# Reciprocal-Space Formulation and Prediction of Misfit Accommodation in Rigid and Strained Epitaxial Systems

MAX W.H. BRAUN and JAN H VAN DER MERWE

Geometrical properties form a key aspect of any description of heteroepitaxial systems in which orientation, symmetry, and lattice parameters differ. An energetically founded epitaxial criterion, which is geometric in nature, for matching at a planar interface is derived from a generalization of the Frank–van der Merwe theory and the rigid models introduced by Reiss and van der Merwe. The criterion is most naturally formulated in reciprocal space as the matching of overgrowth and substrate reciprocal lattice vectors and is visualized with a construction analogous to the Ewald construction. Structure factors are introduced and account for rigid translations and the nonprimitive nature of substrate and overgrowth surface unit cells. This article focuses on the derivation of the epitaxial criterion and its consequences as a basis of a description of epitaxial configurations, pseudomorphism, and the parameters of dislocation or misfit vernier arrays, in terms of crystallographic conventions. The strength of the description is its general nature, as it is general and applicable to any combination of crystal symmetries or mismatch and can be used to predict, or interpret, interfacial structure.

## I. INTRODUCTION

APPLICATIONS of epitaxial systems range from metallurgical materials to semiconductor electronics, optics, and superconducting thin-film devices. Consequently, there is a need for an accessible, theoretically founded formulation of fundamental aspects of epitaxy, particularly to simplify prediction of possible epitaxial configurations in these real and, hence, complex systems.

The development of theoretical descriptions of epitaxy began with Frank and van der Merwe,[1] who accounted for the periodic nature of the crystals of differing lattice parameters and introduced the concept of pseudomorphic strain, misfit accommodation, and misfit dislocations in one-dimensional systems. Since then, many models have been developed from a range of perspectives, usually with models applicable to interfaces with simple geometry: polyatomic crystals have rarely been treated.

Generalization of existing theories to complex symmetries and unit-cell structures has been hampered by the absence of a framework within which the models and predictions can be expressed consistently. There is a need for a description that is general, insensitive to anisotropy of elastic properties, does not rely on simple symmetries, is applicable to polyatomic systems of any size with least complication, and whose results and predictions can be visualized in terms of any preferred or current framework. The reciprocal-space description given here is a strong candidate. While several fundamental aspects of this formalism have been applied by earlier authors, these are significantly extended here.

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Intuitively, the geometries of crystal surfaces on either side of a planar epitaxial interface can be described very generally in terms of surface-reciprocal lattices, and it may be expected that an epitaxial criterion related to the matching of rows of atoms on either side of the interface can be conveniently expressed in terms of these. Here, we derive such a matching criterion from energy considerations.[2] The interfacial energy is minimized in an epitaxial system described with a general, but rigid and essentially atomistic, model.[3,4] The criterion is made particularly useable through the introduction of a geometrical construction analogous to the Ewald construction, common in crystallography.

Consequences of the criterion are discussed, including prediction of ideal epitaxial configurations,[3] and this article introduces useful measures of interfacial misfit related to both direct and reciprocal space. Misfit is accommodated in several ways in real systems: homogeneous strain to allow exact matching of the interface structures (pseudomorphism), both one- or two-dimensionally; periodic relaxation characteristic of arrays of misfit dislocations; or misfit vernier. From the epitaxial criterion we derive a formulation for misfit dislocation spacings, directions and Burgers vectors, and process for the unique characterization of misfit dislocation arrays in terms of their degree of edge and screw character. A real system may be expected to show combinations of these misfit accommodation mechanisms, and their prediction is dealt with elsewhere, where the elastic properties of the systems are taken into account.

## II. THE MODEL

Several models yield expressions which approximate the energy of an epitaxial bicrystal and have been used to predict epitaxial orientations or interfacial structure by minimizing the interaction energy (such as in References 1, 3, 5, and 6).

In the geometric limit, both components of the bicrystal are treated as rigid, retain their bulk or homogeneously deformed lattices, and are in contact at a single interfacial plane. On either side of the interface, each component crystal

presents a crystal plane, with a set of translational and rotational symmetries and two-dimensional periodicities. The set of wave vectors that together form the surface-reciprocal lattice for each crystal face conveniently describes these periodicities. It is useful to refer to the component crystals as substrate and overgrowth, respectively, in particular when one crystal is extremely thick, whereas the other is only an atomic layer or so in thickness.

Fletcher[5] has calculated the energy for a bicrystal system by summing over all the pairwise interactions in the bicrystal while assuming central potentials such as Morse or Lennard–Jones. Novaco and McTague[7] developed a linear-response lattice dynamic formulation based on Fletcher's model, which was applied to this rigid limit. Van der Merwe[3] considered an orientation-dependent contribution to the energy in a rigid overgrowth and substrate system by using a truncated Fourier series to express the overgrowth atom-substrate crystal interaction potential. We present here a short development of an expression for such a bicrystal energy, which is essentially a generalization of Van der Merwe's approach.[2,3] The central result obtainable from these approaches is a necessary criterion for the occurrence of an epitaxial orientation expressed in reciprocal space. It is an energetically founded geometric criterion imposed by the crystalline nature of epitaxial systems and is independent of a particular atomic-force model.

The substrate surface may be described in terms of a two-dimensional Bravais lattice formed by the basis vectors $\mathbf{a}_1$ and $\mathbf{a}_2$, with lengths of $a_1$ and $a_2$, respectively, and an angle of $\alpha$ between them. An associated reciprocal set $\mathbf{a}_1^*$ and $\mathbf{a}_2^*$ is uniquely defined by the condition $\mathbf{a}_i \times \mathbf{a}_j^* = 2\pi\delta_{ij}$, where $\delta_{ij}$ is the Kronecker delta, and by the requirement that these vectors are all coplanar. The lengths $a_1$ and $a_2$ may be expressed in terms of the bulk nearest-neighbor distance $a_{nn}$ as $a_i = C_{ai}\, a_{nn}$ $(i = 1, 2)$ so defining the scaling factors $C_{a1}$ and $C_{a2}$.

The interaction energy between individual interfacial overgrowth atoms (adatoms) and the substrate surface is assumed to be periodically dependent on the adatom position ($\mathbf{r}$) and is conveniently expressed as a Fourier series:

$$V(x,y) = \sum_{\{\mathbf{q}\}} V_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{r}} = \sum_{h,k=-\infty}^{\infty} V_{hk} e^{i2\pi(hx+ky)} \qquad [1]$$

with

$$\mathbf{r} = x\mathbf{a}_1 + y\mathbf{a}_2, \qquad \mathbf{q}_{hk} = h\mathbf{a}_1^* + k\mathbf{a}_2^*$$

$$\mathbf{a}_1^* = 2\pi\frac{\mathbf{a}_2 \times \mathbf{n}}{|\mathbf{a}_1 \times \mathbf{a}_2|}, \qquad \mathbf{a}_2^* = 2\pi\frac{\mathbf{n} \times \mathbf{a}_1}{|\mathbf{a}_1 \times \mathbf{a}_2|} \qquad [2]$$

$$\text{with unit normal,} \qquad \mathbf{n} = \frac{\mathbf{a}_1 \times \mathbf{a}_2}{|\mathbf{a}_1 \times \mathbf{a}_2|}$$

where $\mathbf{q}_{hk}$ is a lattice-translation vector of the substrate surface-reciprocal lattice, $h$ and $k$ are integers, and $\mathbf{r}$ is a position vector expressed in terms of the substrate. The Fourier coefficients can be determined from extensive detailed first-principle calculations, or by using empirical or semiempirical atomic potentials.[8,9] Many-body calculations can lead to values for these coefficients. These single atom–substrate calculations are of interest in absorption and atom-surface migration. Calculations have more recently been extended to atoms belonging to an epilayer using many-body interactions.[10]

