fourier series as (see Appendix A for details)

$$V(\mathbf{r})=\sum_{\mathbf{g}} V_{\mathbf{g}}(z)e^{i\mathbf{g}\cdot\rho} , \tag{1}$$

where $\mathbf{g}=(g_x,g_y)$ are the two-dimensional reciprocal-lattice vectors, and $\rho=(x,y)$. When an incident electron has the wave vector $(\mathbf{k}_{\parallel},k_z)$, the scattered electron wave function by $V(\mathbf{r})$ takes the form

$$\Psi(\mathbf{r})=\sum_{\mathbf{g}} \phi_{\mathbf{g}}(z)e^{i(\mathbf{k}_{\parallel}+\mathbf{g})\cdot\rho} . \tag{2}$$

Substituting Eq. (2) into the Schrödinger equation

$$-\frac{\hbar^2}{2m}\nabla^2\Psi+V\Psi=E\Psi , \tag{3}$$

we obtain the following coupled second-order differential equations:

$$\frac{d^2\phi_{\mathbf{g}}(z)}{dz^2}=\sum_{\mathbf{g}} W_{\mathbf{g}\mathbf{g}}(z)\phi_{\mathbf{g}'}(z) , \tag{4}$$

where

$$W_{\mathbf{g}\mathbf{g}'}(z)=\frac{2m}{\hbar^2}V_{\mathbf{g}-\mathbf{g}'}(z)-k_{\mathbf{g}}^2\delta_{\mathbf{g}\mathbf{g}'} \tag{5}$$

with

$$k_{\mathbf{g}}^2=\frac{2m}{\hbar^2}E-(\mathbf{k}_{\parallel}+\mathbf{g})^2 . \tag{6}$$

Equation (6) has two solutions for $k_{\mathbf{g}}$, but we adopt $k_{\mathbf{g}}$,

which has a positive or zero real part in this paper. Here, E is the incident electron energy; m is the electron mass; and $\hbar$ is Planck's constant divided by 2π. Introducing the column vector Φ as

$$\Phi=\begin{bmatrix}\phi_{g_1}(z)\\ \phi_{g_2}(z)\\ \cdots\end{bmatrix}. \tag{7}$$

We can rewrite Eq. (4) as

$$\frac{d^2\Phi}{dz^2}=\tilde{W}\Phi\ , \tag{8}$$

or

$$\frac{d}{dz}\begin{bmatrix}\Phi\\ \dfrac{d\Phi}{dz}\end{bmatrix}=\begin{bmatrix}\tilde{0} & \tilde{I}\\ \tilde{W} & \tilde{0}\end{bmatrix}\begin{bmatrix}\Phi\\ \dfrac{d\Phi}{dz}\end{bmatrix}, \tag{9}$$

where $\tilde{I}$ is the unit matrix, $\tilde{0}$ is the zero matrix, $\mathbf{g}_1=\mathbf{0}$, and $(\tilde{W})_{gg'}=W_{gg'}$. Defining a column vector $\bar{\Phi}$ to combine Φ and its derivative as

$$\bar{\Phi}=\begin{bmatrix}\Phi\\ \dfrac{d\Phi}{dz}\end{bmatrix}, \tag{10}$$

Eq. (9) can be written simply as

$$\frac{d}{dz}\bar{\Phi}=\begin{bmatrix}\tilde{0} & \tilde{I}\\ \tilde{W} & \tilde{0}\end{bmatrix}\bar{\Phi}\ . \tag{11}$$

The solution of Eq. (11) is formally written as[11,12]

$$\bar{\Phi}(z_l+\tfrac{1}{2}h_l)\simeq\exp\begin{bmatrix}\tilde{0} & h_l\tilde{I}\\ h_l\tilde{W}(z_l) & 0\end{bmatrix}\bar{\Phi}(z_l-\tfrac{1}{2}h_l)\ , \tag{12}$$

where $h_l=z_l-z_{l-1}$. For simplicity, let us divide the system shown in Fig. 1 equally into $(n-1)$ slices. Namely, $h=z_i-z_{l-1}=(0-z_0)/(n-1)$, $z_1+\frac{1}{2}h=z_0$, and $z_n+\frac{1}{2}h=0$, where $z=0$ and z_0 are the coordinates of top and bottom of the system, respectively. Equation (12) now becomes

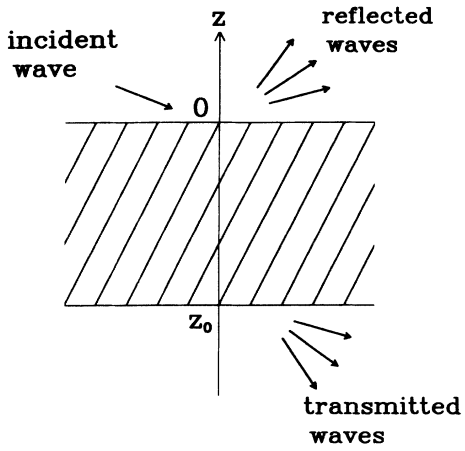

FIG. 1. Schematic view of the electron scattering.

