Dynamical calculations for RHEED from MBE growing surfaces. I. Growth on a low-index surface

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Dynamical diffraction calculations have been made for reflection high-energy electron diffraction (RHEED) from molecular beam epitaxy (MBE) growing surfaces. Effects due to both the diffraction and growth conditions on the RHEED intensity oscillations during MBE growth have been investigated in detail for perfect layer growth, non-diffusive, diffusive growth, and distributed growth on a low-index surface. The results are compared with the kinematic diffraction theory, and are shown to be able to reproduce almost all features of measured RHEED intensity oscillations from low-index surfaces.

1. Introduction

Molecular beam epitaxy (MBE) has become well established as one of the most powerful and versatile techniques for growing thin epitaxial structures made of semiconductors, metals and insulators (Herman & Sitter 1989; Chang & Ploog 1985). The experimental arrangement of MBE is unique among epitaxial thin film preparation methods in that it enables significantly more precise control of the beam fluxes and growth conditions, and allows the studies and control of the growth process in situ in several ways, using reflection high-energy electron diffraction (RHEED) (Larsen & Dobson 1988), ultraviolet photoelectron spectroscopy (Williams et al. 1980) and ellipsometry (Demay et al. 1987; Collins & Cavese 1987). In particular the technique of RHEED intensity oscillations (Harris et al. 1981; Wood 1981) has been used routinely, among other things, to calibrate beam fluxes and alloy composition and to control the thicknesses of quantum wells and superlattice layers. Furthermore, it has been shown that RHEED intensity oscillations also provide a means of studying the mechanisms of crystal growth, and of determining the kinetics of surface diffusion and dopant incorporation under the conditions of MBE (see articles in Larsen & Dobson (1988)).

Although the occurrence of the strong oscillations of RHEED intensity with growth has become an experimentally well-established fact, the theoretical interpretations (Harris et al. 1981; Lent & Cohen 1984; Kawamura et al. 1984; Ichimiya 1987) are still not quite satisfactory and are indeed controversial. In the first place the Philips group (Harris et al. 1981; Joyce et al. 1988) has used a dynamical argument, treating diffraction as a multiple scattering process, and attributed the oscillations in RHEED intensity during steady-state growth to a periodically varying contribution of inelastic or incoherent processes. On the other hand, Cohen and co-workers at the University of Minnesota (Lent & Cohen 1984; Cohen et al. 1986) use a kinematic theory, treating diffraction as a single scattering process, and put much emphasis on the interference of beams reflected from terraces on the crystal surface.
dynamical calculations have also been done for an artificial surface consisting of a periodic array of surface steps (Kawamura et al. 1984; Kawamura & Maksym 1985). However, the enormous amount of computation involved prevents the theory being applied to any more realistic epitaxially growing system.

More recently, a new approach based on comparing the evolution of the step density to that of the measured RHEED specular spot intensities has also been proposed (Clarke & Vvedensky 1988). Although the evolution of the step density is shown to have a remarkable similarity to the measured evolution of the RHEED specular spot intensity, the comparison between the step density and RHEED is largely phenomenological and an unequivocal correspondence between the two quantities is yet to be established (Vvedensky & Clarke 1990).

In a previous paper (Peng & Whelan 1990a) we have developed a practical method for calculating dynamical RHEED from MBE growing surfaces. It is the purpose of this and subsequent papers to report the results of our dynamical diffraction calculations for RHEED from MBE growing surfaces. In this first part, the case of epitaxial growth on a low-index surface will be investigated in detail. Results concerning the effects due to both the diffraction and growth conditions on RHEED intensity evolution during MBE growth will be given, and compared with the kinematic theory and experimental results.

2. Epitaxial growth on a low-index surface

We shall first consider epitaxial growth on a low-index surface. By low-index surface we mean a surface produced by cutting through a single crystal parallel to a low-index plane. While many existing numerical procedures, like Monte Carlo (MC) simulation (Madhukar & Ghaisas 1988; Clarke & Vvedensky 1987) and molecular dynamics (MD) integration (Gilmer & Broughton 1983; Schneider et al. 1987) provide theoretical tools for investigating the effects of various parameters on epitaxial surface growth, as pointed out by Cohen et al. (1989), the calculations are complex and it is difficult to determine the sensitivity and uniqueness of the parameters used in any comparison with experiment.

An alternative and simple approach to the numerical description of epitaxial growth is the rate equation (RE) model (Gilmer et al. 1974; Venables et al. 1984; Kariotis & Lagally, 1989). In the present study we choose to use the birth—death model as proposed by Cohen et al. (1989) to simulate the MBE growth on a low-index surface.

