PHYSICAL REVIEW B VOLUME 43, NUMBER 15 15 MAY 1991-II

X-ray-diffraction measurement of interface structure in GaAs/Si(001)

E. D. Specht, G. E. Ice, C. J. Peters, and C. J. Sparks
Metals and Ceramics Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831-6118

N. Lucas, X.-M. Zhu, and R. Moret*
Department of Physics and Materials Research Laboratory, University of Illinois at Urbana-Champaign, 1110 West Green Street, Urbana, Illinois 61801

H. Morkoç
Coordinated Science Laboratory and Materials Research Laboratory, University of Illinois at Urbana-Champaign, 1101 Springfield Avenue, Urbana, Illinois 68101
(Received 12 July 1990; revised manuscript received 17 December 1990)

We have developed an x-ray-diffraction technique that provides depth sensitivity to the near-interface region of a thick, nonregistered film. By measuring the intensity profiles along the Si[00l] substrate crystal truncation rods, we compare the diffraction from the Si/GaAs interface with a model based on a grid of misfit dislocations. We find that the interface atoms have a root-mean-square displacement of 1.09±0.10 Å and that the interface has a roughness of 2.9±1.0 Å. The diffraction indicates an anomalously small strain perpendicular to the interface in the GaAs near the interface.

I. INTRODUCTION

Heteroepitaxial growth is frequently frustrated by lattice misfit. For thin films, a small misfit may be accommodated by growing a defect-free strained film in registry with the substrate. At a critical thickness, a registered film becomes unstable as dislocations nucleate, taking film and substrate out of registry.[1] Beyond this thickness, a defect-free film can be grown only by localizing these misfit dislocations at the interface.

One heteroepitaxial system of great potential for electronics applications is GaAs on Si.[2,3] Registered GaAs films have not been grown, so a variety of growth methods have been developed to confine misfit dislocations to the GaAs/Si interface, including an initial growth at reduced temperature,[4,5] use of a strained-layer superlattice buffer,[6,7] and growth on vicinally cut substrates.[6–8] This confinement of dislocations has given rise to increased electron mobility.[7]

With proper growth techniques, dislocation density is very low far from the interface; about 10^4 cm^{-2} at a distance near 2 μm in one case.[9] X-ray-diffraction measurements of a thinner sample show a linear gradient in strain normal to the interface of 0.8% across the 900-Å-film thickness,[10] implying that 80% of the misfit is accommodated near the interface.

High-resolution electron microscopy does indeed show an array of dislocations in small areas of the GaAs/Si interface.[9,11] To obtain a quantitative measure of the localization of dislocations over a macroscopic area of interface we have developed an x-ray-diffraction technique for measuring residual registry in incommensurate films.

We obtain sensitivity to the near-interface region by measuring the intensity profile along the Si surface truncation rod. The integrated intensity is proportional to the square of the modulus of the scattering amplitude

$$F(\mathbf{Q})=\frac{a_0^2}{A}\sum_j f_j(\mathbf{Q})e^{i\mathbf{Q}\cdot\mathbf{r}_j}\ , \tag{1}$$

where $a_0=5.431$ Å is the Si lattice constant, A is the area of the interface, and f_j and $\mathbf{r}_j$ are the scattering factor and position of each atom. For the (001) interface studied, F is nonzero only when the reciprocal lattice vector (RLV) $\mathbf{Q}=2\pi(h,k,l)/a_0$ with integral h and k in units of the Si lattice. l varies continuously to form a crystal truncation rod. Because the Si substrate is virtually defect free, it contributes to $F(\mathbf{Q})$ only near its Bragg peaks. Since GaAs has a different lattice constant, the regions of the first few layers of the film lying in registry with the substrate will yield scattering at a somewhat different value of l along the Si rod.

Similar measurements have proven useful in the study of a fully registered thin film.[12] Here the same technique is applied to make depth-sensitive measurements of a thick film, which is in partial registry only near the interface.

II. EXPERIMENTAL

The (001) Si substrate was degreased and subjected to a metal-removal process and a series of oxidation-deoxidation cycles to reduce carbon contamination. The last oxide, which was left on the surface, was grown in a 5:3:3 (H_2O:HCl:H_2O_2) solution. This volatile oxide is removed by thermal outgassing at 1000 °C under vacuum just prior to growth. The GaAs layer was then grown at a substrate temperature of 510 °C and a growth rate of 0.2

 ©1991 The American Physical Society

μm/h to a thickness of 900 Å.