$$\bar{\Phi}(z_l+\tfrac{1}{2}h)\simeq\exp\begin{bmatrix}\tilde{0} & h\tilde{I}\\ h\tilde{W}(z_l) & \tilde{0}\end{bmatrix}\bar{\Phi}(z_{l-1}+\tfrac{1}{2}h)\ , \tag{13}$$

or

$$\bar{\Phi}(i)\simeq M_l\bar{\Phi}(i-1)\ , \tag{14}$$

where

$$M_i=\exp\begin{bmatrix}\tilde{0} & h\tilde{I}\\ h\tilde{W}(z_l) & \tilde{0}\end{bmatrix}. \tag{15}$$

Using Eq. (14) repeatedly, we have

$$\bar{\Phi}(n)=M_n\bar{\Phi}(n-1)\cdots=M_nM_{n-1}\cdots M_2\bar{\Phi}(1)=B\bar{\Phi}(1), \tag{16}$$

where

$$\begin{aligned}B&=M_nM_{n-1}\cdots M_2\\ &=\begin{bmatrix}\tilde{U}_n & \tilde{0}\\ \tilde{0} & \tilde{U}_n\end{bmatrix}\begin{bmatrix}\tilde{U}_n^{-1} & \tilde{0}\\ \tilde{0} & \tilde{U}_n^{-1}\end{bmatrix}M_n\begin{bmatrix}\tilde{U}_n & \tilde{0}\\ \tilde{0} & \tilde{U}_n\end{bmatrix}\begin{bmatrix}\tilde{U}_n^{-1} & \tilde{0}\\ \tilde{0} & \tilde{U}_n^{-1}\end{bmatrix}\cdots\begin{bmatrix}\tilde{U}_2 & \tilde{0}\\ \tilde{0} & \tilde{U}_2\end{bmatrix}\begin{bmatrix}\tilde{U}_2^{-1} & \tilde{0}\\ \tilde{0} & \tilde{U}_2^{-1}\end{bmatrix}M_2\begin{bmatrix}\tilde{U}_2 & \tilde{0}\\ \tilde{0} & \tilde{U}_2\end{bmatrix}\begin{bmatrix}\tilde{U}_2^{-1} & \tilde{0}\\ \tilde{0} & \tilde{U}_2^{-1}\end{bmatrix}\\ &=\begin{bmatrix}\tilde{U}_n & \tilde{0}\\ \tilde{0} & \tilde{U}_n\end{bmatrix}\begin{bmatrix}\cosh(h\lambda_n) & \lambda_n^{-1}\sinh(h\lambda_n)\\ \lambda_n\sinh(h\lambda_n) & \cosh(h\lambda_n)\end{bmatrix}\begin{bmatrix}\tilde{U}_n^{-1} & \tilde{0}\\ \tilde{0} & \tilde{U}_n^{-1}\end{bmatrix}\times\cdots\\ &\quad\times\begin{bmatrix}\tilde{U}_2 & \tilde{0}\\ \tilde{0} & \tilde{U}_2\end{bmatrix}\begin{bmatrix}\cosh(h\lambda_2) & \lambda_2^{-1}\sinh(h\lambda_2)\\ \lambda_2\sinh(h\lambda_2) & \cosh(h\lambda_2)\end{bmatrix}\begin{bmatrix}\tilde{U}_2^{-1} & \tilde{0}\\ \tilde{0} & \tilde{U}_2^{-1}\end{bmatrix}\\ &=\begin{bmatrix}\tilde{B}_{11} & \tilde{B}_{12}\\ \tilde{B}_{21} & \tilde{B}_{22}\end{bmatrix},\end{aligned} \tag{17}$$

$\tilde{U}$ is the unitary matrix which diagonalizes $\tilde{V}(z)$ $\{[\tilde{V}(z)]_{gg'}=\tilde{V}_{g-g'}(z)\}$, and $\tilde{W}$ is also diagonalized by the same $\tilde{U}$ (see Appendix B for details), $\tilde{B}_{ij}$ are defined in Eq. (17), and $[f(\lambda)]_{g_i g_j}=f(\lambda_i)\delta_{ij}$ for any form of function, f, of λ. Equation (16) is then written as

$$\begin{bmatrix} \Phi(n) \\ [\Phi(n)]' \end{bmatrix} = \begin{bmatrix} \tilde{B}_{11} & \tilde{B}_{12} \\ \tilde{B}_{21} & \tilde{B}_{22} \end{bmatrix} \begin{bmatrix} \Phi(1) \\ [\Phi(1)]' \end{bmatrix} . \tag{18}$$

Using the proper boundary conditions, we can determine the unique electron-scattering wave function.

Now, let us study further the following two scattering cases, shown in Fig. 2, so as to reduce the computing time by taking into account the character of $V_g(z)$. The first one is where the incident electron comes from above the slab (case I), and the second one is where it comes from below the slab (case II). In both cases, $h=(z_A-z_B)/(n-1)$ is used.

