Channeling measurements of lattice disorder at the GaAs–InAs(100) heterojunction

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Rutherford backscattering spectrometry (RBS) combined with channeling techniques has been used to analyze the lattice disorder present in InAs thin films less than 1 μm thick grown on GaAs(100) substrates by molecular beam epitaxy (MBE). The axial channeling yields along [100], [110], and [111] reveal that roughly one quarter of the atoms in the thin films are out of registry with the InAs lattice at the heterojunction interface. The amount of lattice disorder decreases rapidly to undetectable ($< 1\%$) amounts at film thicknesses greater than 0.5 μm. The interface disorder arises as a result of the $> 7\%$ lattice mismatch between GaAs and InAs.

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I. INTRODUCTION

Determining the structure of semiconductor heterojunction interfaces is crucial to the understanding of their electronic properties and limitations in device applications. Analysis techniques are required which are relatively straightforward to use so that a large number of samples may be analyzed in the process of optimizing heterojunction fabrication. RBS/channeling techniques have been used successfully as probes of interface disorder in cases where a large mass difference exists between substrate and overlayer[1] or the amount of disorder present involves more than a few percent of the lattice atoms.[2] For example, *in situ* RBS/channeling studies of Ge grown on Si(111) surfaces[3] have shown that the growth for this system (4% lattice mismatch) proceeds according to the Stranski–Krastanov mechanism.[4] Systems such as $InAs_{1-y}Sb_y$–GaAs, which have applications as middle wavelength photodetectors, also fall into this category due to the large lattice mismatch between substrate and epitaxial overlayer. In this paper, we consider the InAs–GaAs(100) heterojunction, which has a lattice mismatch of greater than 7%.

This large mismatch between InAs and GaAs results in significant structural disorder at the heterojunction interface.[5–7] Chang *et al.*[5,6] have observed a high ($\sim 10^{12}$ cm^{-2}) density of misfit dislocations within 2000 Å of the heterojunction, that decreases to $\sim 10^8$ cm^{-2} near the surface of a 2-μm InAs film. Such misfit dislocations have been predicted for epitaxial bicrystals with a large lattice constant mismatch.[8] The high concentration of misfit dislocations has been observed to dominate the majority carrier transport properties of thin InAs films on GaAs.[6,9] Films of 2–4-μm-thick InAs grown on GaAs by MBE for this study, however, show excellent specular morphology, low carrier concentration ($N_D - N_A = 2 \times 10^{15}$ cm^{-2}), and bulklike electron mobilities (60 000 $< \mu_n <$ 100 000 cm^2/V s). Thus, thicker films of InAs grown on GaAs appear to be relatively defect-free. The purpose of the present investigation is to quantify the amount and distribution of lattice disorder in the interface region of InAs–GaAs structures that were grown to produce optimal electronic properties.

II. EXPERIMENTAL

A. Preparation of InAs–GaAs(100) by molecular beam epitaxy

Thin films 0.4–1.0 μm thick were grown on GaAs(100) by MBE. The apparatus and techniques have been described previously[9,10] and will only be summarized here. Resistively heated sources containing elemental indium, gallium, and arsenic are mounted vertically and impinge on a separately shuttered molybdenum substrate holder. The InAs is nucleated under In-stabilized growth conditions at 460 °C and at a growth rate of 1 μm/h. The In-stabilized $C(8 \times 2)$ pattern[11] is observed by reflection electron diffraction at the onset of growth and persists throughout the InAs film deposition. A linear shutter is used to sequentially cover portions of the sample during InAs deposition to produce InAs films of varying thickness on the same substrate. The samples are removed from the MBE growth chamber and sealed in glass

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ampoules under an inert atmosphere to await beam time for RBS analysis.