For a low-index surface, since there is no natural spatial origin, a mean field description is possible. If we go further and use a solid-on-solid (sos) approximation (Weeks & Gilmer 1979) excluding vacancies and overhangs, the coverage \( \theta_n \) of the \( n \)th surface layer then satisfies a set of differential equations (Cohen et al. 1989)

\[
\frac{d\theta_n}{dt} = \tau^{-1}(\theta_{n-1} - \theta_n) + k(\theta_{n+1} - \theta_{n+2})(\theta_{n-1} - \theta_n) - k(\theta_n - \theta_{n+1})(\theta_{n-2} - \theta_{n-1}),
\]

(1)

during the growth, i.e. the rate at which the atoms of an upper layer transfer to a lower layer is proportional to the product of mobile atoms in an upper layer and vacancies in the layer below. After the growth is interrupted we have

\[
\frac{d\theta_n}{dt} = k(\theta_{n+1} - \theta_{n+2})(\theta_{n-1} - \theta_n) - k(\theta_n - \theta_{n+1})(\theta_{n-2} - \theta_{n-1}),
\]

(2)

where \( \tau \) is the time to deposit a monolayer and \( k \) is a diffusion parameter that measures the mobility of uncovered atoms. The initial and boundary conditions of

the sets of equations are $\theta_0(t) = 1, \theta_n(0) = 0$ ($n = 1, 2, \ldots$), and $\theta_\infty(t) = 0$. Perfect layer growth corresponds to an infinite value of $k$ in equations (1) and (2), and the layer coverages are then given by

$$\begin{align*}
\theta_n(t) &= 0, & t < (n-1)\tau, \\
&= t/\tau - (n-1), & (n-1)\tau \leq t \leq n\tau, \\
&= 1, & t > n\tau.
\end{align*}$$

(3)

A non-diffusive growth corresponds to a zero $k$ in equations (1) and (2). The solutions for the layer coverage $\theta_n$ are given by (Cohen et al. 1989)

$$\theta_n(t) = 1 - \exp \left( -t/\tau \right) \sum_{j=0}^{n-1} \frac{1}{j!} (t/\tau)^j$$

(4)
during the growth, and

$$\theta_n(t) = \theta_n(t_0)$$

(5) after the growth is interrupted at time $t_0$.

Shown in figure 1a–c are surface layer coverage curves for epitaxial growth on an As-stable GaAs(001) surface ($0 \leq t \leq 6\tau$). In figure 1a, a diffusion parameter of $k = 1$ is used, and the layer coverage curves are indeed indistinguishable from those of the non-diffusive growth model as shown in figure 2a, for which $k = 0$. In figure 1b, a diffusion parameter of $k = 2000$ is used. The resulting layer coverages as shown in
Figure 2. Surface layer coverage curves (from 1 to 10) for ten growing layers, using (a) a non-diffusive growth model and (b) a perfect layer growth model.

this figure match the perfect layer growth curves of figure 2b \((k = \infty)\) almost exactly. An intermediate value of \(k = 15\) has been used in figure 1c so the growth model is intermediate between perfect layer growth and non-diffusive growth on the surface.

An alternative to the diffusive growth model as described by equations (1) and (2) is the so called distributed growth model (Cohen et al. 1989). In this model the transfer of atoms between layers is treated in accordance of the lateral structure of the layer by distributing adatoms among the layers according to the number of reactive sites available. Equation (1) then becomes

\[
\frac{d\theta_n}{dt} = \frac{1}{\tau} (\theta_{n-1} - \theta_n) + \frac{\alpha_n}{\tau} (\theta_n - \theta_{n+1}) - \frac{\alpha_{n-1}}{\tau} (\theta_{n-1} - \theta_n),
\]

in which

\[
\alpha_n = A \frac{d_n(\theta_n)}{d_n(\theta_n) + d_{n+1}(\theta_{n+1})},
\]

and \(d_n(\theta_n)\) is the perimeter of the \(n\)th layer. When \(A = 1\), this model gives perfect layer growth, and when \(A = 0\) it gives non-diffusive growth. The main advantage of this model is that there is considerable flexibility in defining the dependence of the perimeter on the coverage. A simple approximation is to define

\[
d_n(\theta_n) \propto \theta_n (1 - \theta_n)^{1/4},
\]

or more generally

\[
d_n(\theta_n) \propto \left\{ \begin{array}{ll}
\theta_n^{p_1} & \text{for } \theta_n < \theta_c, \\
(1 - \theta_n)^{p_2} & \text{for } \theta_n > \theta_c,
\end{array} \right.
\]

with

\[
\theta_c^{p_1} = (1 - \theta_c)^{p_2}.
\]

The layer coverage curves for this distributed growth model are shown in figure 3a, b. In figure 3a, the definition of (8) is used for relating the perimeter \(d_n(\theta_n)\) to the layer coverage \(\theta_n\), with an intermediate value of \(A = 0.90\). In figure 3b, the definition of (9) is used, with \(A = 0.9\), \(p_1 = p_2 = 0.5\) and \(\theta_c = 0.5\).