X-ray-diffraction measurements were made at beamline X-14 of the National Synchrotron Light Source.[13] Incident flux was monitored by a N_2-filled ion chamber, calibrated by a *p-i-n* diode, which was in turn calibrated to a scintillation counter using a weaker beam. Typical flux was 10^{11} sec^{-1}; the wavelength was $\lambda = 1.410$ Å. The sample was mounted in vacuum under a 0.02-in.-thick beryllium dome. Data were collected with incident and scattered beams at equal angles to the surface. A 2 mm (in-plane)$\times$4 mm (out-of-plane) slit upstream of the sample ensured that the sample collected the full beam at all angles. The incident beam was focused on a 1×2 mm^2 receiving slit upstream of a scintillation counter. The focal spot is 0.5×1.0 mm^2. By keeping the receiving slit as narrow as possible we collect a minimum of the diffuse scattering associated with short-range order in the film. Even so, our data are restricted to lower angles; at high angles this diffuse scattering obscures the sharp truncation rods.

At each point along the crystal truncation rod we scan across the rod and subtract a smooth background to determine peak intensity. To verify that the features we observe are indeed due to the Si/GaAs interface, we replaced the slits upstream of the counter with a Ge(111) analyzer crystal and reproduced the data from $\mathbf{Q}=2\pi(1,1,0.5)/a_0$ to $\mathbf{Q}=2\pi(1,1,1.2)/a_0$. This confirms that the scattering follows a sharp rod in reciprocal space, matching the Si periodicity to within one part in 10^4. Since we know the GaAs film to be poorly ordered, this long-range order must be at the interface.

Because we are treating weak scattering, we apply the Born approximation. For the out-of-plane polarization used here the cross section is[14]

$$\frac{d\sigma}{d\Omega}=\sigma_T\left|\sum_j f_j(\mathbf{Q})e^{i\mathbf{Q}\cdot\mathbf{r}_j}\right|^2 , \tag{2}$$

where $\sigma_T = 7.94\times10^{-26}$ cm^2 is the Thompson cross section. If the receiving slit is of sufficient area, the detector will integrate over all diffracted beam directions Ω. To convert this to a two-dimensional integral in reciprocal space, we use the relation $d\Omega = L\,dh\,dk$, where

$$L=(\lambda/a_0)^2(\sin\theta\sin\chi)^{-1} \tag{3}$$

is the modified Lorentz factor and θ and χ are goniometer angles as defined in Busing and Levy.[15] Integrating Eq. (2), the ratio of scattered to incident flux is

$$I/I_0=\frac{LA\sigma_T}{A_0a_0^2}\left|\left\langle\sum_j e^{-w_j(\mathbf{Q})}f_j(\mathbf{Q})e^{i\mathbf{Q}\cdot\mathbf{r}_j}\right\rangle\right| , \tag{4}$$

where $\langle\ \rangle$ indicates an average over $a_0\times a_0$ Si unit cells and w_j is a Debye-Waller factor. From our data we extract

$$|F(\mathbf{Q})|^2=\frac{Ia_0^2A_0}{I_0\sigma_T AL} \tag{5}$$

plotted as circles in Figs. 1 and 2; from Eq. (4)

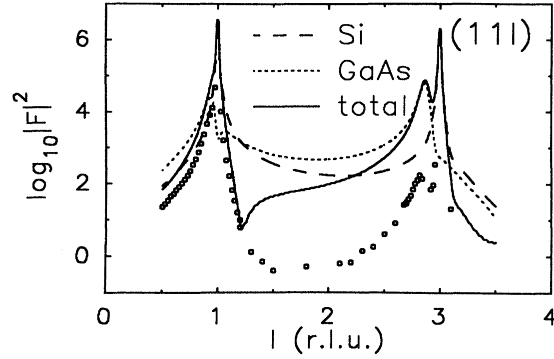

FIG. 1. Scattering intensity along the $(11l)$ Si truncation rod, observed (circles) and calculated for a grid of misfit dislocations, with no adjustable parameters.