B. RBS measurements

The RBS/channeling measurements were performed using instrumentation described previously.[12] The He^+ ion beam energy was 2 MeV. A preliminary investigation involved collecting and analyzing [100] axial channeling and "random" backscattering spectra of the films. In all cases, the random spectra were obtained by rotating the sample to average over azimuthal crystallographic orientations. A sample with a 0.4-μm-thick InAs overlayer was chosen for further analysis since it was the thinnest sample that showed the full dechanneling profile indicating lattice disorder. Channeling and random spectra for the 0.4-μm InAs–GaAs(100) sample and a bulk-grown InAs(100) wafer were obtained along the [100], [110], and [111] axes, as shown in Fig. 1.

III. RESULTS AND DISCUSSION

The dechanneling behavior for several 0.4–1.0-μm-thick films was very similar in the InAs–GaAs region; a large peak in the channeling yield indicated a considerable amount of interfacial lattice disorder. However, for greater than 0.5 μm from the GaAs/InAs interface, the channeling behavior of the InAs film was indistinguishable from that of bulk-grown material, indicating that the crystalline quality sufficiently far away from the heterojunction was relatively good. The 0.4-μm-thick sample was channeled along three different principal axes to see if the lattice defects contained any preferential orientation.

Analysis of the channeling data in Fig. 1 requires separating the contributions to the backscattering from In and As atoms, turning the energy scale in the spectra to a depth scale, and relating the channeling yield to a crystal disorder density. The methods for such data analysis are fairly standard.[13] The As contribution to the backscattering from the thin film was subtracted out of the experimental spectra. The assumption required was that the InAs was stoichiometric and that equal amounts of In and As were disordered. For all the spectra in Fig. 1, the In yield at 3.5-keV intervals was multiplied by $(33/49)^2$, the As/In Rutherford scattering cross-section ratio. The resultant As yield was subtracted from the total scattering yield at a 124-keV lower energy corresponding to scattering from As atoms at the same film depth as the In. The random and channeled yields for In in the 0.4 μ epitaxial films and bulk InAs were collected for the [100], [110], and [111] axes. A depth scale was calculated by assuming linear additivity of stopping cross sections (Bragg's Rule) and the data for 2-MeV scattering from As and In in Ref. (13). An iterative procedure was used to calculate the depth-dependent disorder concentration $N_D(x)$ from the In channeling yield measurements[14]

$$N_D(x)/N = \frac{\chi(x) - \chi_R(x)}{1 - \chi_R(x)}, \tag{1}$$

where N is the atom density of the crystal, $\chi(x)$ is the channeling yield at depth x, and $\chi_R(x)$ is the fraction of dechanneled particles at depth x

$$\chi_R(x) = \chi_V(x) + [1 - \chi_V(x)] \times \left\{1 - \exp\left[-\sigma(\psi_{1/2}) \int_0^x N_D(x')dx'\right]\right\}, \tag{2}$$

where $\chi_V(x)$ is the channeling yield from the "defect-free" substrate material and $\sigma(\psi_{1/2})$ is the cross section for scattering a channeled particle into angles larger than the critical angle for channeling $\psi_{1/2}$. The cross sections were estimated[13] from the Rutherford scattering formula for angles $\psi_{1/2}$ calculated using analytical approximations: $\sigma_{[100]} = 0.011$ Å^2, $\sigma_{[110]} = 0.0078$ Å^2, and $\sigma_{[111]} = 0.0095$ Å^2. The final $N_D(x)/N$ results were only weakly dependent on the values of σ, since $\chi_V(x)$ was the largest part of $\chi_R(x)$.

Equations (1) and (2) were applied to the channeling yield data iteratively to achieve self-consistent results for $N_D(x)$ and $\int_0^x N_D(x')dx'$. The defect distributions calculated from the three different sets of channeling data are shown in Fig. 2. The error in the plots is estimated to be less than 20% of the $N_D(x)/N$ value plotted at any given depth. However, a particular value of $N_D(x)/N$ expresses only the relative concentration of atoms that are displaced far enough from equilibrium lattice sites (>0.1 Å) to be sampled by channeled ions; it does not contain information about the distribution of displaced atoms within a channel. The paper by Barrett in these proceedings discusses an RBS/channeling technique for determining the atomic displacements at an interface,[15] although the system discussed is simpler than the InAs/GaAs heterojunction.

