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Structural and optical features of InGaAs quantum dots grown on Si(001) substrates

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Abstract

A multilayer GaAs/SiGe/Si heterostructure with InGaAs quantum dots (QDs) embedded in a GaAs layer was grown by molecular beam epitaxy (MBE) on a Si(001) substrate. A step-graded Si_{1-x}Ge_x ($0 \le x \le 1$) buffer layer and a GaAs layer with In_yGa_{1-y}As ($y \sim 0.5$) QDs were deposited consecutively in two different MBE systems. The heterostructure exhibits intense photoluminescence in the region of 1.3 μ m at room temperature. Perfect crystal InGaAs islands with height less than 10 nm are the sources of this radiation.

1. Introduction

Achieving direct growth of III–V compounds on Si substrates is one of the crucial problems in producing advanced semiconductor devices. This is required to provide the optical performance needed for interchip and intrachip communication links. There are a few approaches based on hybridization or complex epitaxial growth methods [1–3]. The most promising way to get such integration is by fabrication of III–V-based light emitters on Si substrates for the 1.3–1.55 μ m range [4]. Numerous studies of the growth of InAs quantum dots (QDs) embedded in silicon have been performed during the last few years [5–7]. Recently we have grown a GaAs layer with embedded InGaAs islands on a Si substrate with a Si_{1–x}Ge_x step-graded buffer layer, which exhibited intense photoluminescence (PL) in the region of 1.3 μ m at room temperature [8]. In this work we present results of a study of optical and structural properties of the heterostructure.

2. Experimental details

The epitaxial growth processes for the SiGe and III–V parts of the heterostructure were carried out consecutively in two different molecular beam epitaxy (MBE) systems. A three-inch

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13351



Figure 1. A RHEED image after the deposition of a nominally 3 nm thick In_{0.5}Ga_{0.5}As layer.

Si(001) wafer was used as a substrate. A step-graded Si_{1-x}Ge_x buffer layer was grown in a KATUN MBE installation equipped with two electron beam evaporators for Si and Ge. A 100 nm thick Si buffer was first grown at 750 °C followed by a low-temperature (LT) Si layer deposited at 400 °C with a thickness of 50 nm. Recent reports indicated that the use of a LT Si buffer layer provides high-quality strain-relaxed SiGe buffer layers and could significantly reduce the threading dislocation (TD) density in the SiGe/Si heterostructures [9]. The step-graded Si_{1-x}Ge_x buffer layer was divided into three sublayers with Ge contents x = 0.3, 0.62 and 1.0. Each of these sublayers consisted of a 50 nm LT layer grown at 250 °C followed by a 150 nm layer grown at 500 °C. Then the wafer was capped by a 5 nm thick Si layer and carried through the atmosphere into a TSNA-25 solid-source MBE installation. Prior to the growth of the III–V part, annealing of the sample was accomplished in the growth chamber at 800 °C in Ga flow to remove the native oxide from the surface. After this, a 200 nm thick GaAs layer was grown at 700 °C followed by a In_yGa_{1-y}As ($y \approx 0.5$) layer with effective thickness of 3 nm and a 20 nm GaAs cap layer grown at 650 °C. The InGaAs layer was grown by the cyclical deposition of InAs(2 s)/GaAs(2 s).

During the epitaxial growth, the wafer surface was monitored by *in situ* reflection highenergy electron diffraction (RHEED). After the In_{0.5}Ga_{0.5}As QD layer deposition, a transition from 2D to 3D growth mode was observed due to the coexistence of a streaky and a spotty RHEED pattern (figure 1). RHEED measurements allowed us to determine the lattice constant ratio a_{InGaAs}/a_{GaAs} to be equal to 1.034. This value corresponds to the In content of ≈ 0.5 without considering misfit strains appearing due to the high lattice mismatch between GaAs and InGaAs. PL spectra were measured at 77 and 300 K with the use of an MDR-2 monochromator. A semiconductor laser with wavelength $\lambda = 0.66$ mm (quantum energy $h\nu = 1.87$ eV) served as an excitation source. The emission from the samples was recorded using a liquid-nitrogencooled germanium p–i–n photodiode. The structural studies were performed by transmission electron microscopy (TEM, JEM-200CX) on the cross-sectional and plan-view samples.

3. Results and discussion

The PL spectrum at 77 K shows (figure 2, curve 1) the recombination lines from a 2D wetting layer (1235 meV) and 3D InGaAs QDs (1045 meV). At room temperature (figure 2, curve 2), the PL intensity from QDs is approximately four times lower. The large full width at half-maximum (FWHM) of the QD emission line can be attributed to the fluctuations in size and alloy composition of the InGaAs islands. For the epitaxial growth of III–V alloys, including



Figure 2. PL spectra from InGaAs(QDs)/GaAs/SiGe/Si heterostructure at 77 K (curve 1) and 300 K (curve 2) before and after removing InGaAs/GaAs layers (curve 3, T = 77 K) by selective chemical etching.



