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Thickness-dependent electron accumulation in InAs thin films on GaAs(111)A: A scanning-tunneling-spectroscopy study

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Scanning tunneling spectroscopy has been used to study quantum size effects on the electronic structure of thin InAs films grown on GaAs(111)A substrates, an example of a heterostructure with a relatively large lattice mismatch. The band gap of the InAs films, as measured from current-voltage curves, decreases gradually with film thickness, and electron accumulation occurs in layers that are thicker than 6 nm. Self-consistent calculations suggest the thickness-dependent accumulation is due to quantum size effects and Fermi-level pinning caused by the dislocation network at the InAs/GaAs interface. [S0163-1829(98)51332-X]

Molecular beam epitaxy (MBE) can be exploited to grow semiconductor thin films with unique optical and electrical properties governed by the principles of quantum mechanics. There are many reports of quantum size effects in lattice matched semiconductor thin films, including GaAs/AlAs or InAs/GaSb/AlSb, and also in slightly mismatched systems, such as $\mathrm{In}_x\mathrm{Ga}_{1-x}\mathrm{As/GaAs}$ ($x<0.1$), provided the film thickness is less than the critical layer thickness (CLT) at which plastic deformation occurs.[1] The study of quantum effects in highly mismatched systems, however, has been difficult because three-dimensional (3D) island growth, brought about by the Stranski-Krastanov mechanism,[2,3] prevents the growth of atomically flat semiconductor films. It has recently been demonstrated, however, that in a highly mismatched heteroepitaxial system, InAs/GaAs (lattice mismatch: 7.2%), this difficulty can be overcome by using non-(001) substrates. Two-dimensional (2D) growth of relaxed InAs films on GaAs has been reported to occur on (110)[4,5] and (111)A substrates.[6–8] GaAs(111)A is a particularly useful substrate since the InAs layer relaxes isotropically and misfit dislocations are confined in a network at the InAs/GaAs interface.[7,8] Strain relaxation results in the growth of atomically uniform InAs films for thicknesses greater than the CLT.

This 2D growth mode of InAs on a GaAs(111)A system makes it ideal for the study of quantum size effects in highly mismatched heterostructures, which has the additional advantages of Fermi-level pinning in the conduction band at metal/semiconductor interfaces[9–13] and high electron activation in n-type material of up to $5\times10^{19}\ \mathrm{cm}^{-3}$.[11] It is therefore an excellent system for electrical characterization and in this paper we report studies by scanning tunneling spectroscopy (STS).

STS studies of compound semiconductors are usually carried out on (110)-oriented surfaces and there are several reports on the characterization of bulk semiconductors,[14,15] heterointerfaces,[16,17] points defects,[18] and impurities in bulk materials.[19] Current-voltage (I-V) curves have also been reported for (001) surfaces.[20–22] The basic parameters obtained were the band gap and the position of the Fermi level relative to the gap, but localized states induced by impurities have also been observed.[19] Previous studies of the InAs(110) surface have shown that the Fermi level lies near the conduction-band minimum, but no electron accumulation was found,[15] consistent with results obtained from photoemission spectroscopy[23] (PES) and high-resolution electron-energy-loss spectroscopy.[24] The I-V curve for clean reconstructed InAs(001) surfaces depends strongly on the nature of the surface reconstruction and Ohmic behavior has been confirmed on As-rich (2×4) surfaces, but not on Ga-rich (4×2) surfaces.[25] There are no reports on the surface tunneling characteristics of (111)A surfaces for either GaAs or InAs and in this paper we investigate, as a function of InAs film thickness, the change in band gap and position of the Fermi level at the surface. Thickness-dependent electron accumulation is clearly observed and suggests that misfit dislocations have a significant influence on the electronic properties of InAs films.

A specially designed scanning tunneling microscopy (STM)/MBE system was used for imaging and characterizing the grown surfaces.[26] Si-doped, n-type GaAs(111)A wafers were used as substrates. After loading the wafer into the STM/MBE system the surface oxide was removed by heating the sample to 600 °C. Undoped GaAs buffer layers 100 nm-thick were grown at 500 °C and 0.1 ML/s. A 500-nm-thick GaAs layer grown under identical conditions on a semi-insulating GaAs substrate showed a hole concentration of $1\times10^{16}\ \mathrm{cm}^{-3}$, probably caused by the incorporation of background carbon impurities. STM measurements were per-