An interesting and important property of the set of equations (1) and (6) can be obtained by adding up the equations, i.e.

\[
\frac{d}{dt} \sum_{n=0}^{\infty} \theta_n(t) = \frac{1}{\tau} (\theta_0 - \theta_\infty) = \frac{1}{\tau},
\]

MBE RHEED intensity oscillations. I

Figure 3. Surface layer coverages of ten growing layers (1–10). A distributed growth model is used, and the perimeter of nth layer is related to the layer coverage \( \theta_n \) using (a) equation (8) with \( A = 0.9 \), and (b) equation (9) with \( A = 0.9 \), \( p_1 = p_2 = 0.5 \) and \( \theta_c = 0.5 \).

or

\[
\sum_{n=0}^{\infty} \theta_n(t) = t/\tau,
\]

during the growth, and

\[
\frac{d}{dt} \sum_{n=0}^{\infty} \theta_n(t) = 0,
\]

or

\[
\sum_{n=0}^{\infty} \theta_n(t_0) = t_0/\tau,
\]

after the growth is interrupted at time \( t_0 \). It is thus shown that the growth rate is indeed \( 1/\tau \) monolayers per second during the growth, and after the growth is interrupted the total sum of the layer coverages remains constant.

3. Kinematic and dynamical diffraction from crystals

We now consider the diffraction by an epitaxially growing system consisting of a bulk substrate crystal and several growing surface layers as described by the set of equations (1). The starting point of electron diffraction theory is the following relativistic wave equation which is valid at moderate beam energies (Fujiwara 1961)

\[
[V^2 + U(r) + \mathbf{\chi}^2] \psi(r) = 0,
\]

\( \mathbf{\chi} \) is the relativistic incident wave vector in the vacuum and \( U(r) \) is a scaled lattice potential given by

\[
U(r) = (2m_e/\hbar^2) V(r),
\]

where \(-e\) is the electronic charge, \(-eV(r)\) is the potential energy of the electron inside the crystal, and \( m \) is the relativistic electron mass. As an alternative, we may reformulate the wave equation (14) as an integral equation

\[
\psi(r) = \exp(i\mathbf{\chi}:\mathbf{r}) + \int G(r, r') U(r') \psi(r') \, dr',
\]

where the first term represents a plane incident wave and the integral represents the scattered wave. The approximate form of the Green’s function

\[
G(r, r') = \exp(ik|\mathbf{r} - \mathbf{r}'|)/4\pi|\mathbf{r} - \mathbf{r}'|,
\]
representing the amplitude at a point of observation \( r \), due to a point of unit scattering strength at \( r' \).

### 3.1. Kinematic diffraction

To a first order approximation, we may approximate the incident plane wave as the total wave function within the crystal to calculate the scattered wave as represented by the integral in equation term (16). The scattered wave can then be written down as

\[
\psi_{\text{scat}}(r) = \frac{1}{4\pi} \int \frac{\exp(ik|r-r'|)}{|r-r'|} U(r') \exp(i\mathbf{r}' \cdot \mathbf{r}') \, dr',
\]

(18)

and the amplitude for scattering into a particular final direction \( \mathbf{k}' \) is given by

\[
f(k' - k) = \frac{1}{4\pi} \int \exp[-i(k'-k) \cdot r'] U(r') \, dr'.
\]

(19)

The scattering potential \( V(r) \) for high-energy electron is usually expressed in terms of a sum of contributions of individual atoms

\[
V(r) = \sum_i \phi_i(r-r_i),
\]

(20)

where \( \phi_i(r) \) is the scattering potential associated with the atoms centred at \( r_i \).

Substituting (20) into (19) gives

\[
f(s) = \frac{me}{2\pi \hbar^2} \sum_i u_i(s) \exp(-is \cdot r_i),
\]

(21)

where \( s = k' - k \), and \( u_i(s) \) is the Fourier transform of \( \phi_i(r) \):

\[
u_i(s) = \int \phi_i(r) \exp(-is \cdot r) \, dr.
\]

(22)

Within the kinematic approximation and assuming diffraction only from the exposed surface layer, the diffracted beam amplitude (21) then becomes

\[
f(s_p, s_z) = \frac{me}{2\pi \hbar^2} \sum_{r_p, n} u_i(s_p, s_z) \exp(-is_p \cdot r_p) \exp(-is_z nd),
\]

(23)

where the sum only includes those \( r_p \) and \( n \) that correspond to atoms occupying exposed surface layers, \( r = r_p + nd\hat{z}, s = s_p + s_z\hat{z}, d \) is the interlayer spacing and \( n \) is integer denoting the height of a particular surface layer, the subscript \( \rho \) denotes surface parallel component and \( \hat{z} \) is a unit vector normal to the surface in the positive \( z \) direction. For simplicity we take \( me\hbar^2/2\pi = 1 \) so that

\[
f(s) = \sum_{r_p, n} \exp(-is_p \cdot r_p) \exp(-is_z nd).
\]

(24)