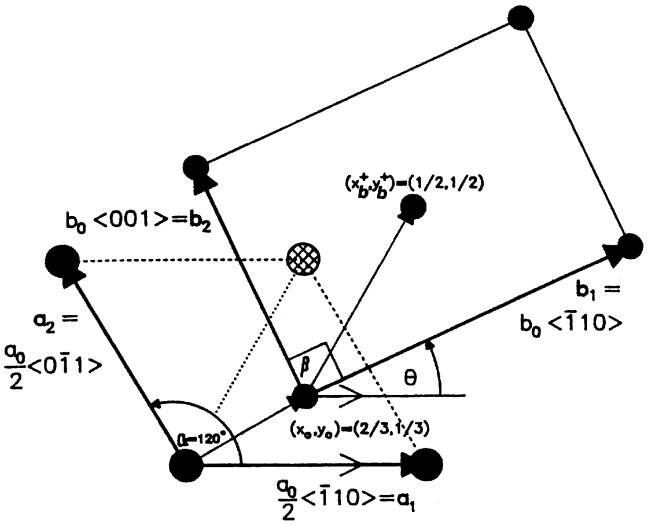


Fig. 1—Transformation parameters for bcc {110} overgrowth (small circles) on fcc {111} substrate (larger circles).

## III. THE EPITAXIAL CRITERION

We extend the relation [1] to deal with an island characterized by primitive interfacial unit cells of $(2M + 1) \times (2N + 1)$ overgrowth lattice points (adatoms C) on a substrate (S) with primitive unit cells (atoms A). This can easily be generalized to crystalline-island overlayers involving this and more complicated cases, as is done subsequently. In this simple case, the overgrowth lattice sites are arranged as 2M + 1 rows of 2N + 1 points each and are generated by displacing a single point by all the vectors in the set

$$\mathbf{r}_{mn} = m\mathbf{b}_1 + n\mathbf{b}_2 \text{: } m = -M, -M+1, \ldots -1, 0, 1, \ldots M, \quad n = -N, -N+1, \ldots -1, 0, 1, \ldots N \qquad [3]$$

The vectors $\mathbf{b}_1$ and $\mathbf{b}_2$, with lengths of $b_i = C_{bi} b_{nn}$ $(i = 1, 2)$ and an angle of $\beta$ between them, form the set of basis vectors of the Bravais lattice of the overgrowth surface; the coplanar vectors, $\mathbf{b}_1^*$ and $\mathbf{b}_2^*$, define the overgrowth surface-reciprocal lattice with $\mathbf{b}_i \times \mathbf{b}_j^* = 2\pi\delta_{ij}$. The relationship between the substrate and overgrowth unit cells, for an example system of a bcc(110) overgrowth on an fcc(111) substrate, are shown in Figure 1.

The total interaction energy for the island is obtained by summing the adatom interaction energy over all the atoms (hence, all $m$ and $n$ terms) in the overgrowth island, which yields a geometric series and, after some simplification, is expressed as

$$V = \sum_{h,k} V_{hk} \left( \frac{\sin \pi(2M+1)p}{\sin \pi p} \times \frac{\sin \pi(2N+1)q}{\sin \pi q} \right)_{hk} \qquad [4]$$

where $p$ and $q$ are functions of $h$ and $k$, given by the expressions

$$p(h,k) = hr_{11}c_\theta + kr_{12}s_\theta,\ q(h,k) = hr_{21}s_{\theta\beta} + kr_{22}c_{\theta\beta} \qquad [5a]$$

Here, $\theta$ is the angle between $\mathbf{b}_1$ and $\mathbf{a}_1$ and determines the relative orientations of the overgrowth and substrate unit cells. The ratios

$$r_{ij} = \frac{b_i}{a_j} = \frac{C_{bi}}{C_{aj}} r, \qquad r = \frac{b_{nn}}{a_{nn}} \quad (i, j = 1, 2) \qquad [5b]$$

define the dimensional relationship between the overgrowth and substrate lattices in terms of the parameter $r$, the ratio of nearest-neighbor distances in the respective lattices, which identifies most readily with the atomic-size ratio introduced by Bruce and Jaeger.[11] Other transformation parameters in Eq. [5a] are

$$c_\theta = \frac{\sin(\alpha - \theta)}{\sin \alpha}, \qquad s_\theta = \frac{\sin \theta}{\sin \alpha}$$
$$s_{\theta\beta} = \frac{\sin(\alpha - \beta - \theta)}{\sin \alpha}, \qquad c_{\theta\beta} = \frac{\sin(\beta + \theta)}{\sin \alpha} \qquad [5c]$$

Implicit to the derivation of Eq. [4] is the assumption that atoms in the overlayer interact independently with the substrate, so that the total may be obtained by simple summation. An equally important assumption is that the atomic interaction across the interface is of rather short range and involves the atoms adjacent to the interface only.

Direct calculation of the transformation between the $\mathbf{b}_1$ and $\mathbf{b}_2$ and $\mathbf{a}_1$ and $\mathbf{a}_2$ systems (by expressing these vectors in terms of a common Cartesian coordinate system, and solving for $p$ and $q$) shows that $p(h, k)$ and $q(h, k)$ in Eqs. [4] and [5] are the coordinates of the substrate wave vector $\mathbf{q}_{hk} = h\mathbf{a}_1^* + k\mathbf{a}_2^*$, expressed in the overgrowth reciprocal lattice as $\mathbf{q}_{hk} = p(h, k)\,\mathbf{b}_1^* + q(h, k)\,\mathbf{b}_2^*$. The energy in Eq. [4] peaks sharply when $p$ and $q$ are *integers*. When this necessary condition is met, the interfacial energy is sharply minimized. Consequently, the translation vector of the substrate reciprocal lattice $\mathbf{q}_{hk}$ must coincide with a translation vector of the overgrowth reciprocal lattice, $\mathbf{q}^{pq}$. The condition

$$\mathbf{a}_{hk} = \mathbf{q}^{pa}, \quad i.e., \mathbf{q}_{hk} \equiv h\mathbf{a}_1^* + k\mathbf{a}_2^* = p\mathbf{b}_1^* + q\mathbf{b}_2^* \equiv \mathbf{q}^{pq} \qquad [6]$$

is a *necessary* condition for an *ideal epitaxial configuration*, which is defined as the orientation and associated lattice parameters at which the interfacial misfit energy is minimized for a rigid system, as introduced by van der Merwe.[3] Note that the essence of the rigidity condition is that the overlayer atomic positions in Eq. [3] form a regular grid. This also includes a homogeneously deformed lattice (epilayer). At equilibrium, systems with ideal lattice parameters will be found in the orientation yielding the least interfacial energy. This necessary condition for interfacial-energy minimization has previously been obtained from a different energy model by Fletcher.[5]

As discussed subsequently, the condition [6] is equivalent to a criterion that epitaxy occurs when sets of lattice rows in the overgrowth and substrate are parallel and have equal spacing in the interface. Atomic rows, as opposed to lattice rows, are governed by the reciprocal-lattice criterion if the reciprocal lattice is appropriately modified by the inclusion of structure factors to account for nonprimitive unit cells and translations. Only reciprocal lattice translation vectors, which do not cause the combined structure factors to vanish, are relevant.