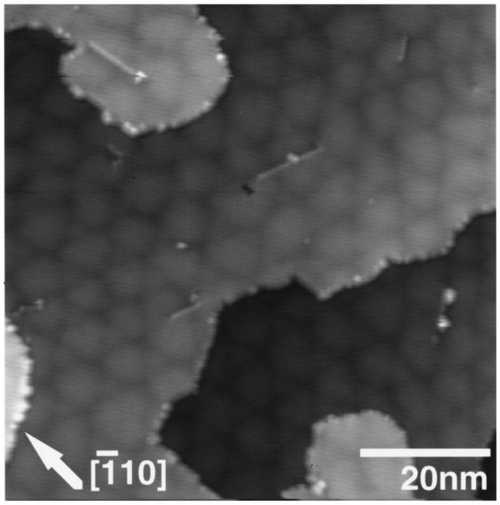

FIG. 1. A STM surface topograph of a 5-ML-thick InAs film grown on GaAs(111)A.

formed at room temperature, at sample voltages of -1.5 V–-3.5 V and tunneling currents of 0.08–0.2 nA. The topographic image and the I-V curve at each sampling point were acquired simultaneously to ensure the reliability of the I-V curves obtained.

A typical STM image of a 1.5-nm-thick InAs film grown on GaAs(111)A is shown in Fig. 1. In contrast to (001) surfaces, where 3D InAs islands are formed, the growth mode remains 2D for all InAs coverages despite the significant lattice mismatch (7.2%).[6] The topographic image shows a dislocation network with a trigonal symmetry at the InAs/GaAs interface. This network consists of partial dislocations and stacking faults, as well as perfect dislocations, buried at the interface.[7] The surface manifestation of the dislocation network disappears completely after growth of an InAs film thicker than 6 nm, presumably because the strain field is screened by a layer of this thickness. Apart from the low density of threading dislocations and inclined stacking faults coming to the surface,[7] the InAs layer is virtually defect free and the thickness is atomically uniform despite the large lattice mismatch.

The precise control of the 2D growth of InAs layers on GaAs(111)A permits the change in band gap and position of the Fermi level at the surface to be monitored by STS. Separate I-V curves for homoepitaxially grown GaAs and InAs were first obtained. The tunneling current I obtained on a 100-nm-thick undoped GaAs film grown on an n-type GaAs substrate, and the measured normalized conductance $(dI/dV)/(I/V)$ are plotted in Fig. 2(a) as a function of bias voltage V. The low-conductivity region corresponding to the band gap of GaAs can be clearly seen and the Fermi level at the GaAs surface is almost in the middle of the band gap. Although the carrier concentration of the GaAs buffer layer is low ($\sim 1\times10^{16}$ cm^{-3}), it can be deduced from the carrier concentration and buffer layer thickness that tip-induced band-bending[15] does not cause an error greater than 0.3 eV in the determination of the conduction-band minimum (CBM) and the valence-band maximum (VBM) relative to the Fermi level. In fact, these positions showed no significant dependence on the thickness of the buffer layer.

The normalized conductance curve obtained from the surface of an undoped 200-nm-thick InAs film grown on an n-type InAs(111)A substrate is shown in Fig. 2(b). A band gap of about 0.35 eV is clearly visible. The position of the surface Fermi level is in the gap, indicating no electron accumulation at the surface, in contrast to recent PES studies of InAs(111)A.[27] This discrepancy may be related to the preparation of the surfaces in the two studies since the surface state density required to move the surface Fermi level of InAs from the midgap to the CBM is less than 10^{12} cm^{-2} for a typical carrier concentration of 10^{16}–10^{18} cm^{-3}. Different preparation procedures could lead to significant differences in the density of surface defects and therefore in the position of the Fermi level at the InAs surface, but without further details of the comparative methods no definitive answer is available.