If we assume that there are \( N \) sites per surface layer (each having a layer coverage of \( \theta_n \) and therefore a total of \( N(\theta_n - \theta_{n+1}) \) uncovered atoms) and that \( s_p = 0 \), the above expression (24) is further simplified to

\[
f(s) = N \sum_{n=0}^{\infty} (\theta_n - \theta_{n+1}) \exp(-is_z nd).
\]

(25)

Until now this kinematic formulation has been the main tool for analysing RHEED diffraction measurements (Van Hove et al. 1983).
3.2. Dynamical diffraction

For an adequate treatment of the dynamical diffraction from MBE growing surfaces, the theoretical framework should be able to incorporate the non-periodic variations of the scattering potential in the surface normal direction, and non-periodically distributed surface disorders within the surface layers parallel to the substrate. There exist many dynamical approaches nowadays which meet the first requirement (Maksym & Beeby 1981; Ichimiya 1983; Peng & Cowley 1986, 1988; Zhao & Tong 1988; Peng & Whelan 1990b). However, a full treatment of surface disorders seems at present to be intractable.

To avoid the complexity of treating the non-periodic surface disorders on the growing surface layers and the often unknown atomic details of the reconstructed surface, in a previous paper (Peng & Whelan 1990a) we proposed to use a 'systematic reflection' approximation, considering only the reflection by planes parallel to the substrate surface. Diffuse diffraction effects, such as those arising when the electron enters on one side of a step and exits on the other side, are not included. This is because when the systematic reflection case is realized the diffusely scattered electrons do not contribute to the specular reflected beam directly (since a lateral momentum transfer is involved). To a first-order approximation the effects can be taken into account, however, by using an effective absorbing potential, and this is the approach we have adopted in the present model.

Although the systematic reflection case in RHEED has often been referred to as an ‘idealized case’, it is practically achievable as has been done nearly sixty years ago by Kikuchi & Nakagawa (1933) on a cleavage face of sphalerite, and more recently by Ichimiya (1985) on the reconstructed Si(111) 7 x 7 surface, and by Cohen et al. (1986) on MBE grown surfaces.

Artificially, we may consider the whole crystal system as composed of a semi-infinite periodic bulk crystal and an assembly of non-periodic growing surface layers. Within the bulk crystal for the systematic reflection case, the crystal lattice can be effectively considered as periodic along the surface normal direction only, and a convenient plane wave expansion can be made of the scaled lattice potential \( U(r) \)

\[
U(r) = \sum_{i} U_i \exp(i l \cdot r),
\]

in which \( l \) are the reciprocal lattice vectors normal to the surface. In the systematic reflection approximation, since one reciprocal lattice rod is involved, only two independent Bloch wave are excited within the crystal. And among the two waves only the one which propagates or decays into the crystal will be physically allowed. The total electron wave field within the bulk crystal can then be written as (Peng 1989; Peng & Whelan 1990b)

\[
\psi(r) = \alpha \sum_{i} C_i \exp[i(K + \gamma n + l) \cdot r],
\]

where \( \alpha \) is the Bloch wave amplitude to be determined from the boundary conditions, and the conventional 'anpassung' \( \gamma \) and Bloch wave coefficients \( C_i \) satisfy the fundamental equation of electron diffraction (Bethe 1928)

\[
(K^2 - k_i^2) C_i + \sum_{k \neq l} U_{k-l} C_l = 0,
\]

where $K$ is the electron wave vector derived from $\chi$ after correction for the mean inner potential $U_0$,

$$K^2 = \chi^2 + U_0.$$  

To simulate the structural variations of growing surface layers along the surface normal direction, we divide the surface layers into an assembly of thin slices parallel to the surface, and assume that the slice at depth $z$ below the surface has an inner potential $U_0(z)$. Within each thin slice the electron wave function has the form:

$$\psi_n(z) = T_n \exp(i k_z z) + R_n \exp(-i k_z z),$$  

and its surface normal derivative:

$$\psi_n'(z) = i k_z T_n \exp(i k_z z) - i k_z R_n \exp(-i k_z z).$$  

In equations (30) and (31) the exponential term $\exp(i k \cdot \rho)$ has been omitted, since it is a common phase term for all slices, and $k_z$ depends on $z$ through the relation

$$k_z(z) = (\chi^2 + U_0(z)).$$  

An explicit expression for $U_0(z)$ in terms of the surface layer coverage parameter $\theta$ and the potential of a single layer has been given by Peng & Whelan (1990a).