## IV. GEOMETRIC CONSEQUENCES OF THE EPITAXIAL CRITERION

### A. *Matching of Lattice Rows*

Discussion of the ideal epitaxial condition and its geometric criterion is simplified with a system of indices for directions and lattice rows in the surface lattice, consistent with Miller indices in crystallography. These indices may be associated with directions and spacings of families of rows of lattice points. Just as reciprocal lattice vectors of a three-dimensional lattice act as wave-propagation vectors of plane-wave fronts which coincide with lattice planes, so in two dimensions reciprocal lattice vectors propagate line fronts that coincide with rows of lattice points. The spacing of these lattice rows is given by the wavelengths of the propagation vectors, while the components of the reciprocal lattice vector provide Miller indices for the lattice rows. In particular, the reciprocal lattice vector $\mathbf{q}_{hk} = h\mathbf{a}_1^* + k\mathbf{a}_2^*$ (denoted here by $[h\ k]^*$) defines a family of direct lattice rows that may be indexed as $(h\ k)$, and the vector $\mathbf{q}_{hk}$ is perpendicular to these rows. The reciprocals of the indices give the intercepts of the first lattice row of the family along the $\mathbf{a}_1$ and $\mathbf{a}_2$ vectors, and integer multiples give the intercepts of the others. A specific direction in direct space parallel to $x\mathbf{a}_1 + y\mathbf{a}_2$ is written as $[x\ y]$. The spacing of the rows propagated by $[h\ k]^*$ is given by

$$\lambda_{hk} = \frac{2\pi}{|\mathbf{q}_{hk}|} = 2\pi \div \sqrt{h^2\mathbf{a}_1^* \cdot \mathbf{a}_1^* + 2hk\mathbf{a}_1^* \times \mathbf{a}_2^* + k^2\mathbf{a}_2^* \times \mathbf{a}_2^*} \qquad [7]$$

In analogy to the zone law of crystallography, it is always true that

$$h\mathbf{a}_1^* + k\mathbf{a}_2^* = [h\ k]^* \perp [k\ \bar{h}] \equiv k\mathbf{a}_1 - h\mathbf{a}_2 \qquad [8]$$

where the overbar indicates a negative index. Lattice rows, indexed as $(h\ k)$, lie parallel to the direct lattice direction $[\mathbf{k}\ \bar{\mathbf{h}}]$.

Consequences of the coincidence of a pair of overgrowth and substrate reciprocal lattice vectors include the following.

(1) If the wave vectors are parallel, then so are the lattice rows they propagate. When crystals are aligned in ideal epitaxial orientation, lattice rows of substrate and overgrowth are aligned in a parallel orientation.

(2) The aligned lattice rows have the same spacing in a direction perpendicular to the lattice rows. Since $\mathbf{q}_{hk} = \mathbf{q}^{pq}$, it follows that $\lambda_{hk} = \lambda^{pq}$ where

$$\lambda^{pq} = \frac{2\pi}{|\mathbf{q}^{pq}|} = 2\pi \div \sqrt{p^2\mathbf{b}_1^* \times \mathbf{b}_1^* + 2pq\mathbf{b}_1^* \times \mathbf{b}_2^* + q^2\mathbf{b}_2^* \cdot \mathbf{b}_2^*} \qquad [9]$$

This is analogous to the Bragg condition of crystallography.

(3) The spacing of atoms *along* the rows is not matched by this single criterion. Matching a second spacing also produces full two-dimensional coherency.

### B. *Construction*

The matching criterion of Eq. [6] is analogous to the von Laue condition of diffraction theory[12] and leads to a

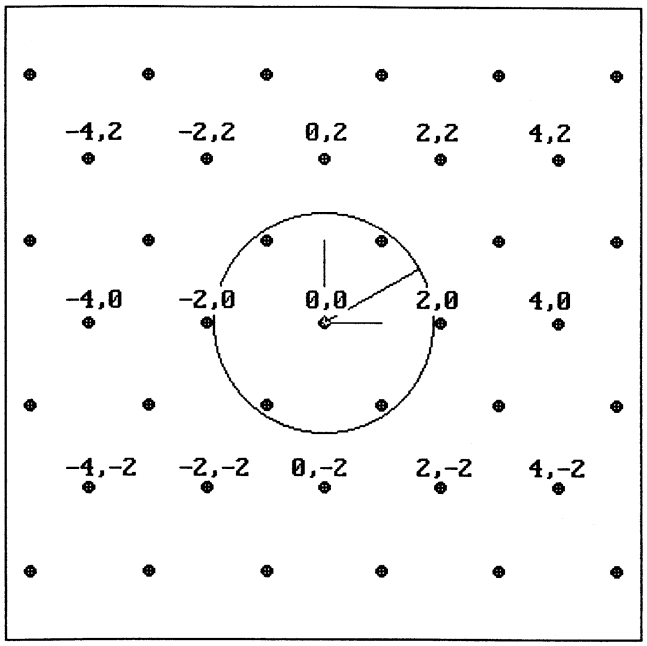


Fig. 2—The "Ewald circle" corresponding to the substrate wave vector [1 0]*. Both overgrowth reciprocal lattice vectors [2 0]* and [1 1]* lie close to the circle. Note also that although the unit cell of the bcc(110) surface was rectangular, the effect of the central point has been to remove some reciprocal lattice points, illustrating the effect of the structure factor.

geometrical realization similar to the Ewald construction, as illustrated in Figure 2. This simplifies the qualitative discussions of epitaxy of real crystals and simultaneously provides a visualization and a tool for quantitative predictions of epitaxial orientations.

The steps in the construction may be described as follows.

(1) Choose the substrate lattice row which is to be matched with the overgrowth. Express its direction as the substrate direct lattice direction [**k** $\bar{\mathbf{h}}$]. Plot $\mathbf{q}_{hk} = [h\ k]^*$ to a suitable scale in the substrate reciprocal lattice. Substrate structure factors, to be considered subsequently, may, depending on their sign and magnitude, respectively, nullify the given vector $\mathbf{q}_{hk}$, or reduce the epitaxial potency associated with it. This must be taken into account.
(2) Draw a circle, centered at the origin, through the end of $\mathbf{q}_{hk}$. This circle forms the locus of the endpoint of $\mathbf{q}_{hk}$ when this vector is rotated through 360 deg.
(3) Plot the overgrowth reciprocal lattice to the same scale and in any suitable orientation, but with the origin at the start of the vector $\mathbf{q}_{hk}$. (Again, take account of structure factors.)