$$|F(\mathbf{Q})|^2=\left|\left\langle\sum_j e^{-w_j(\mathbf{Q})}f_j(\mathbf{Q})e^{i\mathbf{Q}\cdot\mathbf{r}_j}\right\rangle\right|^2 . \tag{6}$$

A_0 is the cross section of the incident beam, and A is the active area of the sample.[16] For larger values of χ the receiving slit admits the entire diffracted beam, so A is simply the footprint of the incident beam $A=A_0/(\sin\theta\sin\chi)$. For smaller χ, the active area is determined by the in-plane (i.e., vertical) widths L_1 and L_2 of the incident beam and receiving slit $A=L_1L_2/(\sin2\theta\cos\chi)$. Uncertainty in the incident-beam profile results in uncertainty of up to 30% in the active area; this is the principle source of experimental error, which has the greatest effect on determination of the Debye-Waller factor.[16]

Our data reduction uses the peak intensity of a scan across the rod, allowing the detector to integrate across the rod, rather than using the established technique using an integrated intensity.[16,17] We may do so here because

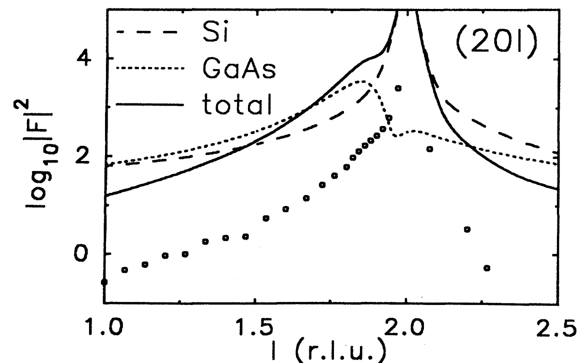

FIG. 2. Scattering intensity along the $(20l)$ Si truncation rod, observed (circles) and calculated for a grid of misfit dislocations, with no adjustable parameters.

incident-beam divergence and sample mosaic are of negligible importance. The advantage is that peak intensity is less sensitive to uncertainty in instrumental resolution than is integrated intensity.

III. MODEL

We compare the observed scattering with that produced by a perfectly ordered grid of misfit dislocations at the interface. Well-ordered GaAs/Si interfaces have been found[11] to develop a lattice of misfit dislocations with Burgers vectors of $[\frac{1}{2}\frac{1}{2}0]$ and $[\frac{1}{2}\frac{\bar{1}}{2}0]$. The strain at such an interface has been calculated by van der Merwe[1] by treating each crystal as an isotropic continuum elastic medium. The continuum approximation is justified for dislocation spacing (96 Å) much larger than the lattice parameter (3.84 Å for the primitive cell). The van der Merwe model treats infinite crystals, a good approximation since the interface strain falls off exponentially far from the interface with a 15-Å decay length. Since Si has a higher modulus than GaAs and the model takes them to be equal, we will overestimate the strain in Si and underestimate it in GaAs. We use a Poisson's ration of 0.30 for both Si and GaAs. The GaAs lattice constant is well approximated by $25a_0/24$, corresponding to the 4.1% misfit.

Figures 3 and 4 show the atom positions calculated using this model for two planes of atoms. Figure 3 depicts the first plane of GaAs atoms, dilated near the dislocation lines (solid lines). The small square outlines a 5.65-Å cubic unit cell. As can be seen in Fig. 4, which shows the plane orthogonal to Fig. 3 through the dashed line in Fig. 3, the Si (solid circles) and GaAs (open circles) atoms are in registry except near the dislocation at the center of the figure. The GaAs within 12 Å of the interface is compressed in the plane of the interface and dilated out of plane between dislocations, dilated in plane and compressed out of the plane near a dislocation line. Further from the interface this behavior is reversed. The interference we observe along the Si truncation rods is due to the regions between dislocations near the interface, where atoms are in registry.

From Eq. (1) we calculate $F(\mathbf{Q})$ using the Ge form factor as an average for As^+ and Ga^- ions.[18] Since the strain falls off exponentially with distance from the interface, we treat atoms within 100 Å of the interface using the van der Merwe model. Silicon atoms below this region are taken to be at their bulk lattice sites; GaAs atoms above do not contribute to the truncation rod. Extending the modeled region to 150 Å in either direction does not significantly alter the results. The small, rapid oscillations in the calculated values of $|F|^2$ are artifacts of this 100-Å limit.

