Structure and optical properties of Si/InAs/Si layers grown by molecular beam epitaxy on Si substrate

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Epitaxial Si/InAs/Si heterostructure grown on (001) Si substrate by molecular beam epitaxy and annealed at 800 °C was investigated by high resolution transmission electron microscopy. Extensive interdiffusion leads to the formation of an InAs solid solution in the Si cap layer. Additionally, InAs-enriched regions with extensions of ~6 nm, which exhibit two kinds of ordering are observed. The ordering of InAs molecules has occurred, respectively, in (101) and (10T̄̄) planes inclined and (110) and (T̄0) planes parallel to the [001] growth direction. It is attributed to the energy gain from the reduced number of mixed Si–As and Si–In bonds. The sample show photoluminescence in the 1.3 μm region, which is tentatively attributed to the recombination of excitons localized in the ordered regions. © 2000 American Institute of Physics. [S0003-6951(00)00719-1]

The potential benefit from combining the advantageous optical properties and flexibility of III–V semiconductors with silicon technology widely used in microelectronics has attracted great interest for decades. Up to now, researchers have focused on the growth of continuous layers of III–V materials on silicon. The large misfit between Si and, e.g., such small InAs islands on Si was still a practically unresolved problem. More recently, the possibility to exploit the formation of narrow-gap III–V materials on Si substrates has been pointed out. Indeed, such small InAs islands on Si(100) surface have been observed by scanning tunneling microscopy and high-resolution transmission electron microscopy (HRTEM). HRTEM investigations of capped InAs/Si structures revealed a high density of coherent InAs clusters with typical dimensions in the 3 nm region at the InAs/Si interface for optimized growth conditions. Such samples exhibit a broad photoluminescence (PL) peak in the 1.3 μm region at 10 K. Detailed optical investigations of this PL line indicated a k indirect type II transition, which has been tentatively attributed to excitons localized in the small coherent InAs clusters. The extreme small size (<3 nm) of these clusters might, however, prevent sufficient carrier localization. The present work presents a detailed structural characterization of such InAs–Si layers providing insight into the origin of the 1.3 μm PL peak.

The InAs/Si heterostructure was grown by molecular beam epitaxy (MBE) on p-type Si(100) substrate using an EP 1203 machine. Conventional evaporation cells were used for In, Si, and As fluxes. The growth rates for InAs and Si were 0.03 and 0.017 nm/s, respectively, and the As4/In flux ratio was ~4. InAs was deposited at a substrate temperature of T s = 350 °C. For these particular growth conditions, the reflection high energy electron diffraction pattern indicates the two- (2D) to three-dimensional (3D) transition at 1.3 monolayers (ML). The nominal thickness of the deposited InAs was 1.6 ML. Immediately after the InAs deposition, a 10 nm Si cap layer was grown at the same T s = 350 °C followed by a 10 min annealing step at 700 °C. Further 40 nm Si cap layer was grown at 700 °C with a final 10 min annealing step at 800 °C to smooth resulting surface. The crystaline quality of the structure and the composition of the grown layers were investigated by techniques of transmission electron microscopy (TEM).

The following electron microscopes were exploited: Philips CM20T and JEOL JEM-4000 EX operating at 200 and 400 kV, respectively. Commercial software package ‘MacTempas’ was used for computer simulations of HRTEM images. PL spectra were measured at a temperature of 7 K using argon laser excitation.

Typical cross-section and plan-view images of the investigated structure are shown in Figs. 1(a) and 1(b), respectively. The plan-view image shows the good structural quality of the sample with a relatively low density (1 × 106 l/cm²) of structural defects, marked A in Fig. 1(b). These defects (A) are located at the InAs/Si interface and do not penetrate into Si cap layer. The nature of the contrast features B in Fig. 1(a) is analyzed below.

First, the average InAs concentration in the Si cap layer can be estimated from selected area diffraction (SAD) taken at once from substrate and cap layer in cross-sections sample as shown in Fig. 1(a). Such SAD pattern reveal a splitting of reflections in [001] direction perpendicular to the layer surface [Fig. 1(c)]. This splitting is attributed to a tetragonal distortion of Si cap layer due to the formation of an InAs solid solution. The magnitude of the observed splitting of the...
reflection (206) measured in SAD corresponds to a tetragonal distortion \( \Delta = \frac{g}{g_{(206)}} = \Delta a/a_{Si} = 0.007 \). The volume of the distorted unit cell is \( V_{i} = a_{Si}^{3}(1 + \Delta a/a_{Si}) \). It immediately follows that average cubic unit cell parameter of the solid solution \( a_{ss} \) is given by:

\[
a_{ss} = \left( \frac{V_{i}}{a_{Si}} \right)^{1/3} = a_{Si}(1 + \Delta a/a_{Si})^{1/3}.
\]  