In case I, the electron wave function is written as

$$\psi_1^-(\mathbf{r})=\begin{cases} e^{i\mathbf{k}_\parallel\cdot\rho-ik_{g_1}z}+\sum_g r^-_{gg_1}e^{i(\mathbf{k}_\parallel+\mathbf{g})\cdot\rho+ik_g z}, & z\geq z_A \quad (19a) \\ \sum_g t^-_{gg_1}e^{i(\mathbf{k}_\parallel+\mathbf{g})\cdot\rho-ik_g z}, & z\leq z_B , \quad (19b) \end{cases}$$

where $r^-_{gg_1}$ and $t^-_{gg_1}$ are coefficients of reflected and transmitted waves, respectively. At $z=z_B$ $(=z_1+\frac{1}{2}h)$, the electron wave function and its derivative are

$$\Phi_1(1)=\begin{bmatrix} t^-_{g_1g_1}e^{-ik_{g_1}z_B} \\ \vdots \\ t^-_{g_Ng_1}e^{-ik_{g_N}z_B} \end{bmatrix} \tag{20}$$

and

$$[\Phi_1(1)]'=\begin{bmatrix} -ik_{g_1}t^-_{g_1g_1}e^{-ik_{g_1}z_B} \\ \vdots \\ -ik_{g_N}t^-_{g_Ng_1}e^{-ik_{g_N}z_B} \end{bmatrix}=-i\tilde{K}\Phi_1(1) , \tag{21}$$

respectively, where

$$\tilde{K}=\begin{bmatrix} k_{g_1} & & 0 \\ & \ddots & \\ 0 & & k_{g_N} \end{bmatrix} \tag{22}$$

is a diagonal matrix. On the other hand, after the calculation of $\tilde{B}_{ij}$ for this slab by Eq. (17), and using Eqs. (18)–(22), at $z=z_A$ $(=z_n+\frac{1}{2}h)$ the electron wave function and its derivative become

$$\begin{aligned} \Phi_1(n)&=\begin{bmatrix} e^{-ik_{g_1}z_A} \\ 0 \\ \vdots \\ 0 \\ 0 \end{bmatrix}+\begin{bmatrix} r^-_{g_1g_1}e^{ik_{g_1}z_A} \\ \vdots \\ r^-_{g_Ng_1}e^{ik_{g_N}z_A} \end{bmatrix} \\ &=\tilde{B}_{11}\Phi_1(1)+\tilde{B}_{12}[\Phi_1(1)]' \\ &=(\tilde{B}_{11}-i\tilde{B}_{12}\cdot\tilde{K})\Phi_1(1) \end{aligned} \tag{23}$$

and

$$\begin{aligned} [\Phi_1(n)]'&=-i\tilde{K}\begin{bmatrix} e^{-ik_{g_1}z_A} \\ 0 \\ \vdots \\ 0 \\ 0 \end{bmatrix}+i\tilde{K}\begin{bmatrix} r^-_{g_1g_1}e^{ik_{g_1}z_A} \\ \vdots \\ r^-_{g_Ng_1}e^{ik_{g_N}z_A} \end{bmatrix} \\ &=\tilde{B}_{21}\Phi_1(1)+\tilde{B}_{22}[\Phi_1(1)]' , \\ &=(\tilde{B}_{21}-i\tilde{B}_{22}\cdot\tilde{K})\Phi_1(1) , \end{aligned} \tag{24}$$

respectively. Equation (24) can be modified as

$$\begin{aligned} &i\tilde{K}^{-1}\cdot(\tilde{B}_{21}-i\tilde{B}_{22}\cdot\tilde{K})\Phi_1(1) \\ &=\begin{bmatrix} e^{-ik_{g_1}z_A} \\ 0 \\ \vdots \\ 0 \\ 0 \end{bmatrix}-\begin{bmatrix} r^-_{g_1g_1}e^{ik_{g_1}z_A} \\ \vdots \\ r^-_{g_Ng_1}e^{ik_{g_N}z_A} \end{bmatrix} . \end{aligned} \tag{25}$$

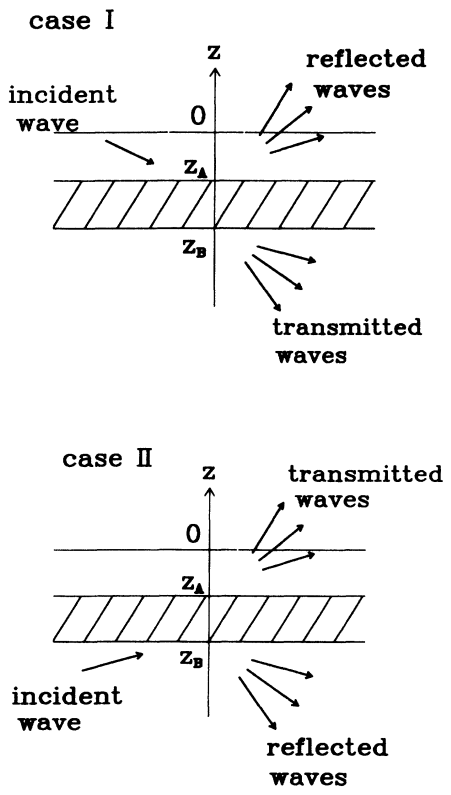

FIG. 2. Schematic view of the electron-scattering process for two cases: case I, where it comes from above the slab; case II, where it comes from below the slab.