In Figs. 1 and 2 we compare our data (circles) to the van der Merwe model (lines), showing $|F_{\rm Si}|^2$ and $|F_{\rm GaAs}|^2$ as well as the total $|F_{\rm Si}+F_{\rm GaAs}|^2$. The model reproduces qualitatively the principal features of the data; after a discussion of these features we will describe how disorder in the interface produces the large quantitative differences between model and data. The model illustrated here includes no adjustable parameters.

In both our calculation and our measurement, GaAs produces a peak on the low-l side of each Si Bragg peak, which we will refer to as the interface peak. Because the GaAs has a larger lattice parameter than Si, its unstrained bulk peaks appear at values of h, k, and l, which are 4% contracted from the Si reciprocal lattice. For the case of a thick GaAs film constrained in plane by the denser Si substrate and smaller Si thermal contraction, peaks are shifted toward higher h and k and lower l relative to the ideal GaAs peaks. This corresponds to in-plane contraction and the resulting out-of-plane Poisson expansion. As the film is not registered, it does not match the substrates in-plane spacing and therefore produces no scattering along the Si truncation rod. Very near the interface, however, the GaAs lies in partial registry and so yields the interface peak along the Si truncation rod.

The positions of the interface peaks are related to strain in the GaAs near the interface, but not in a simple way: The calculated interface peaks are at (1,1,0.935), (2,0,1.845), and (1,1,2.865) Si r.l.u., corresponding to

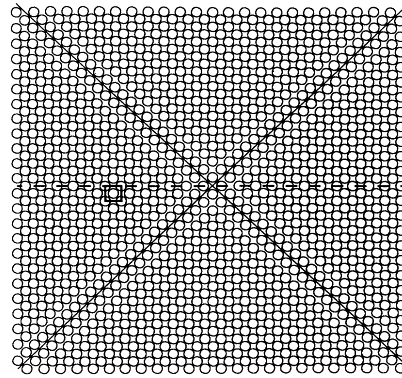

FIG. 3. van der Merwe model of the first [001] plane of GaAs atoms, showing compression near misfit dislocations (solid lines). The dashed line is the plane shown in Fig. 4. The box is a 5.65-Å cubic unit cell.

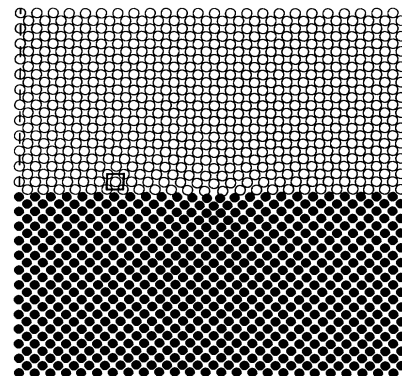

FIG. 4. van der Merwe model of the (100) plane at the position indicated in Fig. 3. Solid circles are Si atoms, open circles GaAs atoms. The box is a 5.65-Å cubic unit cell.

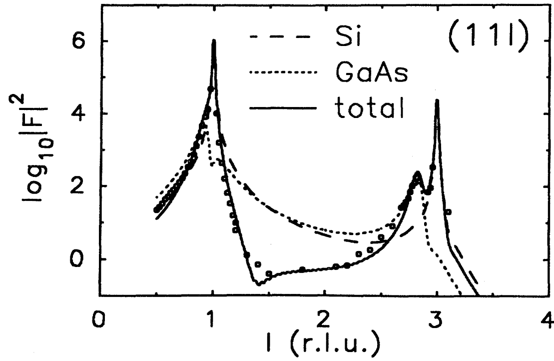

FIG. 5. Scattering intensity along the $(11l)$ Si truncation rod, observed (circles) and calculated for a grid of misfit dislocations with rms displacements of 0.96 Å (Si) and 1.09 Å (GaAs), interface roughness of 2.9 Å, and an added strain of 1.5%.

strains normal to the interface 2.8%, 4.2%, and 0.6% relative to bulk GaAs. Interference of variously strained regions of the interface produces different shifts in the interface peaks.

