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2010 Nanotechnology 21 465701

(http://iopscience.iop.org/0957-4484/21/46/465701)

IOP Publishing | Nanotechnology

Nanotechnology **21** (2010) 465701 (5pp) doi:10.1088/0957-4484/21/46/465701

Cathodoluminescence studies of GaAs nano-wires grown on shallow-trench-patterned Si

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Received 10 May 2010, in final form 26 August 2010
Published 25 October 2010
Online at stacks.iop.org/Nano/21/465701

Abstract

The optical properties of GaAs nano-wires grown on shallow-trench-patterned Si(001) substrates were investigated by cathodoluminescence. The results showed that when the trench width ranges from 80 to 100 nm, the emission efficiency of GaAs can be enhanced and is stronger than that of a homogeneously grown epilayer. The suppression of non-radiative centers is attributed to the trapping of both threading dislocations and planar defects at the trench sidewalls. This approach demonstrates the feasibility of growing nano-scaled GaAs-based optoelectronic devices on Si substrates.

1. Introduction

The heteroepitaxy of a device-quality GaAs layer on Si substrates has recently attracted increasing attention because of its application in monolithic optoelectronic and high speed integrated circuits (ICs). The epitaxial growth of GaAs on Si encounters problems of polarity difference, a lattice mismatch of 4.1%, and a thermal expansion mismatch of 54% [1], which result in the formation of defects such as antiphase disorders [2] and threading dislocations [3]. A possible approach to inhibit the formation of threading dislocations is to open nano-trenches on Si by lithography and then overgrowing the GaAs layers in the trenches [4–7]. The threading dislocations are expected to be trapped at the bottom of the overgrown GaAs. This technique, like the shallow trench insulator (STI) structure in a Si-based process, has been referred to as the aspect ratio trapping (ART) method [5]. Transmission electron microscopy (TEM) results confirm that the threading dislocations are trapped close to the GaAs/Si interface and no defects are present at the surface of the nano-wire-like GaAs layers with a width of ∼300 nm [5, 7]. To meet current technological needs, the trench width should be further reduced without reducing the structural quality. This raises technical challenges for both epitaxial growth and structural characterization. TEM for structural characterization is time consuming, destructive, and limited to the investigation of large areas. However, conventional optical characterizations are limited in terms of the spatial resolution. In this study, high-quality GaAs nano-wires with widths below 300 nm were grown on shallow-trench-patterned Si by metalorganic chemical vapor deposition (MOCVD). Cathodoluminescence (CL) is demonstrated to be very effective for measuring the optical properties of GaAs nano-wires. GaAs nano-wires that are grown in trenches with widths between 80 and 100 nm are shown to have the strongest emission efficiency, because of the effective suppression of non-radiative centers as a result of the successful trapping of threading dislocations and planar defects at the trench sidewalls.

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2. Experimental details

Trenches along $[1\bar{1}0]$ with designed widths ranging between 40 and 1700 nm and a depth of 250 nm were fabricated on 12 inch, p-type, (001) Si wafers through a SiO_2 mask using 193 nm immersion lithography and reactive ion etching (RIE). The GaAs layer was deposited in these trenches using a commercial MOCVD system at 70 Torr, including a low-temperature buffer layer grown at 430 °C and a high-temperature top layer grown at 650 °C. Additionally, GaAs that was grown on a planar Si substrate under the same growth conditions and another homoepitaxial GaAs epilayer that was grown on semi-insulating GaAs substrate by molecule beam epitaxy (MBE) were used as reference samples. Structural defects in these specimens were analyzed by TEM using a FEI Tecnai G2 F20 microscope operated at 200 kV. The optical properties were investigated by obtaining CL spectra and monochromatic mapping using a JEOL JSM-7001F microscope at 300 K, operated at 16 keV and 15 nA. The spot size of the electron beam was less than 10 nm under these conditions. The CL signals were analyzed by a Horiba Jobin-Yvon iHR550 0.5 m monochromator and detected using a LN_2-cooled charge-coupled device (CCD) with an energy resolution of 0.3 meV.