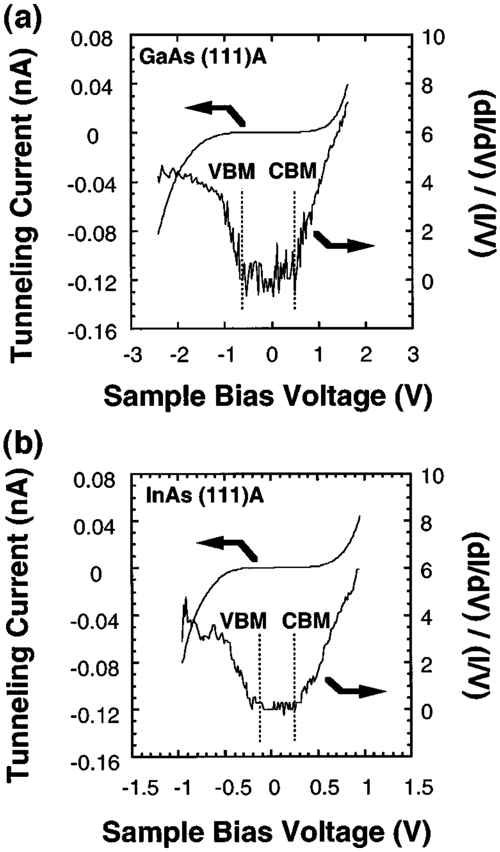

FIG. 2. Tunneling current and normalized conductance $(dI/dV)/(I/V)$ as a function of sample voltage for (a) GaAs and (b) InAs films grown homoepitaxially on (111)A substrates.

Tunneling spectra obtained from STS measurements of InAs layers grown on GaAs(111)A are shown in Fig. 3. The position of the CBM and VBM relative to the Fermi level, determined from the spectra, are plotted in Fig. 4 as a function of layer thickness. Changes in the band gap and position of the Fermi level can clearly be seen as the InAs thickness is increased and the decrease in band gap from GaAs to that of InAs occurs at about 3 nm. The position of the surface Fermi level is above the CBM, indicating that the tunneling of electrons accumulated in the InAs layers leads to a finite conductance even though the Fermi level of the tip lies in the band gap of InAs. This tunneling of the accumulated electrons has also been observed for highly doped GaAs samples.[14,15] Our results show that electrons are accumulated in the InAs layer

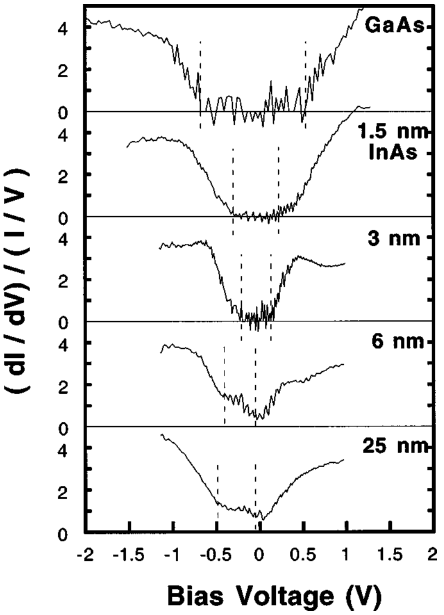

FIG. 3. Normalized conductance $(dI/dV)/(I/V)$ as a function of sample bias voltage for InAs films grown heteroepitaxially on GaAs(111)A.

after the heteroepitaxial growth of 6-nm-thick InAs films without any intentional doping.

As discussed earlier, we have already shown that electron accumulation does not occur for InAs films grown homoepitaxially on InAs(111)A in our system. This suggests that surface states are not responsible for the electron accumulation in InAs/GaAs(111)A heterostructures, but defects at the interface act as donorlike states and supply electrons to the InAs layers. The high density of dislocations at the interface is the most likely source of the accumulated electrons and the density of dangling bonds along the dislocations ($\sim 1 \times 10^{14}$ cm^{-2}), calculated from the model proposed in Ref. 7 for the structure of the dislocation network at the InAs/GaAs(111)A interface, is high enough to generate electron accumulation in the InAs layer. It is reasonable to assume that this kind of dangling bond acts as a donor because the charge neutrality level of InAs is 0.1–0.2 eV above the bottom of the conduction band.[13] Since the dangling-bond density is much higher than that required for electron accumulation (10^{12}–10^{13} cm^{-2}), the interface Fermi level must be pinned at the energy level of the dangling bonds.

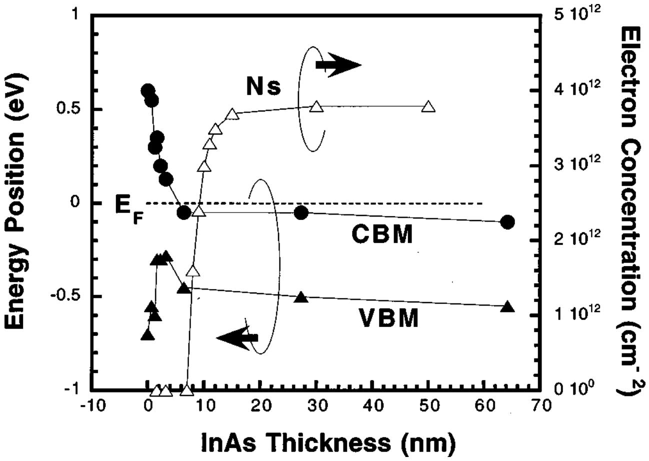

FIG. 4. The measured position of the CBM (closed circles) and VBM (closed triangles) relative to the surface Fermi level as a function of InAs layer thickness. The sheet electron concentration N_S, obtained from self-consistent calculations, is also plotted (open triangles).