Then, using Eqs. (23) and (25), we can obtain the formula for the transmitted waves:

$$\Phi_1(1)=\begin{pmatrix} t^{-}_{\mathbf{g}_1\mathbf{g}_1}e^{-ik_{\mathbf{g}_1}z_B} \\ \vdots \\ t^{-}_{\mathbf{g}_N\mathbf{g}_1}e^{-ik_{\mathbf{g}_N}z_B}\end{pmatrix}=\tilde{T}^{-}\begin{pmatrix} e^{-ik_{\mathbf{g}_1}z_A} \\ 0 \\ \vdots \\ 0 \\ 0\end{pmatrix}, \tag{26}$$

and that for the reflected waves:

$$\begin{pmatrix} r^{-}_{\mathbf{g}_1\mathbf{g}_1}e^{ik_{\mathbf{g}_1}z_A} \\ \vdots \\ r^{-}_{\mathbf{g}_N\mathbf{g}_1}e^{ik_{\mathbf{g}_N}z_A}\end{pmatrix}=\tilde{R}^{-}\begin{pmatrix} e^{-ik_{\mathbf{g}_1}z_A} \\ 0 \\ \vdots \\ 0 \\ 0\end{pmatrix}, \tag{27}$$

where

$$\tilde{T}^{-}=2[(\tilde{B}_{11}-i\tilde{B}_{12}\cdot\tilde{K})+i\tilde{K}^{-1}\cdot(\tilde{B}_{21}-i\tilde{B}_{22}\cdot\tilde{K})]^{-1} \tag{28}$$

and

$$\tilde{R}^{-}=[(\tilde{B}_{11}-i\tilde{B}_{12}\cdot\tilde{K})-i\tilde{K}^{-1}\cdot(\tilde{B}_{21}-i\tilde{B}_{22}\cdot\tilde{K})]\times[(\tilde{B}_{11}-i\tilde{B}_{12}\cdot\tilde{K})+i\tilde{K}^{-1}\cdot(\tilde{B}_{21}-i\tilde{B}_{22}\cdot\tilde{K})]^{-1}. \tag{29}$$

Equations (26) and (27) illustrate that $\tilde{T}^{-}$ and $\tilde{R}^{-}$ take care of the phase advance and change of every beam which is produced by incident $\mathbf{g}_1$ beam. When the whole system is treated as one slab, by setting $z_A=0$ and $z_B=z_0$, $(\tilde{R}^{-})_{\mathbf{g}\mathbf{g}_1}$ calculated by Eq. (29) has sufficient information to obtain the reflectivity. An important point is that $(\tilde{R}^{-})_{\mathbf{g}_i\mathbf{g}_j}$ and $(\tilde{T}^{-})_{\mathbf{g}_i\mathbf{g}_j}$ $(i=1,2,\ldots,N)$ have the scattering information not only for the $\mathbf{g}_1$ incident beam, but also for every $\mathbf{g}_j$ incident beam. If we remember how they were derived for the $\mathbf{g}_1$ beam, it may be easily understood. Namely, $\tilde{R}^{-}$ and $\tilde{T}^{-}$ have the complete information of every scattering process in case I.

Next, we consider the case where the incident electron comes below the slab (case II). The electron wave function can be written as

$$\psi_1^{+}(\mathbf{r})=\begin{cases} e^{i\mathbf{k}_\parallel\cdot\rho+ik_{\mathbf{g}_1}z}+\sum_{\mathbf{g}} r^{+}_{\mathbf{g}\mathbf{g}_1}e^{i(\mathbf{k}_\parallel+\mathbf{g})\cdot\rho-ik_{\mathbf{g}}z}, & z\le z_B \quad (30a) \\ \sum_{\mathbf{g}} t^{+}_{\mathbf{g}\mathbf{g}_1}e^{i(\mathbf{k}_\parallel+\mathbf{g})\cdot\rho+ik_{\mathbf{g}}z}, & z\ge z_A \quad (30b)\end{cases}$$

where $r^{+}_{\mathbf{g}\mathbf{g}_1}$ and $t^{+}_{\mathbf{g}\mathbf{g}_1}$ are coefficients of reflected and transmitted waves, respectively. At $z=z_A$, the electron wave function and its derivative become

$$\Phi_1(n)=\begin{pmatrix} t^{+}_{\mathbf{g}_1\mathbf{g}_1}e^{ik_{\mathbf{g}_1}z_A} \\ \vdots \\ t^{+}_{\mathbf{g}_N\mathbf{g}_1}e^{ik_{\mathbf{g}_N}z_A}\end{pmatrix} \tag{31}$$