3. Results and discussions

The morphologies of these GaAs nano-wires that were grown in trenches were preliminarily characterized by scanning electron microscopy (SEM). Figure 1(a) presents the plan-view SEM image. The bright and dark areas represent GaAs and SiO_2, respectively. GaAs nano-wires were separated by SiO_2 sidewalls of different widths. Figures 1(b)–(d) present the plan-view TEM images of the GaAs nano-wires grown in trenches with widths of 1000, 80, and 40 nm, respectively. Before the TEM measurements were made, the specimens were polished and ion milled on both sides. The TEM images reveal the structural quality of the GaAs nano-wires close to the top of the trenches. Structural defects were observed at the surface of GaAs that was grown in the 1000 nm trenches. The density of defects exceeds 10^9 cm^{-2}. In figure 1(c), no structural defects were found when the width was reduced to 80 nm. This result was verified for several specimens. However, further reducing the trench width to 40 nm again produced a structural defect at the surface, shown in figure 1(d), indicating that the smallest width at which structural defects near the surface are not produced is around 80 nm, which is narrower than reported in recent literature [5, 7]. The presence of structural defects at the surface was also confirmed by the cross-sectional TEM cleft along $[1\bar{1}0]$ for GaAs in 80 and 40 nm wide trenches, shown in figures 2(a) and (b), respectively. Black and white arrows indicate threading dislocations and planar defects, respectively. On top of the GaAs, no dislocation is observed over a length of 1 μm along $[1\bar{1}0]$ in either the 80 or 40 nm wide trenches. In contrast, planar defects propagate to the surface when the trench width is 40 nm, which confirms figure 1(d).

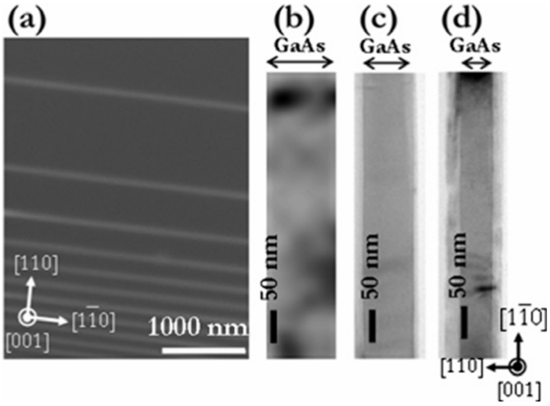

Figure 1. (a) Plan-view SEM image of GaAs nano-wires grown on nano-scale shallow-trench-patterned (001)Si. Plan-view TEM images along $[1\bar{1}0]$ with a trench width of (b) 1000, (c) 80, and (d) 40 nm.

The GaAs nano-wires in the trenches of width 80–100 nm have the best structural quality, for the following reason. Threading dislocations of GaAs are energetically favored starting at the (001) plane, rising up on the (111) planes in the $\langle 110 \rangle$ direction [8], which makes an angle of 45° to the (001) growth plane. Therefore, threading dislocations are trapped in trenches with widths of less than ~300 nm before they reach the surface, because the trenches are in the range of 300–350 nm deep as shown in figures 2(c)–(e). However, planar defects that are formed as a result of deposition mistakes are favored in the {111} atomic planes and propagate to the surface [9, 10]. The respective cross-sectional SEM images of figures 2(c)–(e) for trench widths of 300, 140, and 40 nm, respectively, reveal that as the trench width decreases the basal Si(001) plane is reduced and gradually replaced by inclined facets. Thus, shrinking the trench width reduces the number of threading dislocations at the surface and increases the density of planar defects. For trench widths of between 80 and 100 nm both threading dislocations and planar defects are blocked 150 nm below the GaAs surface. Therefore, defect-free GaAs of depth 150 nm can be achieved.