(1)

Taking \( a_{ss} \) as to be linearly dependent on the InAs concentration in the Si matrix, it follows:

\[
C_{InAs} = (a_{ss} - a_{Si})/(a_{InAs} - a_{Si}),
\]

(2)

where \( C_{InAs} \) concentration of InAs in Si cap layer, \( a_{Si}, a_{InAs} \)-unit cell parameters of Si and InAs, respectively. Substitution of \( \Delta a/a_{Si} = 0.007 \) into Eqs. (1), (2) gives \( C_{InAs} = 0.004 \). Thus the averaged composition of the cap layer can be written as \( Si_{0.996}(InAs)_{0.004} \).

Second, in high resolution cross-sectional images the dark regions marked by B in Fig. 1(a) reveal a doubling of periodicity of \{002\} lattice planes in [110] or [1\bar{1}0] directions [Fig. 2(a)]. It leads to appearance of diffuse maxima situated halfway between \( \pm (220) \) matrix reflections in the Fourier transformed image (FFT) [see insert in Fig. 2(a)]. This result can be interpreted as a partial ordering of InAs in Si. A possible idealized model of such an ordering is shown in Fig. 2(b) where InAs occupies every other atomic (101) plane inclined by 45\(^\circ\) to the surface. Let us define the two-dimensional ordering as \((na \times mb)\), where \(n,m\)-integer numbers and \(a,b\) periodicities in two perpendicular directions without ordering. In our case these directions are \((101),(1\bar{1}0)\) and \(a = b = a_{Si}/2\sqrt{2} = 0.192 \text{ nm} \). It gives \((2a \times 1a)\). A HREM image [Fig. 2(c)] simulated on the basis of this structural model shows that the darker rows correspond to InAs atomic rows. It is obvious that the contrast calculated for an ideal ordering is in a qualitative agreement with the experimental image. These partially ordered regions can also be observed at low magnification using diffraction contrast technique [see features B in Fig. 1(a)]. In this case, the image contrast (dark regions) results from variations of the extinction distance. The size of \((2a \times 1a)\) coherent ordered regions (\(\geq 6 \text{ nm} \)) is about 2 times larger than the size of coherent InAs clusters formed at the InAs/Si interface and described in a former letter. Additionally, a special kind of ordering
was found in the near surface region of cap layer, where InAs occupies (110) and (10 T) planes perpendicular to the layer surface (Fig. 3). Here, however, periodicity is larger with only every third atomic plane occupied by InAs. This kind of ordering (3a×1a) is usually extended over rather large areas being approximately several tens of nm in diameter.

Figure 4 depicts a low temperature PL spectrum of the investigated sample revealing a broad PL peak in the 1.3 μm region. Recently, this luminescence has been studied in detail in a different sample, suggesting a k-independent type II transition in the epitaxial layer. Such a transition is indeed expected for coherent InAs clusters observed near the InAs/Si interface. However, the small size (~3 nm) of such clusters might be too small for sufficient carrier localization. As shown above, the Si-cap layer is actually a Si–InAs solid solution with (2a×1a) and (3a×1a) ordered InAs-rich regions. The ordered regions with a high InAs concentration (and therefore smaller band gap) and a size of ~6 nm, can provide sufficient carrier localization to explain the observed 1.3 μm emission. The incorporation of InAs molecules into the Si is expected to shift the relative positions of the conduction and valence bands leading to a quantum structure.

In conclusion, we have demonstrated that InAs can be epitaxially incorporated in silicon by MBE growth. A solid InAs/Si solution is formed in the Si cap layer. The formation of such a InAs/Si solid solution results from an extensive diffusion of InAs into the Si cap layer during annealing at 800 °C. According to our measurements the average concentration of InAs in the Si cap layer can reach C_{InAs} = 0.4%. In addition to the random distribution of InAs, two similar kinds of ordering have been observed. The (2a×1a) ordered regions have a size of ~6 nm in diameter. They are formed due to condensation of InAs molecules in every second (110) atomic layer. As a result the free energy of the system gets lower due to decreasing the number of mixed Si–As and –In bonds. The appearance of broad PL band at 1.3 μm can be correlated to the formation of InAs/Si ordered regions.

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FIG. 4. PL spectrum of the investigated sample showing a broad luminescence at 1.25 μm. The peak at 1.1 μm correlates to emission from the Si bulk.