Any overgrowth reciprocal lattice point $\mathbf{q}^{pq}$ that lies on this circle will describe an overgrowth reciprocal lattice translation vector, equal in length to $\mathbf{q}_{hk}$, and, hence, yields the $p$ and $q$ values which satisfy the epitaxial criterion of Eq. [6]. In addition, when the overgrowth lattice is rotated so that a lattice point $\mathbf{q}^{pq}$ lying on the circle coincides with $\mathbf{q}_{hk}$, the overgrowth and substrate atomic rows with the same spacings in both lattices that are perpendicular to $\mathbf{q}^{pq}$ and $\mathbf{q}_{hk}$ will be parallel. The overgrowth and substrate will be in an ideal epitaxial orientation.

The angle between the vectors $\mathbf{q}^{pq}$ and $\mathbf{q}_{hk}$ gives the angle through which the overgrowth needs to rotate in relation to the substrate to achieve epitaxy. This angle, $\theta_R$, is given by

$$\cos(\theta_R) = \frac{\mathbf{q}_{hk} \times \mathbf{q}^{pq}}{|\mathbf{q}_{hk}||\mathbf{q}^{pq}|} \qquad [10]$$

The vector cross product $\mathbf{q}^{pq} \times \mathbf{q}_{hk}$ defines the sense of the rotation. The nearest-neighbor ratio that allows a particular pair of vectors to match in length can be calculated from the condition $\lambda_{hk} = \lambda^{pq}$, when the parameters $C_{b1}$ and $C_{b2}$ and the unit-cell angle $\beta$ are unchanged.

The pair of values $\theta_R$ and $r$ (Eq. [5b]) associated with a given pair of surface structures, together with a choice of the orientation for which $\theta = 0$, allows ideal epitaxial configurations to be specified uniquely for a given pair of interfacial planes. Such a convention was used by Bruce and Jaeger[11] and van der Merwe.[3]

To express the epitaxial configuration as parallel crystallographic directions, the lattice row directions must be written in terms of the (three-dimensional) crystallographic indices of the surface unit-cell vectors: if the unit-cell vectors are given as $\mathbf{a}_1 = [u\ v\ w]$ and $\mathbf{a}_2 = [U\ V\ W]$;, respectively, the reciprocal lattice vector $[h\ k]^*$ (itself perpendicular to [**k** $\bar{\mathbf{h}}$]) relates to the row of atoms which lies parallel to the direction $k\mathbf{a}_1 - h\mathbf{a}_2 = [ku\text{-}hU\ kv\text{-}hV\ kw\text{-}hW]$. Similarly, the matched overgrowth reciprocal lattice vector provides the crystallographic indices of the matched direction and the index of the row of lattice points whose spacing is matched with the substrate, but along which lattice points are not necessarily matched.

As an example, consider the bcc(110) surface and its epitaxy with an fcc(111) surface, as in Figure 1. Surface unit-cell basis vectors are $\mathbf{a}_1 = 1/2[\bar{1}\ 1\ 0]$ and $\mathbf{a}_2 = 1/2[0\ \bar{1}\ 1]$ for the fcc substrate and $\mathbf{b}_1 = [\bar{1}\ 1\ 0]$ and $\mathbf{b}_2 = [0\ 0\ 1]$ for the bcc overgrowth, respectively. For perfect matching in the well-known Nishiyama–Wassermann orientation, the overgrowth reciprocal lattice vector [2 0]* coincides with the substrate reciprocal lattice vector [1 0]*. In surface coordinates, the lattice row, whose spacing is matched is then perpendicular to the respective surface reciprocal lattice vectors, is $[0\ \bar{2}]$ and $[0\ \bar{1}]$ for the overgrowth and substrate, respectively. Hence, the crystallographic directions of the overgrowth and substrate, which are parallel, are $[0\ 0\ \bar{1}]$ and [0 1 1], respectively. Lattice positions along these directions are not matched, but the spacing of rows in the perpendicular (overgrowth $1/2[\bar{1}\ 1\ 0]$ and substrate $1/4[\bar{2}\ 1\ 1]$) directions are equal.

## V. MISFIT AND MISFIT ACCOMMODATION

### A. *Measures of Misfit*

Misfit between two crystals with identical structure, meeting at the same crystallographic plane but differing only in an overall scale factor, may intuitively be expressed by a single ratio of lattice parameters. This simple description breaks down when surface symmetries and orientations differ. The row-matching criterion (Eq. [6]) provides a general framework for defining misfit of general interfaces.

Two classes of misfit can be identified. These are *orientational* misfit and *dimensional* misfit (general misfit contains aspects of both). The orientational misfit is given by the angle between nearly coinciding reciprocal lattice vectors as $\theta_R$, defined by Eq. [10].

Measures for the dimensional misfit have been introduced by several authors and are convenient under specific conditions. Consider the following three expressions for misfit, where $\lambda_a$ and $\lambda_b$ are the substrate and overgrowth lattice spacings, respectively.

$$f_a = \frac{\lambda_a - \lambda_b}{\lambda_a}; \qquad f_b = \frac{\lambda_a - \lambda_b}{\lambda_b}; \qquad f_{ab} = \frac{\lambda_a - \lambda_b}{\frac{1}{2}(\lambda_a + \lambda_b)} \qquad [11]$$

The first was introduced by Frank and van der Merwe[1] and applies when the substrate is considerably thicker than the overgrowth and is approximately rigid while the misfit is referred to the substrate lattice spacing, $\lambda_a = \lambda_{hk}$ (Eq. [7]), while $\lambda_b = \lambda^{pq}$ (Eq. [9]) is the overgrowth spacing. The second was used by Matthews[13] and applies most conveniently when the overgrowth strains to partially match the substrate, and the misfit calculated by this expression has the same sense as strain when related to the initial overgrowth lattice spacing. The third averages the lattice spacings and was used by van der Merwe[14] and Jesser and Kuhlmann-Wilsdorf[15] to describe systems in which overgrowth and substrate both strain. While the first and third definitions are actually the negatives of those of the original authors, they are preferred here for the convenience of having the same sense for misfit and strain. Besides the functional advantages of particular definitions of dimensional misfit, each expression is related to a particular choice of Burgers vector. The Burgers vector expresses directly the closure failure (per misfit dislocation) associated with a dislocation array that may accommodate the misfit. These aspects are discussed subsequently.

### B. *Misfit Accommodation by Homogeneous Strain in One and Two Dimensions*

If rows of atoms nearly match in orientation and spacing (the corresponding reciprocal lattice vectors nearly coincide), the overgrowth (with the substrate treated as rigid) may be expected to deform to reduce mismatch if the energy cost due to strain is less than the energy gained when the register is improved.

If the shape of the minimum in the energy function (Eq. [4]) is a very narrow well, then the overgrowth effectively distorts until exact matching is achieved, while for a wide well, the energy will be minimized without exact matching. The overgrowth structure deforms homogeneously toward adopting the substrate lattice spacing. The term pseudomorphism has been adopted if matching has been achieved, and the strain associated with the deformation has been termed misfit strain.