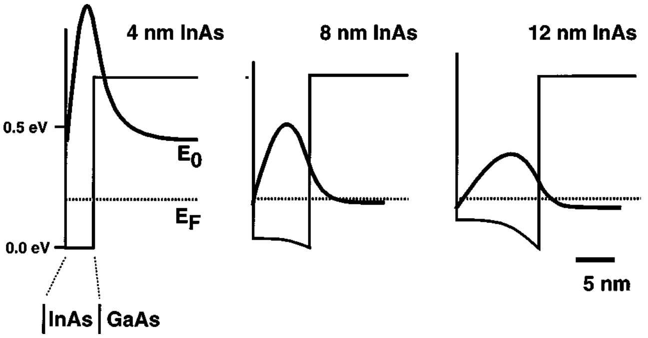

FIG. 5. The wave functions of the lowest quantum levels and potential energy profiles for three different InAs film thicknesses obtained from self-consistent calculations. The position of the Fermi level at the InAs/GaAs interface is assumed to be pinned 0.2 eV above the CBM.

A self-consistent modeling program has been developed and successfully applied to the problem of surface pinning in InAs/GaSb structures.[28] For simplicity, the nonparabolicity of the InAs conduction band was not included and the one-dimensional Schrödinger equation with the effective electron mass obtained for InAs bulk material ($\cong 0.026 m_0$) was solved self-consistently with the one-dimensional Poisson equation, in the calculations described here. They assume a conduction-band discontinuity of 0.8 eV between GaAs and InAs,[8] an infinite potential barrier at the InAs surface,[29] and the presence of interface states that pin the Fermi level at an energy 0.2 eV above the CBM. It is also assumed that the film is unstrained (i.e., no account is taken of any residual strain present following the introduction of misfit dislocations) and that there are no additional defect states apart from those responsible for the pinning.[30] To describe the Fermi-level pinning, a δ functionlike positive carrier profile was assumed at the InAs/GaAs interface to cancel the electric field in the GaAs layers. This reflects the fact that the electrons in the InAs films originated from the defects localized at the interfaces. The wave functions of the lowest electronic subband and the electrostatic potentials obtained are shown in Fig. 5. The calculated electron concentration N_S is also plotted in Fig. 4. For InAs films thinner than 6 nm, the lowest quantum level is higher than the Fermi level and no electrons are accumulated. The lowest level shifts down with increasing film thickness and reaches the Fermi level at around 6 nm. Further increases in InAs thickness pin the Fermi energy at the interface and start to induce electron accumulation. The sheet concentration then increases with film thickness before saturating at about 3.8×10^{12} cm^{-2} (Fig. 4). Saturation occurs when the InAs layer is much thicker than the accumulation layer. The interface Fermi-level pinning and quantum size effect can therefore explain the thickness-dependent electron accumulation observed in InAs layers grown on GaAs(111)A. It should be mentioned that the change in the band gap obtained in our STS characterization cannot compared with the calculation presented here because the valence-band structure is not included. More precise full-band self-consistent calculations[31] are necessary for more detailed analysis of our experimental data.

In conclusion, the band gap and position of the Fermi level at the surface have been obtained as a function of film thickness for a highly mismatched heteroepitaxial system, InAs/GaAs(111)A. The band gap of InAs is established for 3-nm-thick films and the existence of an electron accumulation layer is confirmed after the growth of 6 nm of InAs. This thickness-dependent electron accumulation is a unique property induced by the quantum size effect of this highly mismatched heterostructure, and it is suggested that misfit dislocations at the InAs/GaAs interface are responsible for the electron accumulation.

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[29] This is a reasonable assumption since the work function of III-V compound semiconductors is typically greater than 4 eV.

[30] Strictly speaking, a finite density of surface states should be assumed to explain the STS spectrum for InAs [Fig. 2(b)], but this does not alter the discussion presented here provided the density is sufficiently below the interface state density. This is the case in the present InAs/GaAs system since the density of dangling bonds associated with the dislocations is as high as 10^{14} cm^{-2}.

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