and

$$[\Phi_1(n)]'=\begin{pmatrix} ik_{\mathbf{g}_1}t^{+}_{\mathbf{g}_1\mathbf{g}_1}e^{ik_{\mathbf{g}_1}z_A} \\ \vdots \\ ik_{\mathbf{g}_N}t^{+}_{\mathbf{g}_N\mathbf{g}_1}e^{ik_{\mathbf{g}_N}z_Z}\end{pmatrix}=i\tilde{K}\Phi_1(n), \tag{32}$$

respectively. From (16), $\bar{\Phi}_1(1)$ is connected with $\bar{\Phi}_1(n)$ as follows:

$$\bar{\Phi}_1(1)=M_2^{-1}\bar{\Phi}_1(2)\cdots=M_2^{-1}M_3^{-1}\cdots M_n^{-1}\bar{\Phi}_1(N)=B^{-1}\bar{\Phi}_1(n). \tag{33}$$

Defining

$$B^{-1}=\begin{pmatrix}\tilde{b}_{11} & \tilde{b}_{12} \\ \tilde{b}_{21} & \tilde{b}_{22}\end{pmatrix}, \tag{34}$$

and using Eqs. (31) and (32), Eq. (33) can be written as

$$\Phi_1(1)=\begin{pmatrix} e^{ik_{\mathbf{g}_1}z_B} \\ 0 \\ \vdots \\ 0 \\ 0\end{pmatrix}+\begin{pmatrix} r^{+}_{\mathbf{g}_1\mathbf{g}_1}e^{-ik_{\mathbf{g}_1}z_B} \\ \vdots \\ r^{+}_{\mathbf{g}_N\mathbf{g}_1}e^{-ik_{\mathbf{g}_N}z_B}\end{pmatrix}$$
$$=\tilde{b}_{11}\Phi_1(n)+\tilde{b}_{12}[\Phi_1(n)]'$$
$$=(\tilde{b}_{11}+i\tilde{b}_{12}\cdot\tilde{K})\Phi_1(n) \tag{35}$$

and

$$[\Phi_1(1)]'=i\tilde{K}\begin{pmatrix} e^{ik_{\mathbf{g}_1}z_B} \\ 0 \\ \vdots \\ 0 \\ 0\end{pmatrix}-i\tilde{K}\begin{pmatrix} r^{+}_{\mathbf{g}_1\mathbf{g}_1}e^{-ik_{\mathbf{g}_1}z_B} \\ \vdots \\ r^{+}_{\mathbf{g}_N\mathbf{g}_1}e^{-ik_{\mathbf{g}_N}z_B}\end{pmatrix}$$
$$=\tilde{b}_{21}\Phi_1(n)+\tilde{b}_{22}[\Phi_1(n)]'$$
$$=(\tilde{b}_{21}+i\tilde{b}_{22}\cdot\tilde{K})\Phi_1(n). \tag{36}$$

Equation (36) can also be modified as

$$i\tilde{K}^{-1}\cdot(\tilde{b}_{21}+i\tilde{b}_{22}\cdot\tilde{K})\Phi_1(n)=-\begin{pmatrix} e^{ik_{\mathbf{g}_1}z_B} \\ 0 \\ \vdots \\ 0 \\ 0\end{pmatrix}+\begin{pmatrix} r^{+}_{\mathbf{g}_1\mathbf{g}_1}e^{-ik_{\mathbf{g}_1}z_B} \\ \vdots \\ r^{+}_{\mathbf{g}_N\mathbf{g}_1}e^{-ik_{\mathbf{g}_N}z_B}\end{pmatrix}. \tag{37}$$

From Eqs. (35) and (37), we can obtain the formula for the transmitted waves:

$$\Phi_1(n)=\begin{pmatrix} t^{+}_{\mathbf{g}_1\mathbf{g}_1}e^{ik_{\mathbf{g}_1}z_A} \\ \vdots \\ t^{+}_{\mathbf{g}_N\mathbf{g}_1}e^{ik_{\mathbf{g}_N}z_A}\end{pmatrix}=\tilde{T}^{+}\begin{pmatrix} e^{ik_{\mathbf{g}_1}z_B} \\ 0 \\ \vdots \\ 0 \\ 0\end{pmatrix} \tag{38}$$

and that for the reflected waves:

$$\begin{pmatrix} r^{+}_{\mathbf{g}_1\mathbf{g}_1} e^{-ik_{\mathbf{g}_1} z_B} \\ \vdots \\ r^{+}_{\mathbf{g}_N\mathbf{g}_1} e^{-ik_{\mathbf{g}_N} z_B} \end{pmatrix} = \tilde{R}^{+} \begin{pmatrix} e^{ik_{\mathbf{g}_1} z_B} \\ 0 \\ \vdots \\ 0 \\ 0 \end{pmatrix}, \tag{39}$$

where

$$\tilde{T}^{+} = 2[(\tilde{b}_{11} + i\tilde{b}_{12}\cdot\tilde{K}) - i\tilde{K}^{-1}\cdot(\tilde{b}_{21} + i\tilde{b}_{22}\cdot\tilde{K})]^{-1} \tag{40}$$

and

$$\tilde{R}^{+} = [(\tilde{b}_{11} + i\tilde{b}_{12}\cdot\tilde{K}) + i\tilde{K}^{-1}\cdot(\tilde{b}_{21} + i\tilde{b}_{22}\cdot\tilde{K})] \times [(\tilde{b}_{11} + i\tilde{b}_{12}\cdot\tilde{K}) - i\tilde{K}^{-1}\cdot(\tilde{b}_{21} + i\tilde{b}_{22}\cdot\tilde{K})]^{-1} . \tag{41}$$

