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Analysis of reflection high-energy electron-diffraction data from reconstructed semiconductor surfaces

B. A. Joyce and J. H. Neave
Philips Research Laboratories, Redhill, Surrey RH1 5HA, United Kingdom

P. J. Dobson
Department of Physics, Imperial College of Science and Technology, Prince Consort Road, London SW7 2AZ, United Kingdom

P. K. Larsen
Philips Research Laboratories, 5600-MD Eindhoven, The Netherlands
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Features in reflection high-energy electron-diffraction patterns arising from various types of surface disorder are discussed, with specific examples of each. The relationship between (001)2×4 and (001)-$c(2\times8)$ reconstructions, which are frequently observed on III-V compound semiconductor surfaces, is explicitly demonstrated.

I. INTRODUCTION

It is apparent from several recent publications[1-3] that the analysis of reflection high-energy electron-diffraction (RHEED) data from reconstructed surfaces of semiconductors remains problematical, even when a purely kinematic treatment based on Ewald-sphere—reciprocal-lattice concepts is used. Particular difficulties arise when one-dimensional disorder boundaries or some lack of perfect periodicity are intrinsic features of the reconstruction.[4-6] The occurrence of such effects has, for example, resulted in reports that the 2×4 and $c(2\times8)$ reconstructions observed on (001) surfaces of III-V compound semiconductors are fundamentally different.[1-3,7]

In this paper we show how information on surface morphology, disorder, and topography can be extracted from RHEED patterns, and point out the importance of multiazimuthal measurements. We then explicitly define the relationship between III-V compound (001)2×4 and (001)-$c(2\times8)$ reconstructions in real and reciprocal space, emphasizing that they are not mutually exclusive. Finally, we comment briefly on possible values of the coherence area in RHEED.

II. EFFECTS OF SURFACE MORPHOLOGY, DISORDER, AND TOPOGRAPHY ON RHEED PATTERNS

We should first refer briefly to the appearance of diffraction streaks as opposed to spots in RHEED patterns. For streaks to be observed from a perfectly ordered, perfectly smooth surface, using an ideal instrument (i.e., with no angular or energy spread in the primary beam) they must have an intrinsic origin. The thermal diffuse scattering mechanism proposed by Holloway and Beeby[8] seems the most probable of those advanced so far, but it has not yet been substantiated by experiment. If we consider real surfaces and real instruments, however, several effects can already be explained from simple extensions of the reciprocal-lattice—Ewald-sphere construction. For the cases we are considering here we expect any contribution to streaking from the nonideality of the primary beam to be small.

To obtain the maximum amount of information on overall surface structure from RHEED observations it is also important to obtain diffraction patterns at several azimuthal angles. There are two principal reasons for this.

(i) When there is little or no intensity modulation along the streak it is extremely difficult to determine the complete surface symmetry from a single azimuth. This type of pattern is, however, very frequently encountered with semiconductor surfaces, an example of which is shown in Fig. 1.

(ii) Any one- or two-dimensional disorder in the surface can only be detected and analyzed by using several az-

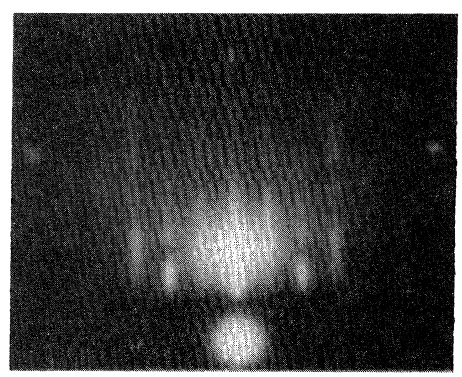

FIG. 1. RHEED pattern from GaAs(001) surface, [110] azimuth showing integral and half-order streaks. Note the effective absence of intensity modulation along the streaks.

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imuths, as we demonstrate below. This multiazimuthal approach is contrary to a recent assertion by Hernández-Calderón and Höchst[1] that it is preferable to use a single azimuth.

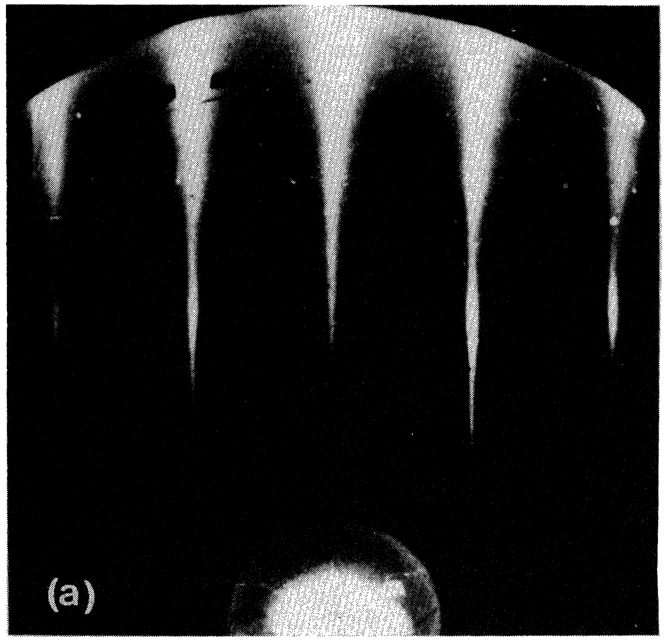
We are now in a position to discuss the effects of various types of surface disorder on RHEED patterns.