Along with TEM, CL is utilized to estimate the defect density of the overgrown GaAs. Figure 3 represents the normalized CL spectra at room temperature. In figure 3(a), the position of the peak at 1.421 eV, associated with the MBE-grown homoepitaxial GaAs on the GaAs substrate is consistent with the near-band-edge emission from the strain-free GaAs epilayer [11]. From GaAs grown on a planar Si substrate, the emission peak is at 1.416 eV, as shown in figure 3(b). According to previous literature [12], the red shift of 5 meV is caused by the tensile strain, which is caused by the mismatch of thermal expansion coefficients of GaAs and Si. For GaAs grown in trenches, as shown in figures 3(c)–(g), the peak position is initially blue-shifted as the trenches become narrower, and is then red-shifted as the width of the trench is further reduced to less than 80 nm. Figure 4(a) plots the peak energy as a function of trench width. The higher energies of peaks from GaAs in trenches with widths of between 80 and 300 nm are attributed to compressive stress that may be induced by the SiO_2 sidewalls.

In addition to the peak energy, the emission efficiency, determined from the CL, is also used to evaluate structural

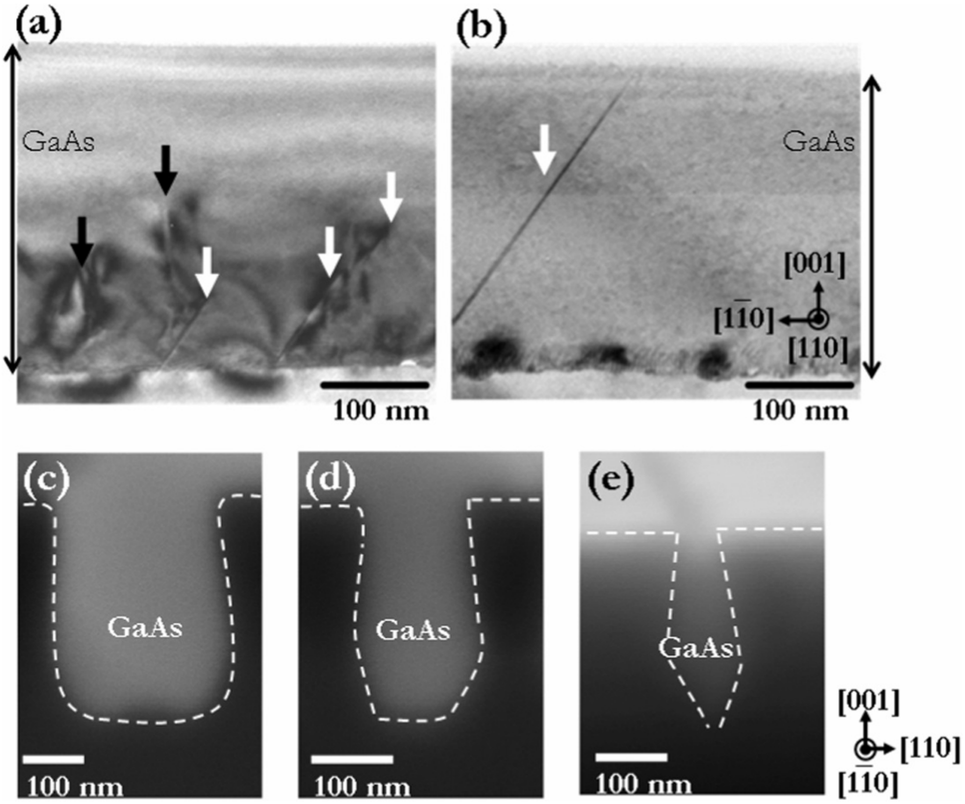

Figure 2. Cross-sectional TEM images of (a) 80 nm and (b) 40 nm wide GaAs nano-wires cleft along [1$\bar{1}$0]. Cross-sectional SEM images with a trench width of (c) 300, (d) 140, and (e) 40 nm.