We may rewrite equations (30) and (31) in matrix notation,

\[
\begin{pmatrix}
\psi_n(z) \\
\psi_n'(z)
\end{pmatrix} = \begin{pmatrix}
\exp(i k_z z) & \exp(-i k_z z) \\
 i k_z \exp(i k_z z) & - i k_z \exp(-i k_z z)
\end{pmatrix} \begin{pmatrix}
T_n \\
R_n
\end{pmatrix}.
\]

On the upper surface of the thin slice, $z = z_{n-1}$, the boundary conditions give

\[
\begin{pmatrix}
\psi_n(z_{n-1}) \\
\psi_n'(z_{n-1})
\end{pmatrix} = \begin{pmatrix}
\exp(i k_z z_{n-1}) & \exp(-i k_z z_{n-1}) \\
 i k_z \exp(i k_z z_{n-1}) & - i k_z \exp(-i k_z z_{n-1})
\end{pmatrix} \begin{pmatrix}
T_n \\
R_n
\end{pmatrix}.
\]

By combining (33) and (34) and eliminating the transmission and reflection coefficients $T_n$ and $R_n$, we obtain

\[
\begin{pmatrix}
\psi_n(z_n) \\
\psi_n'(z_n)
\end{pmatrix} = M_n(t_n) \begin{pmatrix}
\psi_n(z_{n-1}) \\
\psi_n'(z_{n-1})
\end{pmatrix},
\]

in which

\[
M_n = \begin{pmatrix}
\cos(k_z t_n) & \sin(k_z t_n)/k_z \\
-k_z \sin(k_z t_n) & \cos(k_z t_n)
\end{pmatrix}.
\]

and $t_n = z_n - z_{n-1}$ is the thickness of the thin slice.

The scattering matrix $M$ for relating the electron wave function and its surface normal derivative on the upper and lower surfaces of an assembly of thin slices, each having thickness $t_i$ is given by

\[
M = \prod_i \begin{pmatrix}
\cos[k_z(z_i) t_i] & \sin[k_z(z_i) t_i]/k_z \\
-k_z \sin[k_z(z_i) t_i] & \cos[k_z(z_i) t_i]
\end{pmatrix}.
\]

If the total thickness of surface layers is $t(t = \Sigma_i t_i)$, and since the vacuum region above the crystal slab contains only the incident and specular reflected beam, by using (27) and the boundary conditions, we have

\[
\alpha \left( \sum_i C_i \exp[i(K_z + \gamma + l) t] \right) = M \left( \begin{pmatrix}
1 + R_0 \\
i \chi_z (1 - R_0)
\end{pmatrix} \right).
\]
Figure 4. Dynamical reflection rocking curve for 20 keV electrons incident on an As-stable GaAs(001) surface. The imaginary part of the scattering potential is assumed to be 5% of the real part.

and therefore the specular reflected beam amplitudes $R_0$:

$$R_0 = \frac{\sum C_t \exp (ilt) \{ (K_z + \gamma + l) [M_{11} + i\chi_z M_{12}] + i[M_{21} + i\chi_z M_{22}] \}}{\sum C_t \exp (ilt) \{ (K_z + \gamma + l) [M_{11} - i\chi_z M_{12}] + i[M_{21} - i\chi_z M_{22}] \}}.$$  

When an imaginary potential component is added to take into account the anomalous absorption effects, $k_z(z_0)$ in the scattering matrix (37) will become complex, and the electron wave function will be decaying into the crystal. In the case where the slab of surface layers is so thick that the transmitted beam amplitude $T_0$ below the slab is negligible, the true reflected beam amplitude $R_0$ as given by (39) should not be very different from that reflected by the thick slab of surface layers. By analogy to (38) we now have

$$\begin{pmatrix} T_0 \exp (i k_z l) \\ i\chi_z T_0 \exp (i k_z l) \end{pmatrix} = M \begin{pmatrix} 1 + R_0 \\ i\chi_z(1-R_0) \end{pmatrix},$$

and therefore by eliminating $T_0$ from the two equations represented by (40) we obtain

$$R_0 = -\frac{[M_{11} - M_{21}/i\chi_z] - [M_{22} - i\chi_z M_{12}]}{[M_{11} - M_{21}/i\chi_z] + [M_{22} - i\chi_z M_{12}]}.$$  

In figure 4, a systematic reflection rocking curve for 20 keV electrons incident on a perfect As-stable GaAs(001) surface is given. The variation of the specular reflected beam intensity with the incident glancing angle has been presented in both milliradians and Bragg angle ($\theta_B$), and the imaginary part of the scattering potential has been assumed to be 5% of the real part. It should be noted that this type of systematic reflection rocking curve is insensitive to the lateral distribution of atoms and depends only on the projection on the surface normal of the atomic distribution in the various layers of atoms parallel to the surface.

4. RHEED intensity evolution during growth

4.1. Perfect layer growth

As the first case of epitaxial growth, we now consider an extreme where every deposited atom goes into the topmost unfilled surface layer until that layer is

Figure 5. Calculated evolution curves of RHEED intensity during perfect layer growth, using the kinematic theory. 20 keV electrons are incident on a As-stable GaAs(001) surface with a glancing incident angle of (a) 46 mrad, (b) 50 mrad, (c) 53 mrad and (d) 57 mrad. In (a) the kinematic Bragg condition and in (c) the off-Bragg condition are satisfied.

completed. This is the perfect layer growth model as discussed in §2, and the surface growing layer coverage curves have been given in figure 2b.