(a) A polygonized surface, i.e., a mosaic structure which contains a large number of crystallites with a small ($\sim 1°$) angular spread, will produce fan-shaped streaks, as shown in Fig. 2(a). The corresponding Ewald-sphere—reciprocal-lattice construction is shown in Fig. 2(b).

(b) Two-dimensional disorder effects can also be analyzed from the streak shape. Under conditions of grazing incidence a reciprocal-lattice point is drawn out into a one-dimensional rod perpendicular to the surface, i.e., the third Laue condition is relaxed. Any lack of perfect ordering in a particular direction which restricts the average size of the ordered regions leads to the reciprocal lattice rod becoming two dimensional, forming a solid ellipsoidal cylinder. This point is illustrated in Fig. 3(a), where we show the effects along two orthogonal azimuths for the case when the domains are extensive in one direction and restricted in the perpendicular direction. With the beam parallel to the "short" domain side [Fig. 3(ai)] the streaks are long and narrow, which corresponds to the diffraction pattern Fig. 3(bi). When the beam is parallel to the "long" domain side the situation depicted in Fig. 3(aii) prevails, which produces short and broad streaks, corresponding to those in Fig. 3(bii). The domain structure giving rise to these has been discussed in detail elsewhere.[9]

(c) The presence of two-dimensional surface disorder, or domains, implies that they will be separated by one-dimensional (or antiphase) boundaries, which give rise to curved streaks provided the appropriate azimuth is used.[10,11] Such boundaries give planes in reciprocal space, and when the incident electron beam is parallel to the boundaries the Ewald sphere is tangential to the reciprocal-lattice planes and there is only an increase in background intensity. For any other azimuth, however, the planes and the Ewald sphere intersect to give curved streaks, as shown in Fig. 4(a), producing the type of RHEED pattern illustrated by Fig. 4(b). This example was taken in the [010] azimuth from a GaAs(001)2$\times$4 reconstructed surface which contained one-dimensional disorder boundaries along [$\bar{1}$10].[4] We will consider other features of this pattern in Sec. III.

(d) At least four topographic features can be identified from RHEED patterns, but it is important to realize that in general the length and width of streaks are not necessarily related to topography. The simplest case is surface roughness or asperities on such a scale that the glancing incidence beam produces a transmission diffraction pattern, in which there are no streaks but only sharp diffraction spots. The asperities need to be < 1000 Å thick (in the beam direction) to allow a transmission pattern to be formed at typical RHEED energies (< 20 keV). Undulating surfaces can also be identified from the "tailing" of spots towards the shadow edge.[12] The effect of step arrays on RHEED and low-energy electron-diffraction (LEED) patterns has been analyzed in detail by Henzler[13]



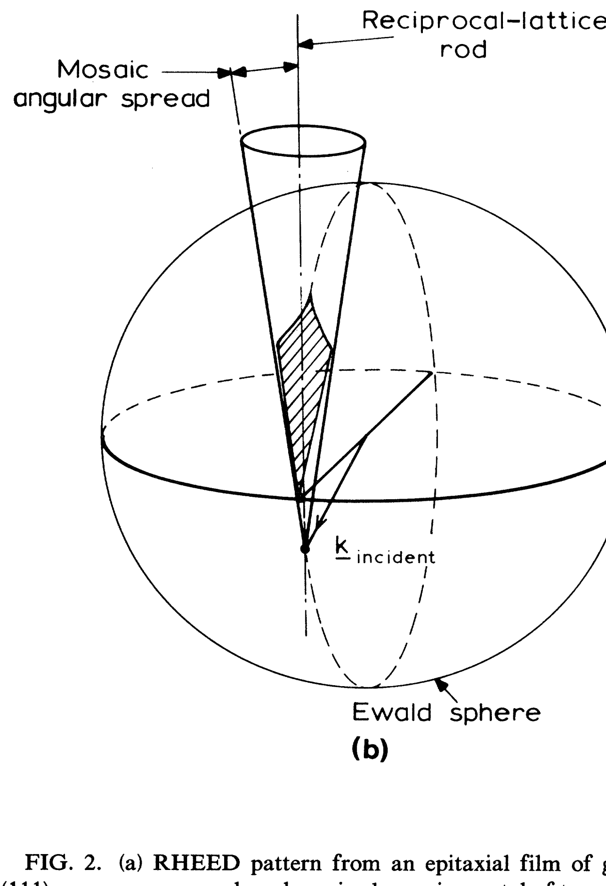


FIG. 2. (a) RHEED pattern from an epitaxial film of gold (111) grown on a severely polygonized mosaic crystal of tungsten (110) showing "fan-shaped" streaks. Mosaic spread $\sim \pm 3°$, beam along [110] at 30 keV. (b) Reciprocal-lattice—Ewald-sphere construction for mosaic structure. Shaded area indicates intersection of Ewald sphere with "mosaic cone."