quality. A higher CL emission efficiency implies better structural quality and a lower density of non-radiative centers [13]. The emission intensity of 80–100 nm GaAs nano-wire is weaker than that in figures 3(a)–(c). However, when the smaller emission volume is considered, the emission efficiency of the 80–100 nm GaAs nano-wire is the best, as shown in figure 4(b). The emission efficiency is defined as the ratio of the CL intensity to the volume of emission. The CL intensity is the average over many spots on the GaAs nano-wires. The volume of the region of luminescence emission in the thin film (wide GaAs) equals the electron–specimen interaction region where carriers were generated. In the GaAs nano-wires, the interaction region is wider than the nano-wires and the real emission volume should be modified, as shown in figures 4(c) and (d). According to a Monte Carlo simulation, when a 16 keV electron beam is focused at the center of the trench, more than 50% of the carriers are generated in a gray cylinder-shaped region with a diameter of 150 nm and a depth of 200 nm [14]. The thickness of all the GaAs nano-wires exceeds 300 nm, which is greater than the electron generation depth. However, when the width of the trench is less than 150 nm, some of the generated electrons are in the GaAs, while the remainder are in the SiO_2 sidewalls. The CL emission from SiO_2 is outside the energy range 1.35–1.55 eV. Only the generated electrons in the GaAs nano-wire contribute to the CL emission. When the width of the trenches exceeds 150 nm, all of the electrons in the electron-interaction region contribute to the CL emission.

In figure 4(b), the emission efficiency initially increases as the width of the trench decreases, and then decreases as the width of the trench decreases further below 80 nm. The width of the trench that yields GaAs nano-wires with the highest structural quality is 80–100 nm, and is consistent with the plan-view TEM measurement. For trenches with widths between 60 and 200 nm, the emission efficiency exceeds that of homoepitaxial GaAs on a GaAs substrate, indicating that GaAs grown on a shallow-trench-patterned Si substrate significantly suppresses the density of non-radiative centers, which generally include both threading dislocations [15] and planar defects [16]. The trapping of threading dislocations and planar defects significantly reduces the density of non-radiative defects close to the surface. The density is even lower than that in the homoepitaxial GaAs thin film and causes a higher CL emission efficiency of GaAs grown in a trench with widths of 80–100 nm. A similar result has been observed for 270 nm wide GaAs using photoluminescence [5]. In this study, the optimum trench width can be further reduced from 270 to 80–100 nm. However, further reduction of the trench width toward 40 nm causes planar defects to propagate to the GaAs surface, degrading the emission efficiency.

Figures 5(a) and (b) show the plan-view SEM image for GaAs in the 1000 nm trench and the corresponding CL images detected at the peak energy. Dark spots, which indicate non-radiative centers, are found in figure 5(b). Figures 5(c) and (d) show the SEM image and the corresponding CL mapping image of GaAs with a trench width of 100 nm. No dark spot

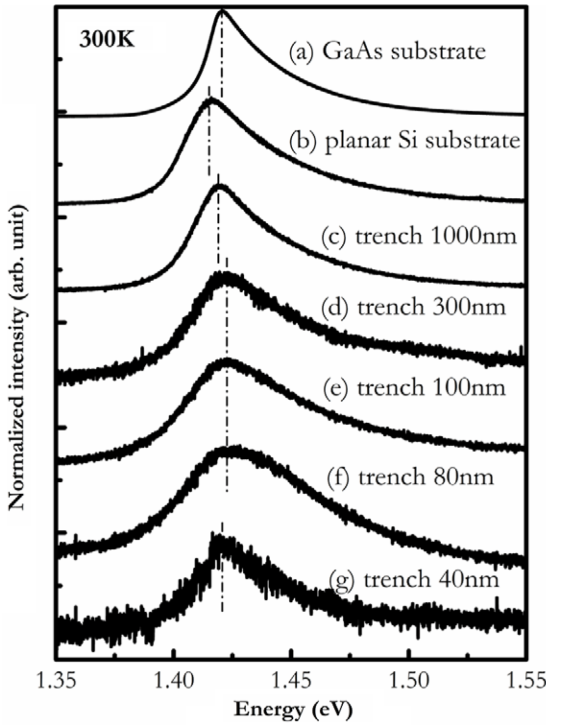

Figure 3. Room temperature CL spectra of GaAs grown on (a) GaAs substrate, (b) planar Si substrate, and nano-scale shallow-trench-patterned Si substrate, with a trench width of (c) 1000, (d) 300, (e) 100, (f) 80, and (g) 40 nm.