Similarly to case I, Eqs. (40) and (41) take care of phase advance and change of every beam, and the complete scattering processes for any **g** incident beam in case II are included in $\tilde{T}^{+}$ and $\tilde{R}^{+}$. Let us illustrate in the next section how the computing time for the RHEED analysis can be reduced by using those scattering matrices given by Eqs. (28), (29), (40), and (41).

III. LAYER-DOUBLING METHOD

Let us consider the scattering matrices for the combined system of two slabs as can be seen from Fig. 3. In LEED, since the scattering matrices are calculated at the center of the slab, phase matching becomes sensitive.

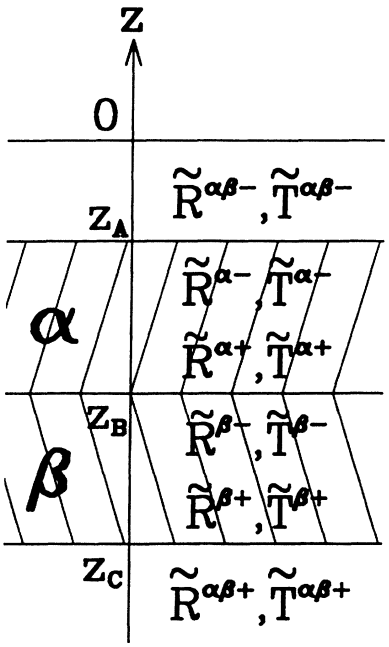

FIG. 3. Layer-doubling scheme of slab α and slab β, where $\tilde{R}^{\alpha-}, \tilde{T}^{\alpha-}$ and $\tilde{R}^{\beta-}, \tilde{T}^{\beta-}$ are scattering matrices defined in Eqs. (28) and (29) for case I. $\tilde{R}^{\alpha+}, \tilde{T}^{\alpha+}$ and $\tilde{R}^{\beta+}$ are those defined in Eqs. (39) and (40) for case II. Furthermore, $\tilde{R}^{\alpha\beta-}, \tilde{T}^{\alpha\beta-}$ and $\tilde{R}^{\alpha\beta+}, \tilde{T}^{\alpha\beta+}$ are those for the combined slab.

But, since Eqs. (28), (29), (40), and (41) take care of the phase advance automatically, we can use the layer-doubling method of LEED without worrying about the phase matching at all. According to the layer-doubling scheme, scattering matrices in cases I and II are given by

$$\tilde{R}^{\alpha\beta-} = \tilde{R}^{\alpha-} + \tilde{T}^{\alpha+}\tilde{R}^{\beta-}(\tilde{I} - \tilde{R}^{\alpha+}\tilde{R}^{\beta-})^{-1}\tilde{T}^{\alpha-} , \tag{42}$$

$$\tilde{T}^{\alpha\beta-} = \tilde{T}^{\beta-}(\tilde{I} - \tilde{R}^{\alpha+}\tilde{R}^{\beta-})^{-1}\tilde{T}^{\alpha-} , \tag{43}$$

and

$$\tilde{R}^{\alpha\beta+} = \tilde{R}^{\beta+} + \tilde{T}^{\beta-}\tilde{R}^{\alpha+}(\tilde{I} - \tilde{R}^{\beta-}\tilde{R}^{\alpha+})^{-1}\tilde{T}^{\beta+} , \tag{44}$$

$$\tilde{T}^{\alpha\beta+} = \tilde{T}^{\alpha+}(\tilde{I} - \tilde{R}^{\beta-}\tilde{R}^{\alpha+})^{-1}\tilde{T}^{\beta+} , \tag{45}$$

respectively, where α and β denote the respective slabs. Equations (42)–(45) have very clear physical meanings. The scattering process should be interpreted from right to left in those equations. For case I, $\tilde{R}^{\alpha\beta-}$ includes the following processes: namely, the incident electron is simply reflected by slab α, or transmits slab α, and after repeating the multiple scattering between slab α and slab β, is reflected by slab β and transmits slab α. Similarly, the following processes are included in $\tilde{T}^{\alpha\beta-}$. Namely, the incident electron transmits slab α and then slab β, or transmits slab α and, after repeating multiple scattering between slab β and slab α, transmits slab β. It may also be easy to find the scattering processes included in $\tilde{R}^{\alpha\beta+}$ and $\tilde{T}^{\alpha\beta+}$ for case II. Since the present theory is naturally incorporated into the layer-doubling scheme, we can reduce the computing time considerably in RHEED analysis as follows. As shown in Fig. 4, we divide the solid into two domains. In domain I, the crystal potential is not periodic in the z direction, but in domain II the crystal has periodic potential in the z direction. Then, treating domain I as a set, we calculate scattering matrices. However, in domain II we calculate them only once for one period of the potential because other scattering matrices are identical due to the periodicity of the potential in the z direction. We then use Eqs. (42)–(45), repeatedly, from the top slab to deep inside the solid until the converged $\tilde{R}^{-}$ is obtained. Considering that the amplitude is proportional to the velocity of an electron, the