The widths of the interface peaks are determined by the distance over which the overlayer falls out of registry with the substrate. The van der Merwe model predicts that strain falls off exponentially with a decay length of 15 Å, giving interface peak widths near 0.12 r.l.u. FWHM.

Although the strain calculated for the Si lattice is equal and opposite to that for the GaAs, the contribution to the scattering along the Si rods is markedly different. The scattering due to Si does not change measurably from that of a truncated crystal near the Bragg peaks. Between the peaks the scattering is reduced by a factor of 2. This is characteristic of a diffuse boundary: The Si periodicity is no longer sharply truncated but falls off over ~ 15 Å due to interfacial strain.

We now consider the difference between calculated and

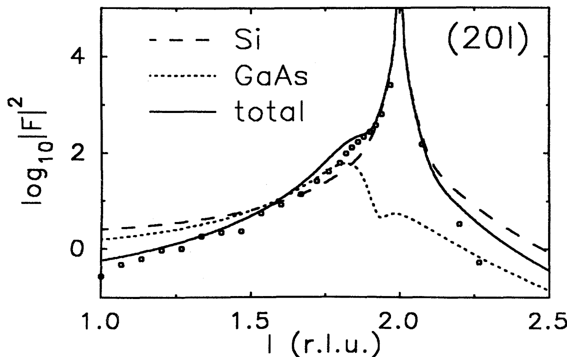

FIG. 6. Scattering intensity along the $(20l)$ Si truncation rod, observed (circles) and calculated for a grid of misfit dislocations with rms displacements of 0.96 Å (Si) and 1.09 Å (GaAs), interface roughness of 2.9 Å, and an added strain of 1.5%.

observed scattering, both the large difference in intensity and a less obvious discrepancy in peak position. While the interface peak at (1,1,0.935) is near to the right intensity, the calculated intensities for those at (2,0,1.845) and (1,1,2.865) are far above the measured intensities (Figs. 1 and 2). Reduced intensity for higher-order peaks is a signature of atomic displacements from lattice sites: A root-mean-square (rms) displacement u will give a scattering factor tailing off as $\exp[-8\pi^2u^2\sin^2\theta/(3\lambda^2)]$.[18] Our final model gives $u_{\mathrm{GaAs}}=1.09\pm0.10$ Å and $u_{\mathrm{Si}}=0.96\pm0.1$ Å.

Making this correction for atomic displacement gives good agreement at the interface peaks but leaves the calculated intensity higher than that observed between the peaks. This is characteristic of interface roughness.

We adapt the model developed by Robinson[19] to describe surface roughening: A smooth surface is covered with a layer with fractional occupancy β, a second layer with occupancy β^2, and so on. The scattering factor is proportional to

$$F(\mathbf{Q})=\sum_{n=0}^{-\infty}(e^{in\mathbf{Q}\cdot\mathbf{b}}+e^{i\mathbf{Q}\cdot(n\mathbf{b}+\mathbf{t})})+\sum_{n=1}^{\infty}(\beta^2ne^{in\mathbf{Q}\cdot\mathbf{b}}+\beta^{2n+1}e^{i\mathbf{Q}\cdot(n\mathbf{b}+\mathbf{t})}) \quad (7)$$

$$=F_0(\mathbf{Q})\left[1+\frac{\beta^2(1+\beta e^{i\mathbf{Q}\cdot\mathbf{t}})(e^{i\mathbf{Q}\mathbf{b}}-1)}{(1+e^{i\mathbf{Q}\cdot\mathbf{t}})(1-\beta^2e^{i\mathbf{Q}\cdot\mathbf{b}})}\right], \quad (8)$$

where $\mathbf{b}=(\frac{1}{2},0,\frac{1}{2})a_0$, $\mathbf{t}=(\frac{1}{4},\frac{1}{4},\frac{1}{4})a_0$, and $F_0(\mathbf{Q})$ is the scattering factor for a flat surface.

We use Eq. (8) to correct our calculated intensities. This correction assumes that the interface position fluctuates in steps of Si lattice spacing $\frac{1}{4}a_0$, with the Si planes well below the interface remaining in alignment while the GaAs planes are misaligned above each step. As a consequence of this assumption, the intensity near the Si peaks is unaffected by roughness while the intensity of the interface peaks is reduced. To convert the roughness parameter β into a distance, we note that the occupancy of substrate falls off as $\beta^{-2z/a_0}=\exp(-z/r)$, where $r=-a_0/(4\ln\beta)$. Our final model gives $\beta=0.62$ or $r=2.9\pm1.0$ Å.