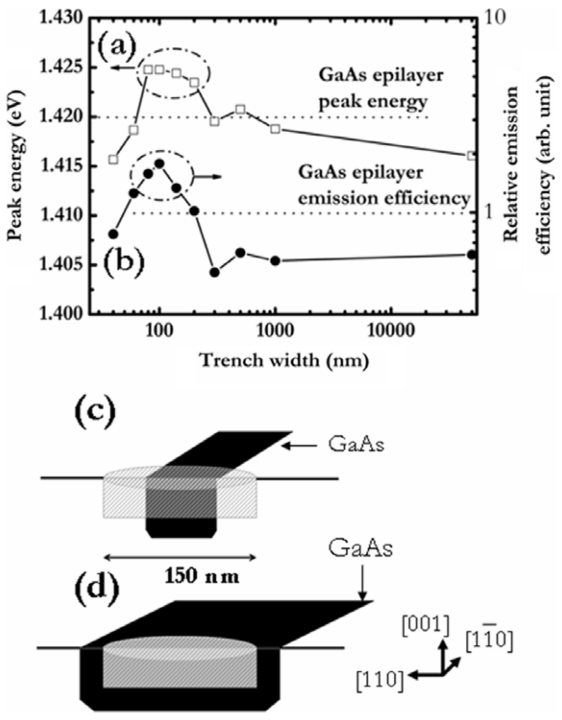

Figure 4. (a) Peak energy and (b) relative emission efficiency of GaAs grown in trenches of different width. Schematic representation of the emission volume for GaAs in (c) narrow and (d) wide trench.

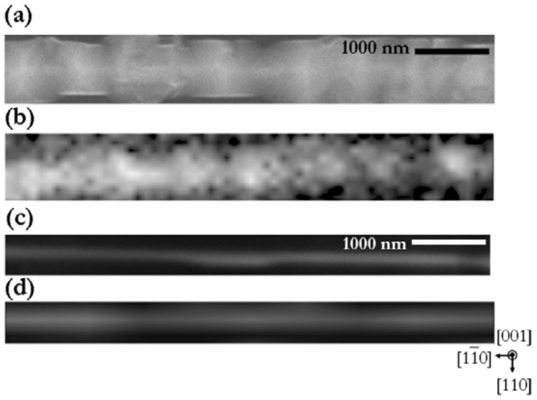

Figure 5. (a) SEM and (b) corresponding CL mapping for a GaAs nano-wire in a trench of 1000 nm. (c) SEM and (d) corresponding CL mapping for a GaAs nano-wire in a trench of width 100 nm.

is observed for 6 μm along the trench. The high-quality GaAs nano-wires are much longer than the feature size of current microelectronic devices. This result demonstrates that CL measurements provide the advantage of characterizing nano-scale structures over the large area of the 12 inch wafer. TEM, however, reveals only local structures.

4. Conclusion

In conclusion, the optical properties of nano-scale GaAs grown on shallow-trench-patterned Si(001) substrates were investigated. The dependence of trench width on the emission efficiency was characterized by CL. When the trench width ranged between 80 and 100 nm, the emission efficiency of defect-free GaAs was the highest, even better than that of the homogeneously grown epilayer. The non-radiative defects close to the GaAs surface are suppressed by the trapping of threading dislocations and planar defects at the trench sidewalls. The results herein demonstrate the feasibility of growing high-quality nano-scaled GaAs-based optoelectronic devices on Si substrates. This work also demonstrates that CL provides an effective method for characterizing the structural quality of nano-scaled material.

Acknowledgments

This work was supported by the National Science Council under grant no. NSC 96-2112-M-009-026-MY3 and no. NSC 99-2731-M-009-001-NPI, Ministry of Education under grant no. MOE-ATU 99W957 and the Taiwan Semiconductor Manufacturing Co., Ltd. The authors would like to thank Precious Instrument Center of National Chiao Tung University for providing the CL instrument.

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