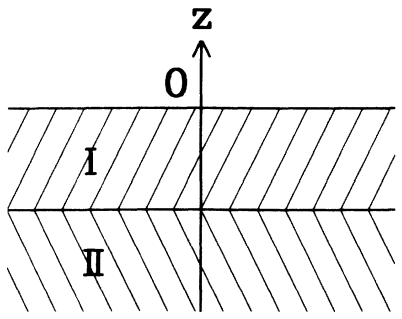

FIG. 4. Domain I, nonperiodic potential domain in the z direction; domain II, periodic potential domain in the z direction.

reflectivity can be obtained by

$$R_{\mathrm{g}}^{\mathrm{ref}}=\left|\frac{k_{\mathrm{g}}}{k_{\mathrm{g}_1}}(\tilde{R}^{-})_{\mathrm{gg}_1}\right|^2 . \tag{46}$$

Similarly, the transmittability can be obtained by

$$T_{\mathrm{g}}^{\mathrm{tras}}=\left|\frac{k_{\mathrm{g}}}{k_{\mathrm{g}_1}}(\tilde{T}^{-})_{\mathrm{gg}_1}\right|^2 . \tag{47}$$

In the case of thin film, $(\tilde{R}^{-})_{\mathrm{gg}_1}$ and $(\tilde{T}^{-})_{\mathrm{gg}_1}$ given by Eqs. (28) and (29) are sufficient to calculate Eqs. (46) and (47).

IV. SUMMARY

We have proposed a new method for RHEED analysis. Since our method takes care of phase advance of the scattering waves automatically, the layer-doubling scheme is incorporated into it very naturally. We can then be very flexible in choosing the way to implement the calculation of RHEED rocking curves.

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APPENDIX A: CALCULATION OF $V_{\mathrm{g}}(z)$

Since the electron form factor can be fitted approximately by a sum of Gaussian functions as[13]

$$f(\mathbf{G})=\frac{2\pi me}{h^2}\int v(\mathbf{r})\exp(i\mathbf{G}\cdot\mathbf{r})d^3r = \sum_{i=1}^{n} a_i\exp\left[-\frac{b_i}{16\pi^2}G^2\right] , \tag{A1}$$

we use it to calculate $V_{\mathrm{g}}(z)$, where $v(\mathbf{r})$ is the electron-ion interaction potential. Thus, after the Fourier transform in x-y plane, we can obtain

$$\begin{aligned} V_{\mathrm{g}}(z)&=\frac{1}{A}\int\sum_{\mathbf{R}}^{w} v(\mathbf{r}-\mathbf{R})\exp(i\mathbf{g}\cdot\boldsymbol{\rho})d\boldsymbol{\rho} \\ &=\frac{1}{a}\sum_{\mathbf{R}}^{u}\int v(\boldsymbol{\rho},z-R_z)\exp(i\mathbf{g}\cdot\boldsymbol{\rho})d\boldsymbol{\rho}\exp(-i\mathbf{g}\cdot\mathbf{R}_{\parallel}) \\ &=-\frac{a_0^2}{a}(2\ \mathrm{Ry})_y\sum_{\mathbf{R}}^{u}\int f(\mathbf{g},G_z)\exp[-iG_z(z-R_z)]dz\exp(-i\mathbf{g}\cdot\mathbf{R}_{\parallel}) \\ &=-\frac{a_0^2}{a}(2\ \mathrm{Ry})\sum_{\mathbf{R}}^{u}\left[\sum_{i=1}^{n} a_i\left[\frac{\pi}{b_i}\right]^{1/2}\exp\left[-b_ig^2-\frac{(z-R_z)^2}{4b_i}\right]\right]\exp(-i\mathbf{g}\cdot\mathbf{R}_{\parallel}) , \end{aligned} \tag{A2}$$

where $\mathbf{R}$ are the ion coordinates; A, the total area; a the area of a unit cell; a_0 the Bohr radius; and Ry the rydberg. In Eq. (A2), $\sum^{w}$ and $\sum^{u}$ indicate that summation is done in the whole volume, or in the unit cell, respectively. In RHEED, inelastic damping of the electron scattering is included by replacing $V_{\mathrm{g}}(z)$ given in Eq. (A2) by $(1+i\epsilon)V_{\mathrm{g}}(z)$. Usually, $\epsilon=0.1$ is taken.