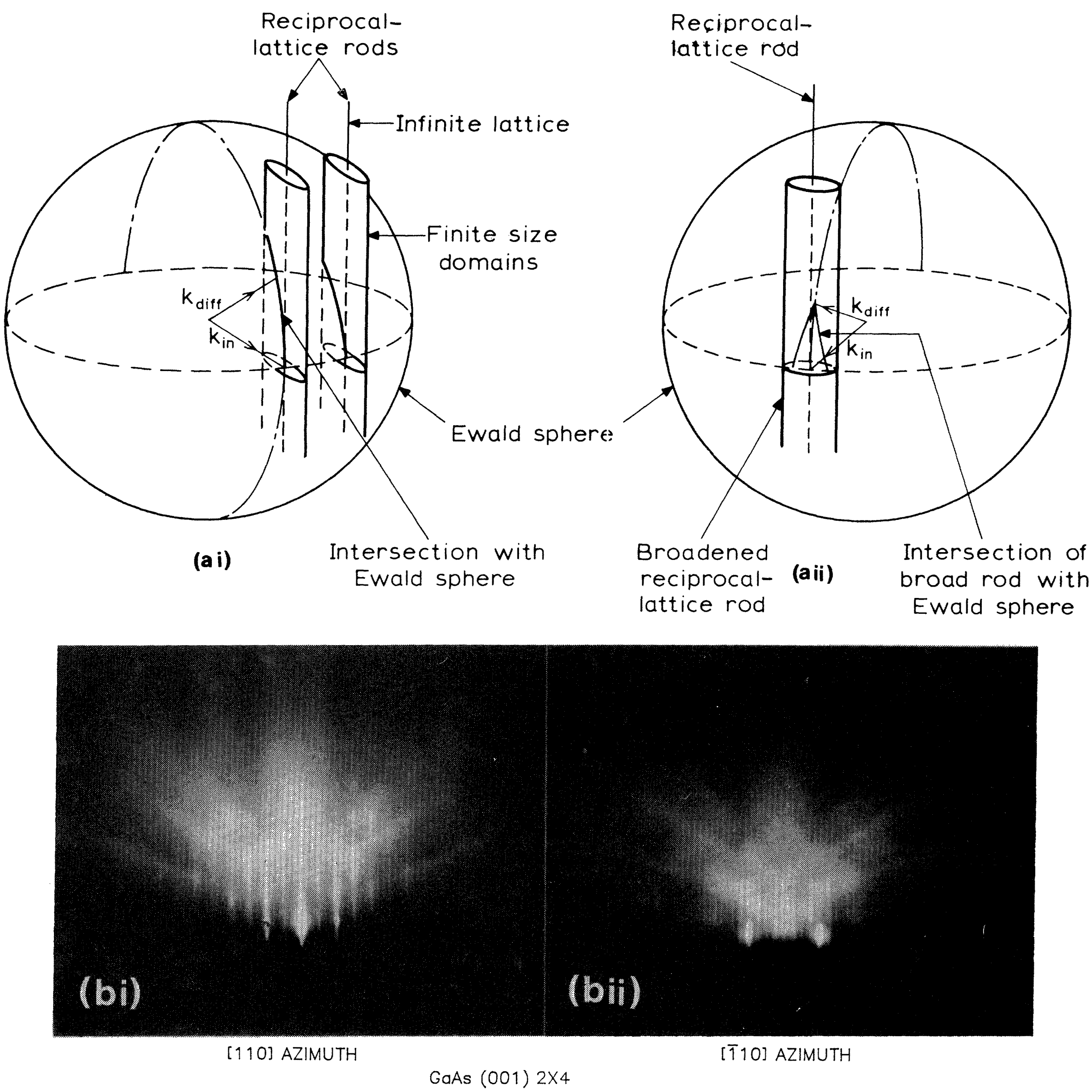


FIG. 3. (ai) and (aii) Reciprocal-lattice—Ewald-sphere construction showing lengthening and broadening of diffraction streaks resulting from lack of perfect ordering in a specific direction. (bi) and (bii) RHEED patterns illustrating this effect, from GaAs(001)2×4 reconstructed surface, [110] and [$\bar{1}$10] azimuths respectively.

and Hottier *et al.*,[14] so we will not consider it further here, beyond the general comment that steps are revealed by splitting of the diffracted beams in a manner characteristic of their orientation and spacing. Finally, the presence of facets shows up as additional streaks in the pattern, formed by diffraction from the facet planes, and so they are not normal to the shadow edge. This has been treated by Simmons *et al.*,[15] and in Fig. 5 we show an example of a RHEED pattern corresponding to the onset of growth by molecular beam epitaxy of an autoepitaxial GaAs film on a slightly contaminated GaAs(001) substrate. The arrowhead features are derived from {511} facets.