Shown in figure 5 are some RHEED intensity evolution curves during the perfect layer growth. RHEED intensities are calculated using the kinematic formulation (25) for 20 keV primary beam energy, and the intensities have been normalized to unity for the perfect crystal surface prior to the start of deposition. The calculated RHEED intensities at all incident angles decrease from unity to a minimum at half layer coverage, and then increase back to unity at complete layer coverage. The amplitude of intensity oscillations varies from zero at Bragg incidence (ca. 46 mrad) to unity at the off-Bragg condition (ca. 53 mrad). By ‘off-Bragg’ we mean that the phase difference \( \phi_d \) in equation (25) is \((2m + 1)\pi\), where \( m \) is an integer. It should also be noted that the kinematic diffraction theory gives a cusp-like shape to all intensity oscillation curves (Van Hove & Cohen 1987).

Shown in figures 6 and 7 are the kinematic phase and amplitude diagrams, i.e. the variations of RHEED intensity maxima and minima positions with the incident angle of the primary beam (phase diagram), and the variation of the amplitude of RHEED intensity oscillations (amplitude diagram). Under the kinematic approximation, the phase and amplitude behaviour is relatively simple. As shown in figure 6, for all incident angle ranges from 40 to 58 mrad, the RHEED intensity maxima are always at zero or complete layer coverage, while the intensity minima are always at half layer coverage. The amplitude of the intensity oscillation, on the other hand, varies in a sinusoidal manner, having its minima (zero) at Bragg incident angles and maxima (unity) at off-Bragg conditions (see figure 7) (Lent & Cohen 1984).

To compare with the kinematic behaviour of RHEED intensity evolution during perfect layer growth, four RHEED intensity evolution curves for glancing incident angle of 46, 50, 53 and 57 mrad are given in figure 8, and the dynamical phase and
Figure 6. Kinematic phase diagram of RHEED intensity oscillations, showing the intensity maxima (*) are always at zero layer coverage and intensity minima (o) at half layer coverage.

Figure 7. Kinematic amplitude diagram of RHEED intensity oscillations, showing a sinusoidal variations of the amplitude of the intensity oscillations with the incident angle. The amplitude of the intensity oscillations drops to a minimum at the Bragg condition (ca. 46 mrad) and goes to maximum at the off-Bragg condition (ca. 53 mrad).

Figure 8. Calculated dynamical RHEED intensity evolution curves for a perfect layer growth model. The primary incident beam energy is 20 keV, and the glancing incident angle at the GaAs(001) growing surface is (a) 46 mrad, (b) 50 mrad, (c) 53 mrad and (d) 57 mrad.

amplitude diagrams are plotted in figures 9 and 10 respectively. Although the intensity evolution curves in figure 8 also exhibit cusp-like behaviour, it is seen that a cusp can be irregular (figure 8a) or turned upside down (figure 8d). The dynamical phase diagram and the amplitude diagram (figures 9 and 10 respectively) show a complex behaviour with changing incident condition, compared with the kinematic diagrams of figures 6 and 7.

To some extent this dynamical behaviour can be understood qualitatively with reference to the reflection rocking curve of figure 4, if we assume that the effect of depositing a small number of atoms on the surface is equivalent to a shift of the dynamical rocking curve slightly towards the high incident angle side. For example,
Figure 9. Dynamical phase diagram of intensity oscillations for 20 keV electrons incident on GaAs(001) system with the incident angle range from 40 to 58 mrad. *, maxima; o, minima.

Figure 10. Dynamical amplitude diagram of intensity oscillations, showing the variation of the intensity oscillation amplitude with the incident angle.

Figure 11. Dynamical RHEED intensity surface showing the intensity variations with the incident angle and with time for the growth of a monolayer. A perfect layer growth model is used, and the diffraction calculation has been made for 20 keV electrons incident at a GaAs(001) growing surface. Intensity contours at 0.02, 0.04, 0.06, 0.08.

at an incident angle between 50–53 mrad the initial behaviour of the RHEED intensity will be to go down toward the lower angle side of the rocking curve at 46–50 mrad, that is to decrease the intensity, giving a cusp-like oscillations. On the other hand, at 57 mrad incidence, the intensity will increase, giving a reverse cusp-like behaviour.