We introduce a third correction to make the calculated interface peak positions match those observed. We include a homogeneous contraction of the GaAs film normal to the interface by $(1.5\pm0.2)\%$. Here the model includes four adjustable parameters: strain, interface roughness, and Debye-Waller factors for Si and GaAs. As shown in Figs. 5 and 6, these corrections produce good agreement with observations. We will discuss these corrections below.

IV. DISCUSSION

We find a high degree of disorder at the interface. From the falloff of interface-peak intensity at high angles we infer a random rms displacement near 1 Å of the atoms near the interface from their positions in the van der Merwe model structure. This is larger than the 0.80-Å periodic rms displacement of atoms in the layer nearest

the interface for the model structure from their bulk lattice positions. This is consistent with the observation[11] that inclined dislocations and stacking faults occur at GaAs/Si interfaces with frequency comparable to that of the edge dislocations in our model. We measure slightly smaller random displacements for Si (0.96 Å) than for GaAs (1.09 Å). For Si we are combining scattering from undisplaced atoms deeper in the crystal with scattering from highly displaced atoms near the interface, so we measure some sort of average.

Due to the large interface roughness and random atomic displacements, these data cannot be taken as confirmation of the van der Merwe model on small length scales: The atoms in the dislocation cores are disordered. Moreover, the approximations used in the model itself are not valid in the dislocation core. The strain which occurs on longer length scales between dislocations is accurately measured by this technique: When measuring a strain over a 50-Å region, we average over small displacements.

We find the GaAs near the interface to be contracted $(1.5\pm0.2)\%$ normal to the interface, relative to the calculated structure. In the van der Merwe model, the GaAs and Si are strained in plane by equal and opposite amounts (2.0%) between dislocation lines. The Poisson response[20] to this in-plane contraction of the GaAs is a 1.8% expansion out of plane. We expect a somewhat larger expansion, for two reasons. First, since GaAs has a lower elastic modulus than Si, strain will be greater in GaAs and less in Si than calculated. Second, the misfit is not accommodated at the interface only. X-ray measurements of the widths of the GaAs Bragg peaks show a 0.8% linear gradient across the thickness of the film in the strain normal to the interface,[10] implying that some 20% of the strain is accommodated in the film rather than at the interface. Thus the GaAs near the interface will again be more strained than the model suggests, the Si less strained. We observe the opposite. Subtracting the $(1.5\pm0.2)\%$ correction from the 1.8% strain predicted by the van der Merwe model, we arrive at an out-of-plane expansion of only $(0.3\pm0.2)\%$.

This anomalously small strain may be an intrinsic feature of the GaAs/Si interface; relaxation is a common feature at surfaces. We cannot rule out two other possibilities, however. It may be the high degree of disorder near the interface rather than the interface itself which modifies the elastic properties of the GaAs. Alternatively, the material close to the interface may indeed be strained as predicted by the van der Merwe model. The atoms nearest the interface suffer the most displacement from their calculated positions, so the scattering will reflect primarily the less displaced atoms further from the interface.

Finally, we compare the technique used here, measuring substrate truncation rod intensities, with other diffraction techniques which are sensitive to buried interfaces. The most direct means of determining an interface structure is to measure the scattering from the interface reciprocal lattice. The model that we have developed for GaAs/Si(001) gives the interface a 136-Å periodicity, but scattering on its reciprocal lattice was too weak to measure. This is consistent with the disorder we observe: The dislocations do not form an ordered lattice.

Another technique which exploits the interference between substrate and overlayer is x-ray standing-wave fluorescence (XSWF).[21] XSWF is complementary to the measurement of substrate truncation rods. While the truncation rods contain no scattering from a nonregistered film, XSWF contains no fluorescence from the substrate. Thus XSWF is an effective technique when the film is very thin. Fluorescence from a 900-Å film would swamp the weaker interface signal.