The defect distributions indicate that (23 ± 4)% of the InAs atoms at the heterojunction interface are displaced sufficiently with respect to their normal lattice sites to backscatter channeled ions. The displacements are mainly due to the misfit dislocations observed in the work of Chang *et al.*[5,6] An exact comparison of the disorder as measured by RBS and TEM on the samples grown for this study is not yet available.

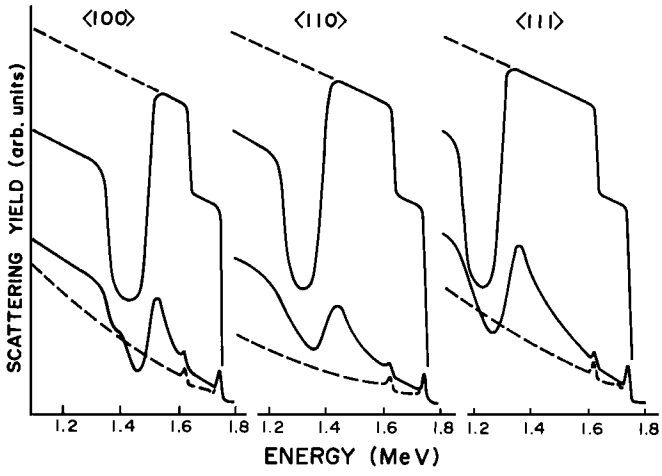

FIG. 1. He^+ ion backscattering: Random and channeled spectra for a 0.4-μm InAs film grown epitaxially on GaAs(100) (solid lines) and corresponding spectra from a high-quality bulk-grown InAs(100) wafer (dashed line) for the [100], [110], and [111] channeling axes. The incident beam energy was 2 MeV and the total beam dose was 21.3 μC for each spectrum. The channeled spectra are the backscattered ion energy distributions with lower intensity for each pair of spectra shown.

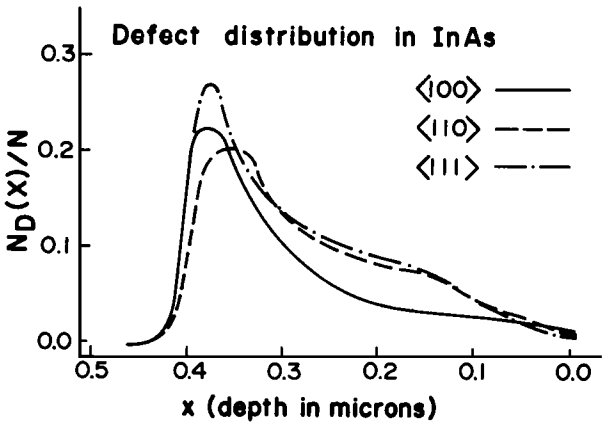

FIG. 2. Lattice disorder as sensed by RBS/channeling calculated from the three sets of spectra in Fig. 1. The disorder $N_D(x)/N$ is the density of atoms displaced sufficiently to scatter channeled ions divided by crystal atomic density. The depth resolution of the profile at the interface is about 300 Å.

The slope of the InAs defect distribution obtained from the [100] channeling data indicates an interface width of ~300 Å, which is also the calculated depth resolution[13] of the backscattering distribution due to energy straggling of scattered He ions and the 18-keV energy resolution of the Si barrier height detector. Thus, the interface between the GaAs and InAs is relatively sharp, indicating that little or no alloying has taken place between the two semiconductors.

The defect concentration as measured by RBS decreases to half the maximum concentration at a distance of 0.1 μm from the interface and is less than 2% near the surface of the 0.4-μm film. RBS measurements on thicker films and the mobility measurements both indicate that, after a sufficiently thick buffer layer has been grown, the crystal quality of the epitaxial InAs is excellent.

At a location of 0.2 μm from the heterojunction, the defect concentration measured along the [110] and [111] axes is nearly a factor of 2 larger than that measured along the [100] axis. This difference appears to be significant and indicates that there are more defects for which the atomic displacements are parallel to the [100] axis than those with displacements perpendicular to [100].