Matching may involve a single direction in the crystal in which the overgrowth strains to match the spacing of a family of rows, while the lattice spacing along the rows remains mismatched (one-dimensional pseudomorphism). Alternatively, matching may be achieved in all directions (two-dimensional pseudomorphism). This may include coincidence matching in the sense of Frank or O-lattice matching in the sense of Bollmann,[16] where some lattice rows may be skipped in the overgrowth or the substrate.

The strains necessary to achieve matching may be calculated directly from the condition for ideal epitaxy (Eq. [6]), while predictions of strains in perpendicular (free) directions and associated energy densities may be calculated within the assumptions of elasticity theory.[2,17,18] This requires estimates of elastic constants for the overgrowth region, and even if they are somewhat uncertain for very thin overgrowths, the energy density does provide a measure of the likelihood that a particular configuration will be observed: the greater the deformation energy, the less the likelihood that the configuration will be observed. Elastic constants must be transformed to a coordinate system suitable for the overgrowth as a two-dimensional system, and plane-stress boundary conditions must be enforced to account for the free surface parallel to the interfacial plane to yield a suitable expression for the energy density in terms of two-dimensional strains:

$$\xi = \frac{1}{2}(D_{11}\varepsilon_x^2 + D_{22}\varepsilon_y^2 + D_{33}\gamma_{xy}^2) + D_{12}\varepsilon_x\varepsilon_y + D_{13}\varepsilon_x\gamma_{xy} + D_{23}\varepsilon_y\gamma_{xy} \qquad [12]$$

where the $D$ terms are appropriately transformed, two-dimensional elastic constants. It is sufficient to point out here that, where the intention is to calculate the spacing, orientation, and character of arrays of misfit dislocations which accommodate *residual* strain, the strained lattice parameters can be substituted into expressions [1] through [4].

### C. *Misfit Dislocations and Misfit Vernier*

The third misfit accommodation mode, besides simple rotation and homogeneous strain, occurs when the energy associated with misfit strain exceeds that to be gained by exact matching. Local relaxation will occur if possible, but overall lattice periodicities will not be the same in overgrowth, and substrate and reciprocal wave vectors will not coincide. Local relaxation does imply alternate regions of good and poor matching. This pattern is associated with misfit dislocations if the regions of fit are larger than those of the mismatch. "Misfit Vernier" is the term used by van der Merwe[3] to characterize the pattern that occurs if the regions of good and bad fit are of nearly equal size with essentially no relaxation. In both cases, these patterns repeat, and the period is known as the *dislocation spacing* or *vernier period*, as appropriate. The period can be calculated by exploiting the analogy between misfit dislocation arrays arising from the growth of crystals with different lattice spacings and the superposition of two waves of different wavelengths to produce beats. Similar geometric considerations have shown these associations with Moiré patterns both in direct space, as observed by Bollmann,[16] and in reciprocal space, as observed by Jesser.[19]

From the superimposed wave analogy, the beat wave vector is given by the difference of the wave vectors (Figure 3):

$$\delta\mathbf{q} = \mathbf{q}_b - \mathbf{q}_a \qquad [13]$$

where $\mathbf{q}_b$ and $q_a$ are nearby wave vectors from the overgrowth and substrate, respectively. The wave vector $\delta\mathbf{q}$ determines the spacing of the beats, or dislocations, and their orientation. The spacing (similar to Eq. [7]) is

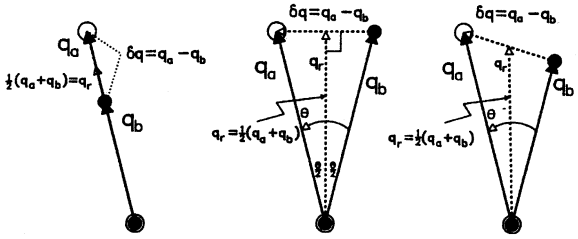


Fig. 3—(*a*) through (*c*) Characteristics of misfit dislocations, which can be determined from the reciprocal lattice. Note how the reference Burgers vector $\mathbf{B}_r$ and the dislocation line sense vector $\mathbf{Z}$ determine the character of the misfit dislocation array uniquely. These are obtained from the vectors $\mathbf{q}_r$ and $\delta\mathbf{q}$, where $\mathbf{B}_r \parallel \mathbf{q}_r$, while $\mathbf{Z} \perp \delta\mathbf{q}$.

$$\lambda_D = \frac{2\pi}{|\delta\mathbf{q}|} = \frac{2\pi}{\sqrt{\delta\mathbf{q} \times \delta\mathbf{q}}} = \frac{2\pi}{\sqrt{(\mathbf{q}_a - \mathbf{q}_b) \times (\mathbf{q}_a - \mathbf{q}_b)}} = \frac{\lambda_a\lambda_b}{\sqrt{\lambda_a^2 + \lambda_b^2 - 2\lambda_a\lambda_b \cos\theta_R}} \quad [14]$$

while dislocation lines are parallel to the wave front propagated by the wave vectors. Applying Eq. [8], the lines of coinciding phases (the wave fronts) lie along direct-space lattice directions given by $\mathbf{Z} = [\delta q_2, \delta\bar{q}_1]$, which gives the *line sense* of the dislocation and may be expressed in substrate or overgrowth coordinates. The dislocation lines themselves intersect the basis vectors at integer multiples $1/(\delta q)_{a_1}\mathbf{a}_1$ and $1/(\delta q)_{a_2}\mathbf{a}_2$ in the substrate coordinates, where the substrate reciprocal lattice coordinates of the vector $\delta\mathbf{q}$ are used. Similarly, overgrowth coordinates provide the intercepts in the overgrowth lattice.

Misfit dislocations and misfit vernier share the property that the superimposed lattices are in exact phases repeatedly after a constant distance of $\lambda_D = (1/\lambda_b - 1/\lambda_a)^{-1} = P\lambda_r = (P + 1/2)\lambda_b = (P - 1/2)\lambda_a$ ($P$ is an integer when the ratio between $\lambda_a$ and $\lambda_b$ is rational) from which it follows that $1/\lambda_r = 1/2(1/\lambda_a + 1/\lambda_b)$ and that the misfit $f_{ab} = 1/P$. This is generalized to two dimensions by introducing a reference lattice (or, continuing the beat analogy, the wavelength of the superimposed wave) as

$$\mathbf{q}_r = \frac{1}{2}(\mathbf{q}_b + \mathbf{q}_a) \quad [15]$$

The Burgers vector can be expressed in terms of the reference lattice $\mathbf{q}_r$ or in terms of $\mathbf{q}_a$ or $\mathbf{q}_b$ as

$$\mathbf{B}_i = \lambda_i \frac{\mathbf{q}_i}{|\mathbf{q}_i|}, \quad \text{with } i = a, b, \text{ or } r \quad [16]$$

Definitions of the Burgers vector in terms of overgrowth or substrate lattice spacings have the convenient feature that crystallographic directions may be associated with them. The reference lattice definition has the useful characteristic that it expresses the character of the misfit dislocation directly and that the symmetrical measure of dimensional misfit, $f_{ab}$, is directly related to it.