III. (001)2×4 AND (001)-*c*(2×8) RECONSTRUCTIONS OF III-V COMPOUND SEMICONDUCTORS

There has been considerable emphasis in the literature that (001)2×4 and (001)-*c*(2×8) surface symmetries, which occur on many III-V compound semiconductors, represent different structures which are mutually exclusive.[1–3,7] Critical examination of RHEED and LEED data shows that this is not the case, but that they are in fact simply related by a surface disorder effect. This has been implied in several publications,[4–6,1] and an example of the disorder can also be seen in Fig. 1 of Ref. 2, which was published without comment, but where the streaks in

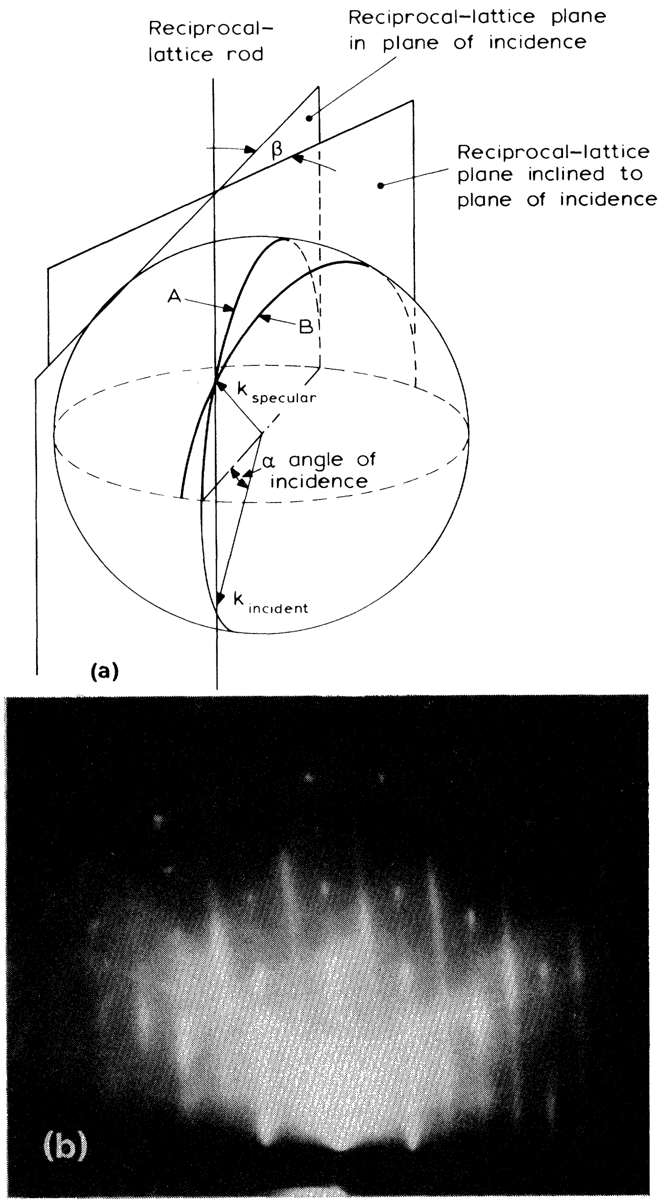


FIG. 4. (a) Reciprocal-lattice—Ewald-sphere construction showing the origin of curved streaks. A and B define the streaks originating from the reciprocal-lattice plane in the plane of incidence and inclined at an angle β, respectively. (b) [010] azimuth RHEED pattern from a GaAs(001)2×4 reconstructed surface. Note the curved streaks, and that extended streaks are only present in the half-order positions, i.e., they do not pass through the origin of reciprocal space.

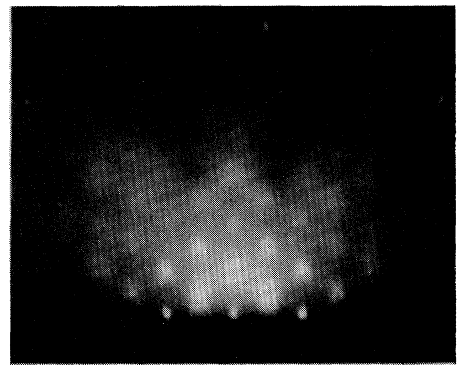


FIG. 5. RHEED pattern from a GaAs(001) surface, [110] azimuth. Facet formation is indicated by the arrowhead structure, in which the streaks are not normal to the shadow edge. For the angle between these streaks and the surface normal ($\sim 19°$) the facet planes are $\sim\{511\}$.

the [010] azimuth are clearly curved. Here we stress the important results and illustrate the relationship in real and reciprocal space. There are two features of the RHEED patterns which enable the analysis to be made.