It should be pointed out, however, that this interpretation of RHEED intensity evolution behaviour is not rigorous. A more comprehensive way is to use the dynamical phase and amplitude surface as shown in figure 11. For example, from this figure an oscillation frequency doubling effect is expected for an incidence from 40–43 mrad, a regular cusp-like behaviour is expected for an incidence from
4.2. Diffusive and non-diffusive growth

We now consider the more realistic model of diffusive epitaxial growth on a low-index surface. Once the atom is deposited onto an unfilled surface layer, the atom can jump to a lower level, and the rate at which the atoms of an upper layer transfer to a lower layer is described by the diffusion parameter $k$ in equation (1). At a very low primary beam energy of 20 keV is used, and the incident glancing angle is 50 mrad. (a), (b) $k = 1$; (c), (d) $k = 5$; (e), (f) $k = 10$; (g), (h) $k = 20$. 45–50 mrad, and for almost all incident angles the RHEED intensity will not decrease to a minimum at half-layer coverage. It should also be noted that the intersection of the intensity surface with a plane surface at a fixed point $\theta$ on the monolayer deposition axis is the reflection rocking curve corresponding to reflection from a rough surface with that value of $\theta$. In particular, at zero monolayer deposition the rocking curve is identical to that shown in figure 4.
jumping rate, this model is equivalent to the non-diffusive growth model for which the atom is not allowed to cross the boundary defined by a step edge, as previously discussed in §2.

The RHEED intensity evolution curves for the diffusive growth model during the growth, and the corresponding growth front profiles at $t = 4\tau$ are shown in figure 12. In figure 12a, b, a very low value of $k = 1$ is used, corresponding to the layer coverage curves of figure 1a. Effectively about six to seven surface layers are involved during the growth, as shown in figure 12b, and the RHEED intensity evolution curve exhibits no obvious oscillations. In figure 12c, d, a small value of $k = 5$ is used. Although, as can be seen from the growth front of figure 12d, at least four surface layers are involved, slight but obvious oscillations are seen in figure 12c. From $k = 10$ to $k = 20$, only two or three surface layers are effectively involved during the growth (figure 12f, h), and the RHEED intensity oscillations achieve their steady states effectively after two or even one monolayer deposition (see figure 12e, g).

For the lower values of $k$ as used in figure 12c–h, and even for a moderate value of $k = 100$ used in figure 13, the steady-state intensity oscillations are very nearly sinusoidal, in contrast to the cusp-like behaviour for perfect layer growth (figure 8) or for a very high value of $k$, for example 2000 as shown in figure 14. It is also shown in figures 13 and 14 that for all incidences the initial behaviour of RHEED intensity evolution is independent of $k$. The amplitude of the intensity oscillations, however, depends strongly on $k$, in particular for $k < 200$ as shown in figure 15. Figure 16 shows that RHEED intensity maxima and minima positions also depend on $k$.

Several points are worth noting concerning the intensity oscillation curves shown in figures 13 and 14. In contrast to the kinematic diffraction analysis (Cohen et al. 1989), the dynamical RHEED intensity does not always decrease as soon as the growth begins (see figures 13d and 14d), depending on the diffraction condition. Also, the amplitude of the intensity oscillations does not drop to zero at the Bragg condition (figures 13a and 14a), and the intensity minima do not reach zero intensity at the off-Bragg condition (figures 13c and 14c). For all incidence and all growth conditions for

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Figure 13. Dynamical RHEED intensity oscillations with time for the growth of four monolayers of GaAs. A diffusive growth model with $k = 100$ is used. The incident beam energy is 20 keV, and the incident angle is (a) 46 mrad, (b) 50 mrad, (c) 53 mrad and (d) 57 mrad.
mbe
rheed
intensity oscillations.

Figure 14. Same as figure 13, but a higher value of \( k = 2000 \) is used for the diffusive growth on GaAs(001) growing system.

Figure 15. The variation of the amplitude of RHEED intensity oscillations with the diffusion parameter \( k \) for a diffusive growth model and 20 keV electrons incident on the GaAs(001) surface at 50 mrad.

Figure 16. The variation of the intensity maxima (*) and minima (○) positions with \( k \). Diffraction and growth conditions are the same as for figure 15.

which \( k > 5 \), the results show that one period of RHEED intensity oscillation corresponds exactly to the growth of one GaAs monolayer on an As-stable (001) oriented substrate, in agreement with the kinematic prediction and experimental observations.

4.3. Distributed growth

Although the diffusive growth model predicts a number of features of measured RHEED intensity oscillations, it failed in producing one of the most important features of RHEED intensity evolution behaviour, i.e. the damping of the measured envelope of intensity oscillation. This is because in the diffusive growth model previously discussed, the effects of surface step distribution on the rate of transfer of atoms between growing surface layers are explicitly excluded.

An improvement to the diffusive growth model is to treat the transfer of atoms

Figure 17. Dynamical RHEED intensity for 20 keV electrons incident at a glancing angle of 50 mrad, plotted as a function of time for the growth of nine monolayers. A distributed growth model and definition (8) are used. In (a) $A = 0.85$, (b) $A = 0.90$, (c) $A = 0.92$, and in (d) $A = 0.95$.

Figure 18. RHEED intensity oscillations during distributed epitaxially growth on a GaAs(001) substrate. Definition (8) and a value of $A = 0.93$ are used in the distributed growth model. Shown in this figure are the variations of RHEED intensity with time for 20 keV electrons incident on the surface at (a) 30 mrad, (b) 40 mrad, (c) 50 mrad and (d) 60 mrad.

between layers in accordance with the lateral structure of the layer, and this is the distributed growth model as discussed in §2. There are, among others, two simple ways of relating the rate of transfer of atoms between layers to the total perimeters or step densities of the surface layers. These are through equations (8) and (9) of §2.