Referring to Figure 3, when $|\mathbf{q}_a| = |\mathbf{q}_b|$, there is no dimensional difference between the lattices, but only an orientational difference. Here, $\mathbf{q}_r \perp \delta\mathbf{q}$, and a *pure screw* dislocation array is described, with the Burgers vector parallel to the dislocation line, in correspondence with the properties of a general dislocation and misfit dislocation theory.[14,15,19] The other extreme occurs when $\mathbf{q}_b \parallel \mathbf{q}_a$ with no orientational difference, but only dimensional misfit. This produces a *pure edge* misfit dislocation with the Burgers vector perpendicular to the dislocation line. Characterization of the screw and edge character of the misfit dislocations is a property of the Burgers vector $\mathbf{B}_r$, based on the reference lattice only, together with the sense of the dislocation array, $\mathbf{Z}$, given by the difference vector.[20]

A convenient approach may be to describe dislocation orientations and Burgers vectors crystallographically in whichever system (overgrowth or substrate) is preferred, but to determine the analytically important properties, such as the fraction of edge or screw character, from the reference lattice. Table I summarizes several of the important parameters.

Variations which can be considered include dislocation interactions whose Burgers vectors of arrays with equal spacing can be added to produce other, equivalent arrays or distended rows of misfit.

## VI. STRUCTURE FACTORS

The foregoing considerations on ideal epitaxial configurations and their reciprocal lattice description and construction are generalized to include island displacements and nonprimitive overlayer and substrate surface unit cells.

### A. *Substrate Structure Factors of Nonprimitive (Atomic Sites A and B) Substrate Surface Unit Cells*

Consider a primitive overgrowth island, formed of C atoms in position $\mathbf{r}$, while the substrate has atomic sites (or atoms) of two kinds, *A* at the origin and *B* in position $\mathbf{r}_+$, as measured in the surface plane. The overgrowth atom C is in a position of $\mathbf{r} - \mathbf{r}_+$ with respect to B. The interaction energy of C with respect to the pairs A and B is accordingly given by ($V \equiv V^C$), from Eq. [1]:

$$V(x, y) = \sum_{h,k=-\infty}^{\infty} V_{hk}\left(e^{i2\pi(hx+ky)} + \frac{V_{hk}^{+}}{V_{hk}} e^{i2\pi(h(x-x_+)+k(y-y_+))}\right) \equiv \sum_{h,k=-\infty}^{\infty} V_{hk}F_{hk}e^{i2\pi(hx+ky)} \quad [17]$$

One can introduce the following definitions:

$$F_{hk} = 1 + \omega_{hk}e^{-i2\pi(hx_+ + ky_+)}, \quad \omega_{hk} \equiv \frac{V_{hk}^{+}}{V_{hk}}$$

$$F_{hk} = F_{hk}^{c} - iF_{hk}^{s} = 1 + \omega_{hk}\cos 2\pi(hk_+ + ky_+) - i\omega_{hk}\sin 2\pi(hx_+ + ky_+) \quad [18]$$

to derive compact expressions for the potential given in Eq. [17] as well as real and imaginary parts which correspond to interactions described by cosine and sine functions, respectively. (The interaction potentials for the cosine and sine series are assumed to have real coefficients in the expressions given in Eq. [19].)

**Table I. Summary of Misfit Dislocation Descriptors Obtainable from the Reciprocal Lattice**

| Absolute Misfit | Dislocation Spacing | Reference Lattice |
|---|---|---|
| $\delta\mathbf{q} = \mathbf{q}_b - \mathbf{q}_a = [\delta q_1, \delta q_2]^*$ | $\lambda_D = \dfrac{2\pi}{\lvert\delta\mathbf{q}\rvert} = \dfrac{\lambda_a\lambda_b}{\sqrt{\lambda_a^2 + \lambda_b^2 - 2\lambda_a\lambda_b \cos\theta_R}}$ | $\mathbf{q}_r = \dfrac{1}{2}(\mathbf{q}_b + \mathbf{q}_a)$ with $\lambda_r = \dfrac{2\lambda_a\lambda_b}{\sqrt{\lambda_a^2 + \lambda_b^2 + 2\lambda_a\lambda_b \cos\theta_R}}$ |
| **Line Sense Vector** | **Burgers Vectors** | **Character** |
| $\mathbf{Z} = [\delta q_2, \delta\bar{q}_1]$ | $\mathbf{B}_i = \lambda_i \dfrac{\mathbf{q}_i}{\lvert\mathbf{q}_i\rvert}$, with $i = a$, $b$, or $r$ | Pure screw: $\mathbf{q}_r \perp \delta\mathbf{q}$<br>Pure edge: $\mathbf{q} \parallel \delta\mathbf{q}$<br>Screw fraction $= \cos^2\gamma$, where $\gamma$ is the angle between $\mathbf{B}_r$ and the line sense vector, $\mathbf{Z}$ |

$$
\begin{aligned}
V^c(x, y) &= \sum_{h,k=-\infty}^{\infty} V_{hk}(F^c_{hk} \cos 2\pi(hx + ky) \\
&\quad + F^s_{hk} \sin 2\pi(hx + ky)) \\
V^s(x, y) &= \sum_{h,k=-\infty}^{\infty} V_{hk}(F^c_{hk} \sin 2\pi(hx + ky) \\
&\quad - F^s_{hk} \cos 2\pi(hx + ky))
\end{aligned}
\qquad [19]
$$

The extension to more than one additional feature is straightforward and has more terms in each of the structure factors defined in Eq. [18], without changing the essential form of Eqs. [17] and [19].

### B. *Overgrowth Structure Factors of Island Size*

In this section, the inclusion of structure factors due to the overgrowth island is developed. As a first step, consider an asymmetrical island which is constructed from atoms at overgrowth lattice points defined by all the vectors in the set: $\mathbf{r}_{mn} = m\mathbf{b}_1 + n\mathbf{b}_2$:

$$
\begin{aligned}
m &= -M, -M + 1, \ldots -1, 0, 1, \ldots M' - 1, M', \\
n &= -N, -N + 1, \ldots -1, 0, 1, \ldots N' - 1, N'
\end{aligned}
\qquad [20]
$$

(Here $M'$, $M$, $N'$, and $N$ are not necessarily equal.)

Summing individual interaction terms of the exponential form given by Eq. [1] leads directly to

$$
V = \sum_{h,k} V_{hk}F_{hk}\left(e^{i\pi(M'-M)} \times e^{i\pi(N'-N)q} \times \frac{\sin\pi(M + M' + 1)p}{\sin\pi p} \times \frac{\sin\pi(N + N' + 1)q}{\sin\pi q}\right)_{hk} \qquad [21]
$$

The leading exponential expressions become 1 for a symmetrical lattice with $M = M'$ and $N = N'$. The quotients in the sine functions, as well as the leading exponentials, are responsible for island-size effects in the misfit energies. The delta function–like behavior of the quotients again leads directly to the *ideal epitaxial configurations*, as obtained earlier.