(a) The presence of domains having a strong ordering direction is indicated by the lengthening and broadening of the fractional and integral order beams in a specific direction for two orthogonal $\langle 110 \rangle$ azimuths, as shown in Figs. 3(a) and 3(b).

(b) The observation of curved streaks in intermediate azimuths, as shown in Figs. 4(a) and 4(b), confirms the presence of one-dimensional disorder boundaries, but the periodicity of the disorder can also be deduced from the diffraction patterns. For these azimuths, the extended streaks are only present in the half-order positions, i.e., they do not pass through the origin of reciprocal space. This requires that the 1×4 lattice order is maintained, but that the periodicity along the twofold reconstruction direction is random. The real and reciprocal space representations of these boundaries are illustrated in Figs. 6(a) and 6(b), respectively, and in the latter case the disorder is shown as sheets in the half-order positions. The real space lattice shows quite clearly that 2×4 and $c(2\times8)$ domains can coexist, and are simply related by random positioning in the direction of twofold periodicity.

We can be rather more specific about the random positioning if we consider the presently accepted model for this reconstruction, shown schematically in Fig. 7 for GaAs. In it, the twofold periodicity is created by tilted As-As dimers, which is fully consistent with angle-resolved photoemission data and a tight-binding calculation of the surface structure.[9] The randomness then corresponds to the sequencing of dimer chains in the [110] direction, which can form 2×4, $c(2\times8)$, or less regular domains.

An identical result can be deduced from the LEED data of Drathen *et al.*[16] and Massies.[17] The results presented recently by Hernández-Calderón and Höchst[1] for InSb are not, however, very clear from their sketched RHEED patterns. The reciprocal-lattice section which they derive from the InSb(001) pattern does not account for the continuous streaks connecting the zero-order and first Laue zones. We suggest that such streaks are indicative of one-dimensional disorder (i.e., sheets in reciprocal space)

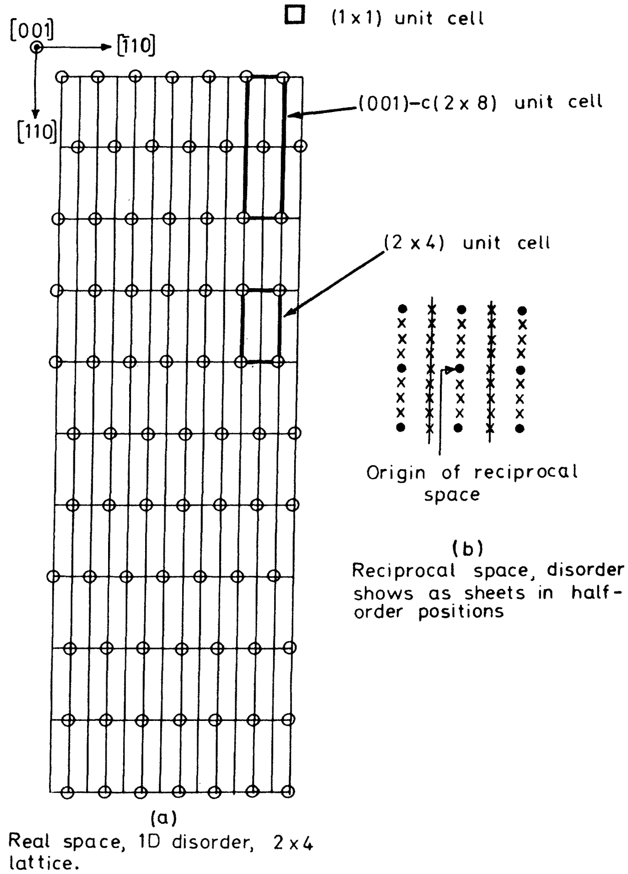


FIG. 6. (a) Real-space representation of one-dimensional (1D) disorder in a 2×4 lattice, with disorder in the direction of twofold periodicity. Not all lattice points are shown. (b) 2×4 reciprocal lattice section showing sheets of intensity resulting from this disorder.