APPENDIX B: CALCULATION OF EQ. (15)

$\tilde{W}(z)$ is not in general a Hermitian matrix. However, since $[\tilde{V}(z)]_{\mathrm{gg}'}=V_{\mathrm{g}-\mathrm{g}'}(z)$, given by Eq. (A2), forms a Hermitian matrix, the unitary matrix, $\tilde{U}$, to diagonalize $\tilde{V}(z)$ can be found. Even if we include the inelastic damping by replacing $V_{\mathrm{g}}(z)$ by $(1+i\epsilon)V_{\mathrm{g}}(z)$, the same matrix $\tilde{U}$ can diagonalize $(1+i\epsilon)\tilde{V}(z)$. Besides, $-k_{\mathrm{g}}^2\delta_{\mathrm{gg}'}$ is already diagonal. Therefore, as Zao *et al.* have pointed out, the same matrix can diagonalize $\tilde{W}(z)$, too. Then, $\tilde{W}(z)$ can be diagonalized as follows:

$$\tilde{U}^{-1}\tilde{W}(z)\tilde{U}=\begin{pmatrix}\lambda_1^2 & 0 & 0\\ 0 & \lambda_2^2 & 0\\ & & \ddots\\ 0 & & \lambda_N^2\end{pmatrix}\equiv\lambda^2 , \tag{B1}$$

where using the eigenvalues of $\tilde{V}(z)$, λ_{0i}, λ_i^2 can be written as follows:

$$\lambda_i^2=\frac{2m}{\hbar^2}(1+i\epsilon)\lambda_{0i}-k_{\mathrm{g}_i}^2 . \tag{B2}$$

Defining a matrix $\tilde{X}$ as

$$\tilde{X}=\begin{pmatrix}\tilde{0} & h\tilde{I}\\ h\tilde{W}(z) & \tilde{0}\end{pmatrix} , \tag{B3}$$

we can conduct the following calculations:

$$\begin{aligned}
\begin{bmatrix} \tilde{U}^{-1} & \tilde{0} \\ \tilde{0} & \tilde{U}^{-1} \end{bmatrix} \exp X \begin{bmatrix} \tilde{U} & \tilde{0} \\ \tilde{0} & \tilde{U} \end{bmatrix} &= \begin{bmatrix} \tilde{U}^{-1} & \tilde{0} \\ \tilde{0} & \tilde{U}^{-1} \end{bmatrix} \left[\tilde{I} + \tilde{X} + \frac{\tilde{X}^2}{2!} + \cdots \right] \begin{bmatrix} \tilde{U} & \tilde{0} \\ \tilde{0} & \tilde{U} \end{bmatrix} \\
&= \begin{bmatrix} \tilde{I} & \tilde{0} \\ \tilde{0} & \tilde{I} \end{bmatrix} + \frac{h^2}{2!} \begin{bmatrix} \lambda^2 & \tilde{0} \\ \tilde{0} & \lambda^2 \end{bmatrix} + \frac{h^2}{4!} \begin{bmatrix} \lambda^2 & \tilde{0} \\ \tilde{0} & \lambda^2 \end{bmatrix} + \cdots \\
&\quad + h \begin{bmatrix} \tilde{0} & \tilde{I} \\ \lambda^2 & \tilde{0} \end{bmatrix} \left[\begin{bmatrix} \tilde{I} & \tilde{0} \\ \tilde{0} & \tilde{I} \end{bmatrix} + \frac{h^3}{3!} \begin{bmatrix} \lambda^2 & \tilde{0} \\ \tilde{0} & \lambda^2 \end{bmatrix} + \frac{h^5}{5!} \begin{bmatrix} \lambda^4 & \tilde{0} \\ \tilde{0} & \lambda^4 \end{bmatrix} + \cdots \right] \\
&= \begin{bmatrix} \cosh(h\lambda) & \tilde{0} \\ \tilde{0} & \cosh(h\lambda) \end{bmatrix} + \begin{bmatrix} \tilde{0} & h\tilde{I} \\ h\lambda^2 & \tilde{0} \end{bmatrix} \begin{bmatrix} (h\lambda)^{-1}\sinh(h\lambda) & \tilde{0} \\ \tilde{0} & (h\lambda)^{-1}\sinh(h\lambda) \end{bmatrix} \\
&= \begin{bmatrix} \cosh(h\lambda) & \lambda^{-1}\sinh(h\lambda) \\ \lambda\sinh(h\lambda) & \cosh(h\lambda) \end{bmatrix} . \qquad \text{(B4)}
\end{aligned}$$

Therefore, we can obtain

$$M = \begin{bmatrix} \tilde{U} & \tilde{0} \\ \tilde{0} & \tilde{U} \end{bmatrix} \begin{bmatrix} \cosh(h\lambda) & \lambda^{-1}\sinh(h\lambda) \\ \lambda\sinh(h\lambda) & \cosh(h\lambda) \end{bmatrix} \begin{bmatrix} \tilde{U}^{-1} & \tilde{0} \\ \tilde{0} & \tilde{U}^{-1} \end{bmatrix} , \qquad \text{(B5)}$$

where $[f(\lambda)]_{ij} = f(\lambda_i)\delta_{ij}$ for any type of function of λ.

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