### C. *Structure Factor Expressing Translation of the Overgrowth Island*

If the origin of the overgrowth island undergoes a displacement of $x_0\mathbf{a}_1 + y_0\mathbf{a}_2$ from the origin of the substrate surface lattice, the $m$th and $n$th lattice points in the overgrowth are given as $m\mathbf{b}_1 + n\mathbf{b}_2 + x_0\mathbf{a}_1 + y_0\mathbf{a}_2$. It is seen that the translation term is common to all overgrowth lattice points, and, correspondingly, acts as a common multiplier of the quotient functions in Eq. [17] and produces a further set of structure factors:

$$
\begin{aligned}
F^o_{hk} &= e^{i2\pi(hx_0 + ky_0)} = F^{co}_{hk} + iF^{so}_{hk} \\
F^{co}_{hk} &= \cos 2\pi(hx_o + ky_o) \\
F^{so}_{hk} &= \sin 2\pi(hx_o + ky_o)
\end{aligned}
\qquad [22]
$$

Expression [21] now becomes

$$
V = \sum_{h,k} V_{hk}F_{hk}F^o_{hk}\left(e^{i\pi(M'-M)p} \times e^{i\pi(N'-N)q} \times \frac{\sin\pi(M + M' + 1)p}{\sin\pi p} \times \frac{\sin\pi(N + N' + 1)q}{\sin\pi q}\right)_{hk} \qquad [23]
$$

### D. *Nonprimitive Overgrowth Unit Cells*

Nonprimitive unit cells are characterized by the presence of more than one atom in a unit cell, or more than one lattice point in a unit cell. These are at positions displaced from overgrowth lattice positions. We derive the effect of this displacement by considering an atom displaced from a lattice site by $x^+\mathbf{b}_1 + y^+\mathbf{b}_2$. If the total interaction energy of these displaced atoms is considered, every $m$ term is shifted by $x^+$ and every $n$ term by $y^+$. This appears again in every exponent and can be taken out as common structure factor. In the simplest case, the essential symmetry of the substrate potential is retained, but may be subject to a multiplier, such as $\kappa$. Atoms at lattice positions do not contain this term, and a two-atom unit cell thus produces an unaltered energy expression, plus a second expression in which each Fourier term is multiplied by $\kappa$ and a displacement factor. As the displacement is expressed in terms of the basis vectors of the overgrowth, the displacement term is most compactly expressed in terms of the pair $p$, $q$. Overgrowth structure factors may then be defined as

$$
\begin{aligned}
F^{pq} &= 1 + F^{pq}_{+} = 1 + \kappa e^{i2\pi(px^+ + ky^+)} = F^{pq}_c + iF^{pq}_s \\
F^{pq}_c &= 1 + F^{pq}_{c^+} = 1 + \kappa \cos 2\pi(px^+ + qy^+) \\
F^{pq}_s &= F^{pq}_{s^+} = \kappa \sin 2\pi(px^+ + qy^+)
\end{aligned}
\qquad [24]
$$

These structure factors are readily generalized to a basis of more than one atom by including more terms in each expression.

E. *Most General Structure Factors*

The general expressions for the misfit energy of a multisite substrate, displaced, asymmetric, multiatom overgrowth is, finally, given by

$$V = \sum_{h,k} V_{hk} F_{hk} F^{o}_{hk} F^{pq} e^{i\pi(M'-M)p} \times e^{i\pi(N'-N)q} \times \left( \frac{\sin \pi(M + M' + 1)p}{\sin \pi p} \times \frac{\sin \pi(N + N' + 1)q}{\sin \pi q} \right)_{hk} \quad [25]$$

where the real part of the expression refers to interactions defined in terms of cosines only, and the imaginary part refers to interactions in terms of sines only ($V^c$ and $V^s$ of Eq. [19] respectively).

The combined structure factors may be shown to be

$$((F^{c}_{hk} F^{co}_{hk} + F^{s}_{hk} F^{so}_{hk})(F^{pq}_{c} F^{M,N}_{c} - F^{pq}_{s} F^{M,N}_{s}) - (F^{c}_{hk} F^{so}_{hk} - F^{s}_{hk} F^{co}_{hk})(F^{pq}_{s} F^{M,N}_{c} + F^{pq}_{s} F^{M,N}_{s})) \quad [26a]$$

for the real part, and

$$((F^{c}_{hk} F^{so}_{hk} - F^{s}_{hk} F^{co}_{hk})(F^{pq}_{c} F^{M,N}_{c} - F^{pq}_{s} F^{M,N}_{s}) + (F^{c}_{hk} F^{co}_{hk} + F^{s}_{hk} F^{so}_{hk})(F^{pq}_{s} F^{M,N}_{c} + F^{pq}_{c} F^{M,N}_{s})) \quad [26b]$$

for the imaginary part, with

$$F^{M,N}_{c} = \cos \pi((M' - M)p + (N' - N)q) \quad \text{and} \quad F^{M,N}_{s} = \sin \pi((M' - M)p + (N' - N)q) \quad [26c]$$

The structure factors due to the nonprimitive nature of the unit cells, namely, $F_{hk}$ and $F^{pq}$, will be zero for many combinations of the integers $h,k$ and $p,q$ and, thus, remove reciprocal lattice points from the substrate and overgrowth reciprocal lattices, respectively. Added atoms reduce the possible epitaxial-matching configurations otherwise predicted from consideration of the lattices alone. The translation structure factor $F^{o}_{hk}$ determines the phase of the overgrowth with regard to the substrate. A bad choice may put the overgrowth and substrate into direct opposition rather than coincidence and is characteristic of a rigid model. (This is significant when misfit dislocations are not allowed.)

In practice, when $h,k$ and $p,q$ are integers (as happens in ideal epitaxial configurations), the structure factors can be precalculated, only the relevant $V_{hk}$ terms need to be retained in the interaction potential, and some complexity can be removed from analytical descriptions of even complex structural pairs. In all cases, the role of the sine quotients in $p$ and $q$, which lead to matching of rows of atoms in ideal epitaxial configurations, remains critically important.

## VII. PREDICTION OF INTERFACIAL CHARACTER

Exact prediction of the final interfacial structure would require a calculation that includes details of both the dynamics of growth and detailed knowledge of interatomic many-body interactions, or, within simplified models, knowledge of elastic constants of the systems and the active Fourier coefficients of the interaction potential (Eq. [1]). However, several qualitative considerations can be applied with the geometric considerations which are a consequence of the epitaxial criterion (Eq. [6]) to identify (and rank) strong candidates for epitaxial configurations for particular pairs of overgrowth and substrate.

These qualitative considerations can provide a preliminary ordering of candidate ideal epitaxial orientations into a *hierarchy*.[21] The ability to predict interfacial character can be improved somewhat if some broad quantitative considerations are added into the calculations. For example, elastic-energy densities (Eq. [12]) for the one- and two-dimensional pseudomorphic fit modes arising from the predicted ideal epitaxial configurations can be calculated; misfit dislocation strain energies can be estimated from well-known expressions, such as those of van der Merwe[1,15] and Matthews;[13] and structure factors (including size effects) can be precalculated.