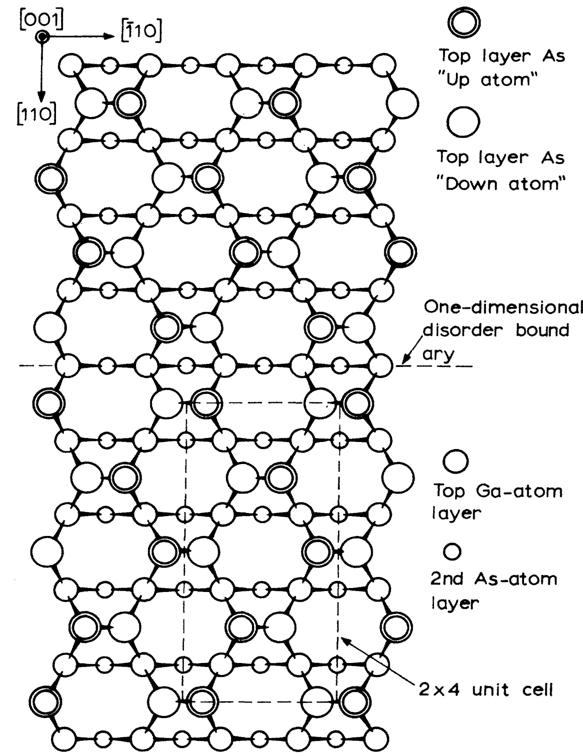


FIG. 7. Tilted dimer modèl of the GaAs(001) reconstructed surface, showing a one-dimensional disorder boundary, with all lattice points on the 1×4 lattice. The dimers are represented by open circles in Fig. 6(a).

due, for example, to atomic steps or to the type of boundary discussed above.

Finally, we add a cautionary note on coherence area values used in RHEED, which may be significant when discussing domain sizes. Hernández-Calderón and Höchst[1] very recently quoted values based only on the finite convergence and energy spread in the incident electron beam which indicated that RHEED could detect ordered regions <1000 Å in diameter, compared with regions <100 Å in diameter in LEED. However, it has been shown by Beeby[18] that it is only the dimension of the electron wave packet which is important in determining the coherence area, and the calculation of the spatial extent of a wave packet for a particular experiment is extremely difficult. General values based only on the energy and angular divergence of the primary beam may not be valid.

ACKNOWLEDGMENTS

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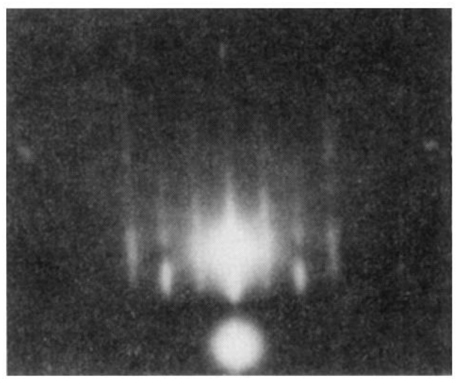
[1] I. Hernández-Calderón and H. Höchst, Phys. Rev. B 27, 4961 (1983).
[2] R. Ludeke, IBM J. Res. Dev. 22, 304 (1978).
[3] A. Y. Cho, J. Appl. Phys. 47, 2841 (1976).
[4] J. H. Neave, B. A. Joyce, P. J. Dobson, and N. Norton, Appl. Phys. A 31, 1 (1983).
[5] J. M. van Hove and P. I. Cohen, J. Vac. Sci. Technol. 20, 726 (1982).
[6] J. M. van Hove, P. I. Cohen, and C. S. Lent, J. Vac. Sci. Technol. A 1, 546 (1983).
[7] T. C. Chiang, R. Ludeke, M. Aono, G. Landgren, F. J. Himpsel, and D. E. Eastman, Phys. Rev. B 27, 4770 (1983).
[8] S. Holloway and J. L. Beeby, J. Phys. C 11, L247 (1983).
[9] P. K. Larsen, J. F. van der Veen, A. Mazur, J. Pollmann, J. H. Neave, and B. A. Joyce, Phys. Rev. B 26, 3222 (1982).
[10] P. Delescluse and A. Masson, Surf. Sci. 100, 423 (1980).

[11]P. J. Dobson, J. H. Neave, and B. A. Joyce, Surf. Sci. 119, L339 (1982).
[12]H. Raether, Ergeb. Exakten Naturwiss. 24, 54 (1951).
[13]M. Henzler, Appl. Phys. 9, 11 (1976).
[14]F. Hottier, J. B. Theeten, A. Masson, and J. L. Domange, Surf. Sci. 65, 563 (1977).
[15]G. W. Simmons, D. F. Mitchell, and K. R. Lawless, Surf. Sci. 8, 130 (1967).
[16]P. Drathen, W. Ranke, and K. Jacobi, Surf. Sci. 77, L162 (1978).
[17]J. Massies (private communication).
[18]J. L. Beeby, Surf. Sci. 80, 56 (1979).