The RHEED intensity evolution curves shown in figures 17–19 are calculated using equation (8), and in figure 19 using (9). Almost all features of measured intensity oscillations from a low-index surface are reproduced here. Among other features, there is an initial transient, after which the intensity oscillation maxima and mean RHEED intensity damp slowly to a nearly constant but non-zero value (Van Hove & Cohen 1987). At moderate surface diffusion rates the oscillations are sinusoidal (figures 17a–c, 18a–d and 19a, b), while at higher rates they are more cusp-like.
5. Conclusion

Dynamical diffraction calculations have been performed for RHEED from MBE growing surfaces, using a systematic reflection approximation. Although the diffraction condition has been chosen so that the reflected beam intensity is insensitive to the lateral distribution of atoms or to the step density, the transfer of atoms between surface layers during growth is sensitive to the step density and therefore so are the RHEED intensity oscillations. Furthermore, the complexities of treating a non-periodic distribution of surface clusters or disorders on the growing surface layers and the sometimes unknown atomic details of reconstructed surfaces are avoided, making a practical dynamical diffraction analysis of RHEED measurements possible.

Using a perfect layer growth model of epitaxy, we have shown that the kinematic approximation to RHEED fails in many qualitative and almost all quantitative aspects concerning the initial behaviour, phase and amplitude variations with the diffraction conditions of the intensity oscillations. On the other hand, our dynamical calculations have successfully reproduced most of the features of measured intensity oscillations from a low-index surface including, among others, the initial transient behaviour of the intensity oscillation, the damping envelope of the intensity maxima or mean intensity, the phase and amplitude variations of the intensity oscillations, the doubling of oscillation frequency and the transition between sinusoidal behaviour at low temperatures (low surface diffusion rates) to cusp-like behaviour at higher temperatures (higher diffusion rates). We have also shown that the oscillation in the RHEED intensity follows a layer by layer epitaxial growth, and that one period of intensity oscillation corresponds exactly to the deposition of one complete monolayer.

The authors thank Professor Sir Peter Hirsch for the provision of laboratory facilities, and Professor B. A. Joyce, Dr J. Zhang, Dr D. D. Vvedensky and Dr S. Clarke for helpful and valuable discussions. One of us (L. M. P.) is supported by the UK Science and Engineering Research Council, through a Research Assistantship, and by Wolfson College, Oxford, through a Junior Research Fellowship, both of which are gratefully acknowledged.

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Received 9 July 1990; accepted 13 September 1990

Rotational motions, or vorticity, can be created within a fluid dammed by two mechanisms: baroclinic torque and viscous-shear torque. Both baroclinic and viscous-shear torques require the presence of fluid density gradients. It is important that vertical motions in the surface roller of a bore are opposed by baroclinic torque acting along the front face of the bore; this baroclinic torque is caused by the density pressure gradient along the air-water interface. On the other hand, vorticity is generated in an internal bore, with a small density difference between the upper and lower fluids, are generated by baroclinic torque caused by the static pressure gradient along the interface of two fluids. Vorticity generated in an internal bore has the opposite rotation to that of a bore in the air-water environment. In both cases the viscous-shear torque plays an insignificant role in the generation of vorticity.

1. Introduction

Consider a layer of water bounded by the free surface from above and an impermeable boundary from below. The flow depth may increase to a greater extent in a short distance without alternating its discontinuity for a fluid jet. A sudden increase in depth occurs at the transition from the surface to the bottom, and the inertial force is dominant in the vertical direction; the centrifugal force is negligible. Based on the shallow-water wave theory, the existence of a discontinuity across the jump is assumed to be a mathematical discontinuity of the flow depth, and usually referred to as a hydraulic jump. The total momentum energy dissipation is attributed to turbulence generated in the jet. The characteristics of turbulence generated at the jet are hard to model with a classical theory of turbulence. A modelled a hydraulic jump as a flow expansion and contraction across a separation region. Raper (1963) and Jirka (1983) modelled the flow as a wall jet. Persyn & Krieger (1978) suggested that the flow resembles that of a shallow-layer. The hydraulic jump flow transitions and transitions elaborated by Blevins & Settles (1986).

A fundamental question is addressed in this paper: how vertical or horizontal flow leads to the formation of a turbulent flow in a fluid jet. Because of this objective, instead of a stationary hydraulic jump, we consider a base fluid at a quasi-steady broken water wave of an infinite water depth propagating into a quiescent water of a uniform depth as shown in figure 1. A bore is also a panel phreatic and, under the one-dimensional flow assumption the flow and fluid properties being uniform in a plane perpendicular to the mean flow direction, the mathematical description of a bore motion can be reduced essentially to that of a stationary hydraulic jump by taking the galactic transformation with this bore.