The present studies are not very sensitive to disorder induced in the GaAs substrate by the epitaxial overlayer. The study of disorder in the substrate material by ion channeling is complicated by dechanneling of the ion beam in the InAs overlayer.[2] The amount of backscattering and dechanneling at the InAs–GaAs interface will also depend strongly on the details of the atomic structure at the interface. Attempting to channel the interface from the GaAs side, i.e., through the back of a thinned wafer, will give information about the bulk GaAs but the interfacial region will be masked by spectral overlap of the scattering from the heavier mass of In. Thus, the best prospect of learning about the GaAs substrate material is by channeling through thin InAs overlayers, and such studies would be best performed in the growth chamber itself.

IV. CONCLUSIONS

RBS/channeling techniques have been used to examine the GaAs–InAs(100) heteroepitaxial interfaces grown by MBE. The backscattering spectra show that the compositional interface width is less than 300 Å, which is the depth resolution of the probe. Channeling spectra reveal that 23% of the In and As atoms are displaced by at least 0.1 Å with respect to the InAs lattice at the interface. The defect density decreases rapidly away from the interface for films ~1 μm thick and is essentially not detectable 0.5 μm from the heterojunction. Thus, the 7% lattice mismatch between GaAs and InAs is accommodated by lattice imperfections in the first 0.5 μm of the InAs film, after which the crystalline quality of the InAs film is excellent. Thus, the results of this study are in excellent qualitative agreement with those of Chang *et al.*,[5–7] but a detailed comparison is not possible because of possible differences in the growth of the films. RBS/channeling has been shown to be an excellent technique to characterize the amount of interface disorder in lattice mismatched epitaxial systems and can be applied rapidly to large number of samples in the optimization of materials properties.

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[1] K. C. R. Chiu, J. M. Poate, L. C. Feldman, and C. J. Doherty, Appl. Phys. Lett. **36**, 544 (1980).
[2] R. S. Williams, L. C. Feldman, and A. Y. Cho, Radiat. Eff. **54**, 217 (1981).
[3] T. Narusawa and W. M. Gibson, Phys. Rev. Lett. **47**, 1459 (1981).
[4] J. A. Venables and G. L. Price, in *Epitaxial Growth*, edited by J. W. Matthews (Academic, San Francisco, 1975), Part B, p. 381.
[5] C. -A. Chang, C. M. Serrano, and L. L. Chang, Appl. Phys. Lett. **37**, 538 (1980).
[6] C. -A. Chang, C. M. Serrano, L. L. Chang, and L. Esaki, J. Vac. Sci. Technol. **17**, 603 (1980).
[7] C. -A. Chang and A. Segmüller, J. Vac. Sci. Technol. **16**, 285 (1979).
[8] J. H. Van der Merwe, in *Epitaxial Growth*, edited by J. W. Matthews (Academic, San Francisco, 1975), Part B, p. 493.
[9] W. J. Schaffer and A. L. Berg, in Proceedings of the IRIS Specialty Detector Group on IR Detectors, Syracuse, 1981.
[10] S. P. Kowalczyk, W. J. Schaffer, E. A. Kraut, and R. W. Grant, J. Vac. Technol. **20**, 705 (1982).
[11] R. Ludeke, IBM J. Res. Develop. **22**, 304 (1978).
[12] J. W. Mayer, M. -A. Nicolet, and W. K. Chu, in *Material Characterization Using Ion Beams*, edited by J. P. Thomas and A. Cachard (Plenum, New York, 1976), p. 333.
[13] W. -K. Chu, J. W. Mayer, and M. -A. Nicolet, *Backscattering Spectroscopy* (Academic, San Francisco, 1978).
[14] S. U. Campisano, G. Foti, E. Rimini, and S. T. Picraux, Nucl. Instrum. Methods **149**, 371 (1978).
[15] J. H. Barrett, these proceedings.