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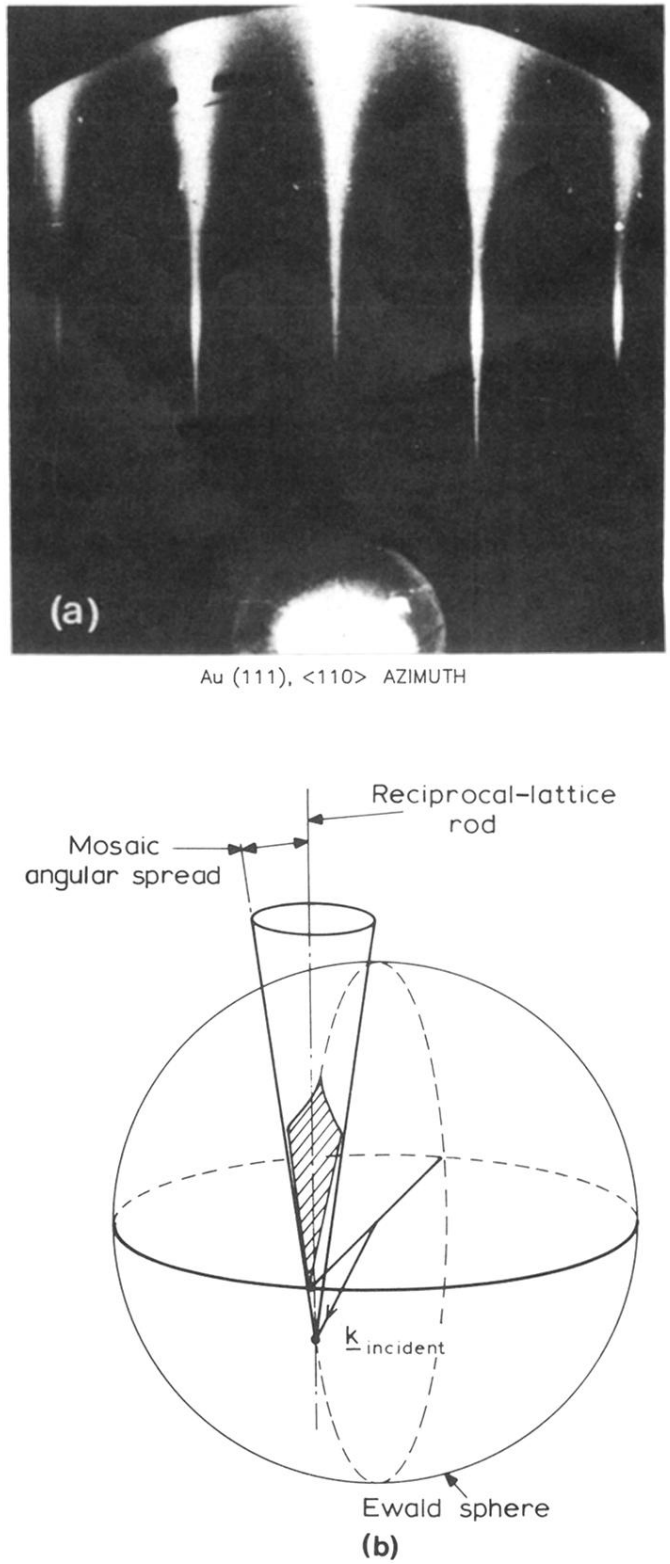

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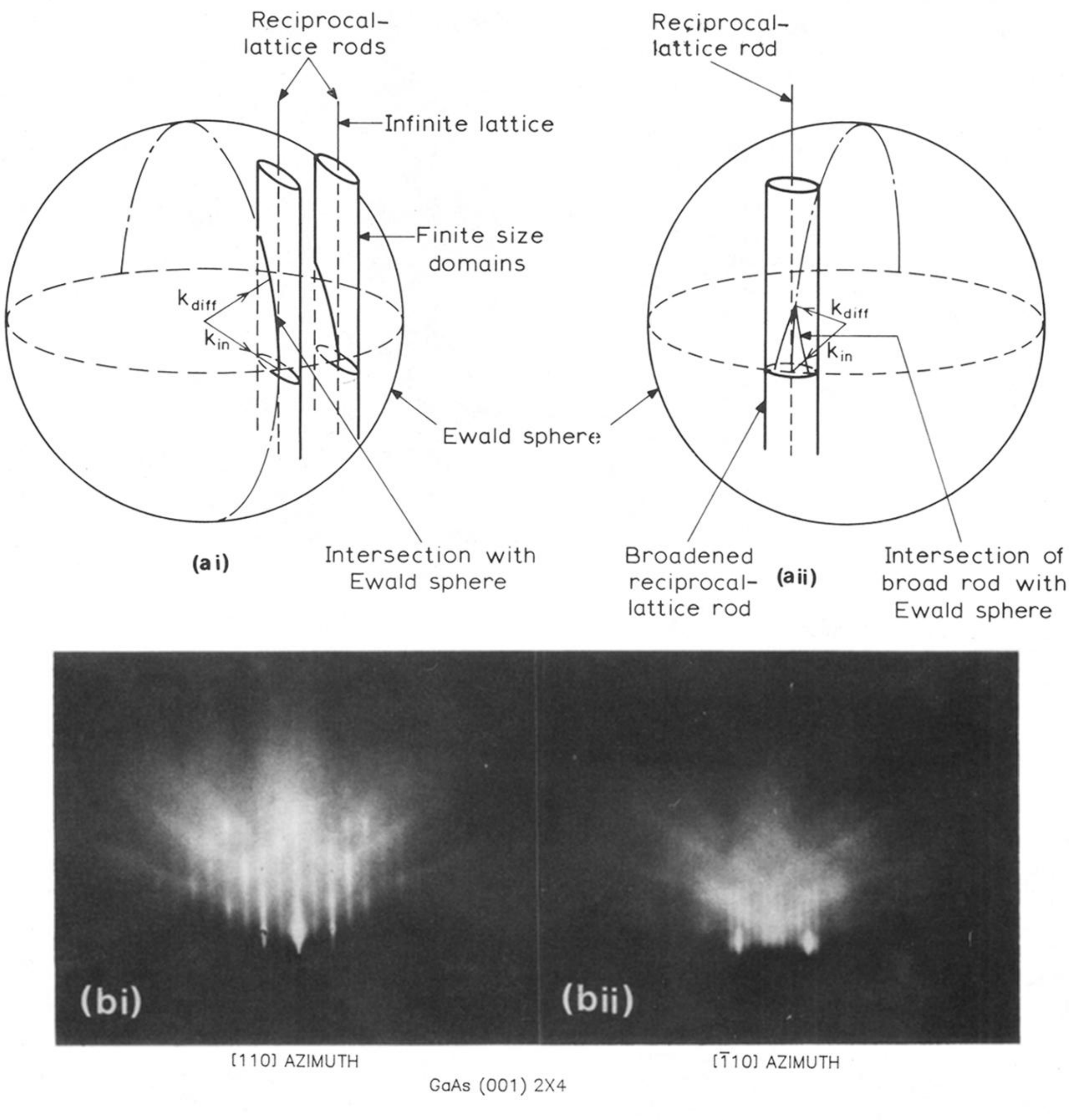