Specular x-ray reflectivity gives a measure of interface roughness. This technique is not directly sensitive to structural defects such as strain and dislocations. The sharpest GaAs/Si interfaces found by this technique have about 10 Å roughness, greater than the 2.9 ± 1.0 Å found here.[22]

ACKNOWLEDGMENTS

We thank F. J. Walker for helpful discussions. This research was supported by the Division of Materials Sciences, U.S. Department of Energy under Contract No. DE-AC05-84OR21400 with Martin Marietta Energy Systems, and under Contract No. DE-AC02-76ER01198 with the University of Illinois. NSLS is supported by the U.S. Department of Energy under Contract No. DE-AC02-76CH00016.

*On leave from the Laboratoire de Physique des Solides, VA 02, Université Paris XI, 91405 Orsay, France.

[1]J. H. van der Merwe, Proc. Phys. Soc. London, Sect. A **63**, 616 (1950).

[2]H. K. Choi, G. W. Turner, and B.-Y. Tsaur, IEEE Electron Device Lett. **EDL-7**, 241 (1986).

[3]H. Shichijo and J. W. Lee, in *Proceedings of the Materials Research Society Symposia on Heteroepitaxy on Silicon,* edited by J. C. C. Fan and J. M. Poate, MRS Symposia Proceedings No. 67 (Materials Research Society, Pittsburgh, PA, 1986), pp. 173–180.

[4]M. Akiyama, Y. Kawarada, and K. Kaminish, J. Appl. Phys. **23**, L843 (1984).

[5]W. T. Masselink, T. Henderson, J. Klem, R. Fisher, P. Pearah, H. Morkoç, M. Hafich, P. D. Wang, and G. Y. Robinson, Appl. Phys. Lett. **45**, 1309 (1984).

[6]R. Fisher, D. Neuman, H. Zabel, H. Morkoç, C. Choi, and N. Otsuka, Appl. Phys. Lett. **48**, 1223 (1986).

[7]J. W. Lee, in *Proceedings of the Materials Research Society Symposia on Heteroepitaxy on Silicon* (Ref. 3), pp. 29–36.

[8]G. M. Metze, H. K. Choi, and B.-Y. Tsaur, Appl. Phys. Lett. **45**, 1107 (1984).

[9]R. Fischer, H. Morkoç, D. A. Neumann, H. Zabel, C. Choi, N. Otsuka, M. Longerbone, and L. P. Erickson, J. Appl. Phys. **60**, 1640 (1986).

[10]A. S. Bommannavar, C. J. Sparks, A. Habenschuss, G. E. Ice, A. Dhere, H. Morkoç, and H. Zabel, in *Proceedings of the Materials Research Society Symposium on Epitaxy of Semiconductor Layered Structures,* edited by R. T. Tung, L. R. Dawson, and R. L. Gunshor, MRS Symposia Proceedings

No. 102 (Materials Research Society, Pittsburgh, PA, 1988), p. 223.

[11]H. L. Tsai and J. W. Lee, Appl. Phys. Lett. **51**, 130 (1987).

[12]I. K. Robinson, R. T. Tung, and R. Feidenhans'l, Phys. Rev. B **38**, 3632 (1988).

[13]A. Habenschuss, G. E. Ice, C. J. Sparks, and R. A. Neiser, Nucl. Intrum. Methods **A266**, 215 (1988).

[14]B. E. Warren, *X-Ray Diffraction* (Addison-Wesley, Reading, MA, 1969), p. 28.

[15]W. R. Busing and H. A. Levy, Acta Crystallogr. **22**, 457 (1967).

[16]I. K. Robinson, Aust. J. Phys. **41**, 359 (1988).

[17]R. Feidenhans'l, Surf. Sci. Rep. **10**, 105 (1989).

[18]*International Tables for X-Ray Crystallography,* edited by K. Lonsdale (Kynoch, Birmingham, England, 1962), Vol. III, p. 204.

[19]I. K. Robinson, Phys. Rev. B **33**, 3830 (1986).

[20]N. Lucas, H. Zabel, H. Morkoç, and H. Unlu, Appl. Phys. Lett. **52**, 2117 (1988).

[21]N. Hertel, G. Materlik, and J. Zagenhagen, Z. Phys. B **58**, 199 (1985).

[22]N. Lucas, H. Zabel, S. V. Iyer, and H. Morkoç (unpublished).