Figure 3. TEM micrographs of structural defects in the heterostructure: (a) a cross-sectional image (dark field); (b) a plan-view image of the top GaAs layer with InGaAs islands. The white arrow indicates the antiphase boundary in the GaAs layer. Black arrows indicate nanoparticles in the SiGe buffer layer. Small (1) and large (2) InGaAs islands have the same moiré contrast.

InGaAs, it is well known that different migration lengths of different kinds of adatom on the rough surface results in lateral composition inhomogeneity of a layer [10]. After removing a GaAs layer by etching in a $5H_2SO_4$: $1H_2O_2$: $1H_2O$ etchant, we observed the recombination lines from a $Si_{1-x}Ge_x$ buffer layer and a weak line from a bound exciton with emission of a TO phonon in the PL spectrum at 77 K (figure 2, curve 3). It is evident that the radiative recombination of interest is related to the InAs/GaAs layers.

The TEM study shows that a highly developed relief has been formed at the heterostructure surface because of a corrugation of the interfaces in the SiGe buffer layer (figure 3(a)). Moreover, all interfaces in the multilayer heterostructure degraded during the epitaxial growth. This effect can be attributed to a diffusion intermixing of the alloys due to the large proportion of the LT layers supersaturated with the intrinsic point defects. Nevertheless, a high degree of strain relaxation has been achieved in this buffer layer, which allowed us to get an almost unstrained GaAs layer. The GaAs layer consists of antiphase domains (figure 3(b)) and contains a high density, $\sim 10^9$ cm⁻², of TDs. Numerous islands with the same parallel moiré contrast are observed in both plan-view and cross-sectional micrographs. There is a great spread in



Figure 4. A plan-view sample with the GaAs layer selectively removed by chemical etching: (a) a TED pattern with extra spots 1, 2, 3 from crystalline nanoparticles (1, 2—extra spots arranged symmetrically with respect to the transmitted electron beam; 3—from crystalline nanoparticles); (b) a dark-field micrograph of the SiGe layer in one of the extra spots (1, 2—nanoparticles with different contrast).

the height and lateral size of the islands. Small islands with height less than 10 nm are nonuniformly arranged on the surface with the density $\sim 10^8$ cm⁻². Such islands are free of extended defects. Large islands with height of about 10–60 nm possess pyramidal shape and contain dislocations and microtwins (figure 3(a)). They are agglomerations of small islands. More than 70% of the small islands are included in the large agglomerates, which can be attributed to the influence of a corrugated surface on the island nucleation.

The results obtained show that the small InGaAs islands are the QDs responsible for the radiation near 1.3 μ m. Small islands are free of extended defects because, on one hand, defect generation does not occur in these thin islands and, on the other hand, the islands themselves do not nucleate in places with TDs. The latter fact can be attributed to the reduction of elastic strains in GaAs layers near to the dislocations, which in turn leads to the reduction of the driving force for island nucleation. In addition, recently we have grown some InGaAs(QDs)/GaAs heterostructures on GaAs substrates. The QDs density was more than 10¹⁰ cm⁻², and the PL intensity of a similar band was two orders of magnitude higher than that in the sample described. This fact indicates that the relatively low intensity of the PL band in the heterostructure grown on Si substrate is mainly caused by the low island density.

Interestingly, we have found nanoparticles of an unknown nature randomly distributed over the SiGe buffer layer (figures 3(a) and (b)). They possess an oblong shape and they are characteristically 30-300 nm in length and 20-100 nm in diameter. The density of the nanoparticles is about 3×10^8 cm⁻². The transmission electron diffraction (TED) patterns from the regions with such nanoparticles always contain extra spots (figure 4(a)). In dark-field micrographs obtained from the extra spots, some of the nanoparticles look like bright spots whereas others have very weak bright contrast (figure 4(b)). Their contrast can be easily changed by observing them in another extra spot. The TED patterns and dark-field micrographs indicate that these nanoparticles are crystalline. They accommodate coherently to the SiGe matrix; however, there is no strict order in their arrangement in the matrix with regard to the crystallographic directions (figure 4(b)). We suppose that these nanoparticles can be enriched by Ge and may originate due to the alloy diffusion intermixing described above. A study is in progress and detailed results will be published elsewhere.

4. Conclusions

The structural and optical properties of the multilayer GaAs/SiGe/Si heterostructure with InGaAs QDs embedded in the GaAs layer, grown by MBE on the Si(001) substrate, were investigated. Practically full strain relaxation has been achieved in the step-graded Si_{1-x}Ge_x $(0 \le x \le 1)$ buffer layer grown with the use of the LT growth technique. Surface corrugation and interface degradation have been found to occur during the growth of this layer, which can be attributed to the diffusion intermixing of the alloys. We demonstrated that intense PL in the region of 1.3 μ m at room temperature can be achieved in such heterostructures despite the presence of a high TD density, ~10⁹ cm⁻², in the GaAs layer. Small In_yGa_{1-y}As ($y \sim 0.5$) islands (QDs) were found to be defect free and responsible for the radiation. The majority of InGaAs is concentrated into the large islands which are agglomerations of small islands. We suppose that this effect can be caused by surface corrugation. We have found crystalline nanoparticles of an unknown nature in the SiGe buffer layer.

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