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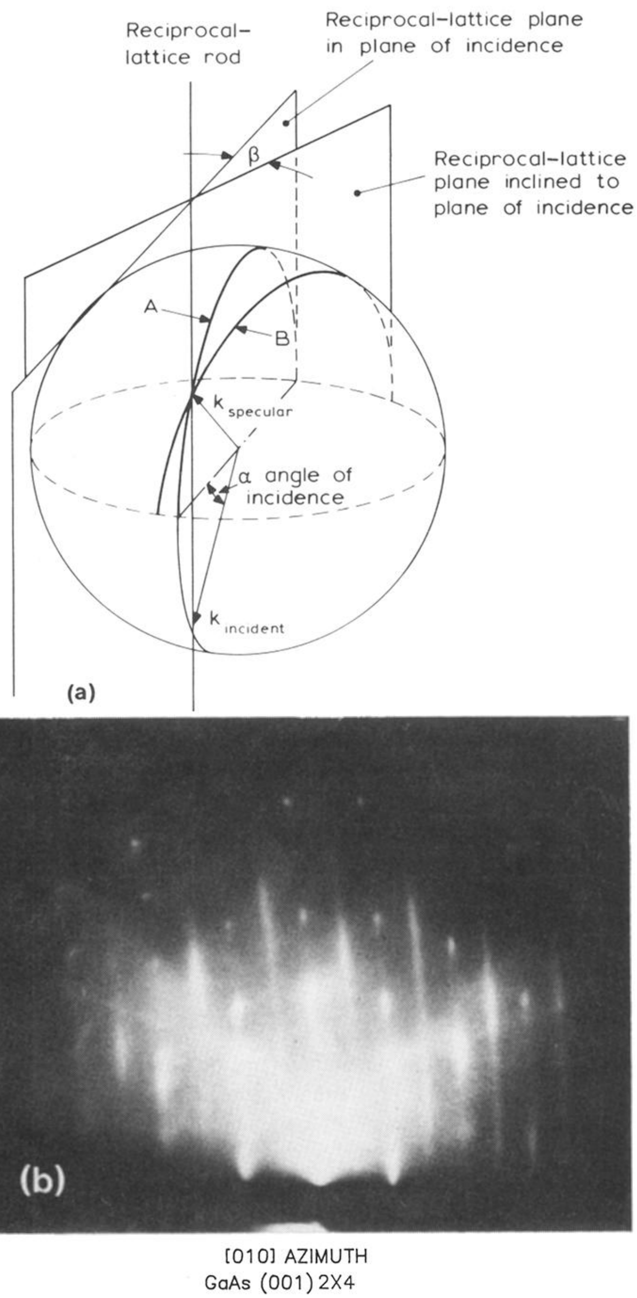

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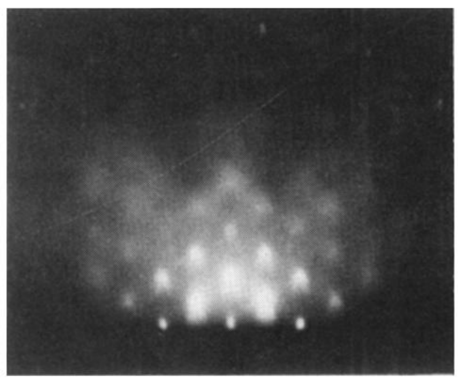

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