The total interfacial energy given by (Eq. [5]) shows strong minima at ideal epitaxial configurations. This energy reduction provides the driving force to both orient and deform the unit cells on either side of the interface. While wave vectors match in reciprocal space and produce a periodic structure in direct space, matching of a particular pair of wave vectors also produces matching with multiples of these vectors—there is also a periodic structure produced in reciprocal space. The misfit-energy reduction is produced not only with the low-order Fourier coefficient, but also to an infinite number of higher-order terms. The higher the fraction of all possible vectors that are matched, the greater the energy reduction. Therefore, the *density* (in reciprocal space) *of matched vectors* is a qualitative parameter for prediction of good epitaxial candidates.

The misfit energy reduction is directly proportional to the Fourier coefficient $V_{hk}$. Stoop has shown that these Fourier coefficients decrease approximately exponentially with order of the Fourier term. The order has been defined as $|h| + |k|$ by Stoop,[8,22] which is more specifically expressed by the *length* (in reciprocal space) *of wave vectors*. It follows that the shorter the wave vectors which are matched, the more likely it is that the epitaxial orientation will be observed. It is true, though, that the criterion has to be applied with due caution, as Fourier coefficients of the same order may differ appreciably in magnitude and may even differ in sign.[23] The shortest wave vectors provide the longest range of order, and, hence, ideal epitaxial configurations can be ordered by the length of reciprocal wave vectors, or order.

Pseudomorphism is predicted for many epitaxial pairs and is a well-known concept since Frank and van der Merwe's articles of 1949.[1] The strain energy associated with the deformation of the overgrowth to matching the substrate must be obtained from the reduction of the misfit energy from the mismatched case. The smaller this energy, the greater the chance of the epitaxial configuration being realized in practice. The *elastic-strain-energy densities* (Eq. [12]) can be used to rank possible pseudomorphic configurations: the higher the strain-energy density, the less likely is the configuration to occur.

Polyatomic systems include atoms that exhibit varying bonding to the substrate (as expressed through the parameter $\kappa$), or one might include bonding sites of varying strength in the substrate potential, for example, to model stacking-fault energies (the parameter $\omega$). These are included in the *structure factors* of Eqs. [18] and [24]. The smaller or more negative the structure factors (Eq. [26]) the less likely is the

configuration, although it is to be noted that the effects of translation (Eq. [22]) of the unit cell must also be fully examined, as appropriate translations may change the sign of the interaction term.

Finally, *size effects* must be considered within the context of the growth mechanism and history. When the islands are small, two effects on the misfit-energy function are evident. First, the quotients of sines in Eq. [5] are not sharp, and the growing island can conceivably orient and strain to match the substrate with a less sharply defined orientation than would apply to a large island. Second, the sine quotients themselves show secondary minima that, although shallower, may orient the growing overgrowth island toward them.[3] Linked to the size effect is the effect of higher-order terms in the Fourier expansion (long-wave vectors). The higher the order of the wave vectors, the greater the number of candidate configurations (now properly described as coincidence configurations) which are close to one another. The minima of several of these configurations may indeed overlap while islands are small, leading to a range of orientations within which the island may grow during its early stages.

The bcc(110)/fcc(111) interface provides an example of effects which may be ascribed to growth history. Two well-described configurations are close to one another, known as the Nishiyama–Wassermann and the Kurdjumov–Sachs configurations. Calculations from reciprocal space show that if an island is originally in two-dimensional coherence, it is strained to match the reciprocal pairs associated with both configurations. However, once the island gets too large to match both (the strain energy being too high), a rotation of 5.26 deg is needed to retain a match with the Kurdjumov–Sachs pair, while perfect orientation with the Nishiyama–Wassermann configuration is achievable without rotation. Gaigher and van der Berg[24] have reported observations on substances which fall between the ideal lattice parameters for the Kurdjumov–Sachs and the Nishiyama–Wassermann configurations. They show that orientations found lie in a small range of 2 deg around the former orientation, while the Nishiyama–Wassermann configuration is usually sharply defined. This range may be ascribed to growth history if the small island assumes near-pseudomorphism in early stages, then ceases to match with one of the vector pairs as the energy minimum becomes more sharply defined with larger island size. Any impediment to rotation would mean that the island is discovered away from an exact orientation. Also, the Fourier coefficients responsible for the Kurdjumov–Sachs orientation have larger magnitudes than the two coefficients—one of which is positive—responsible for the Nishiyama–Wassermann orientation. Consequently, the range of misfit within which the coefficients for the Nishiyama–Wassermann orientation is effective is narrowed, and narrows down faster with increasing thickness, than that generating the Kurdjumov–Sachs orientation.[25] The qualitative criteria allow a hierarchy of possible epitaxial configurations to be established, which allows some prediction of likely candidates.

In addition to providing a basis for the prediction of candidates for epitaxial configurations, the reciprocal space considerations provide a *tool for the analysis* of experimental observations. If, for example, a system is known to have a particular (strained) lattice parameter, this may be used to calculate the reciprocal spaces of the overgrowth, and the residual misfits can be determined by identifying and examining reciprocal lattice points which are in near-match conditions. These provide the parameters of expected misfit dislocation arrays (Table I), against which the actual interfacial structure can be evaluated.

## VIII. CONCLUSIONS

The reciprocal-space condition $\mathbf{q}^{pq} = \mathbf{q}_{hk}$, which expresses row matching as a necessary condition for exact epitaxial matching, has produced a powerful technique for analyzing epitaxial systems. Although it expresses a geometric relationship, it is obtained from energy considerations. When these vectors do not coincide, their difference can be used to calculate the orientational and dimensional misfits, the misfit strain and misfit dislocation structures including Burgers vectors, the spacings and orientation of dislocation arrays, and the edge and screw character in any given interface within a single formulation.

General considerations lead to a qualitative hierarchy of ideal epitaxial configurations which can be ordered by the density of matched reciprocal lattice points, length of matched wave vectors, elastic strain energy densities, structure factors, size effects, and dislocation spacings.

The strength of the formalism lies in its generality, the uniqueness with which an epitaxial configuration can be described, and the quantity of detail that can be obtained from it. The disadvantages are that the two-dimensional nature requires vector manipulations and that, inherently, reciprocal space is not quite as intuitively natural as direct space. Favorable, once more, is that descriptions of periodic structures generally yield simpler expressions in reciprocal space, and that is exploited here.

A computer program[26,27] (known as Orpheus since 1985 and not related to the commercial software of the same name) for analyzing epitaxial interfaces and using all the relationships given here can be obtained from the authors (MWHB: mbraun@scientia.up.ac.za). It is written in Microsoft Quick-Basic* (MSDOS and MACINTOSH** versions). It automates a search for candidate epitaxial configurations with the construction of the Ewald type described in this article, provides strains for one- and two-dimensional coherency, strain energy densities, and values for structure factors, and gives a full list of crystallographic information on Burgers vectors, dislocation spacings, and screw and edge characters that can be expected.

*Microsoft Quick-Basic is a trademark of Microsoft Corporation.

**MACINTOSH is a trademark of Apple Computer Corp., Cupertino, CA.


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