

1 Optical properties of Self-assembled InAs Quantum Dots based P-I-N  
2 Structures Grown on GaAs and Si Substrates by Molecular Beam  
3 Epitaxy  
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25 **Abstract**

26 Extensive work on InAs quantum dots grown on GaAs substrates has been reported in the  
27 literature. However, research in the use of different substrate materials such as silicon to  
28 achieve an ideal and full integration of photonic and electronic systems is still a challenge. In  
29 this work we have investigated the effect of the substrate material (Si and GaAs) and strain  
30 reducing layer on the optical properties of InAs quantum dots for possible applications in laser

1 devices grown by Molecular Beam Epitaxy. Two InAs quantum dots structures with similar  
2 active regions grown on GaAs and Si substrates using strain reducing layer consisting of InAs  
3 QDs/6nm  $\text{In}_{0.15}\text{Ga}_{0.85}\text{As}$  have been investigated. Atomic Force Microscopy, Transmission  
4 Electron Microscopy, and photoluminescence have been used for the characterization of the  
5 samples. We have observed a red shift of the InAs QD photoluminescence peak energy for the  
6 sample grown on Si substrate as compared to the sample grown on GaAs substrate, which was  
7 associated with residual biaxial strain from the Si/GaAs heterointerface. This red-shift of the  
8 photoluminescence peak energy is accompanied by a broadening of the photoluminescence  
9 spectrum from  $\sim 31$  meV to a value of  $\sim 46$  meV. This broadening is attributed to the quantum  
10 dots size inhomogeneity increase for samples grown on Si substrate. This result open new  
11 insights for the controlling the emission of InAs quantum dots for photonic devices integration  
12 using Si substrates.

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## Introduction

15 Considerable efforts have been made to investigate the optical properties of self-  
16 assembled quantum dots (QDs) due to their wide range of applications in optoelectronics such  
17 as lasers, photodetectors, amplifiers, and solar cells [1-3]. Among the QDs systems, InAs QDs  
18 attracted an intensive research activity motivated by the possibility to achieve light emission  
19 covering the optical communication wavelength bands [4-6]. Many strategies have been used  
20 for the extension of the wavelength including growing larger QDs [7] and InGaAs metamorphic  
21 buffers (MB) which behave as virtual substrates where the lattice parameter can be controlled  
22 by an adroit design of the composition profile of the MB, keeping them separated from the  
23 active region of the device [8-12]. Another adopted strategy is the strain reducing layer (SRL)  
24 [6,13]. The SRL preserves the size of QDs during capping by reducing the indium dissolution  
25 [14]. In spite of photoluminescence (PL) emissions closer to  $1.3 \mu\text{m}$  have been achieved [6,7-  
26 13], the larger lattice-mismatch strain between GaAs and InAs ( $\sim 7\%$ ) had resulted in  
27 inhomogeneous dot size distribution and smaller dot density which limiting the device  
28 performance. It was found that the best way to preserve InAs QD size is the use of SRL [15-  
29 17]. Huang et al. [18] reported that  $\text{GaAs}_{1-x}\text{Sb}_x$  SRL improved the performance of InAs/GaAs  
30 quantum-dot infrared photodetectors. Recently, Salhi et al. [6,15] have shown that the emission  
31 wavelength reached  $1.32 \mu\text{m}$  when the InAs QDs are either covered by InGaAs or GaAsSb,  
32 while the incorporation of 1% of Sb in the InGaAs SRL extends further the wavelength to  $1.37$   
33  $\mu\text{m}$ . Extensive work on InAs QDs grown on GaAs substrates has been reported in the literature,

1 however, research in the use of different substrate materials such as silicon to achieve an ideal  
 2 and full integration of photonic and electronic systems [19, 20-23] is still under development.  
 3 Therefore, studies to find suitable capping layer (CL) or SRL materials for covering InAs QDs  
 4 grown on both GaAs and Si substrates are highly motivated by an enhancement of their  
 5 morphology quality and optical properties, as well as exploring possibilities for monolithic  
 6 photonic integration on silicon platform. On the other hand, it is well known that there are  
 7 many challenges to achieve high-quality epitaxial growth of III-V materials on Si substrates.  
 8 The lattice and thermal expansion mismatches between silicon and most III-V materials are the  
 9 most important of these challenges. The 4% lattice constant mismatch between GaAs and Si  
 10 introduces a build-up of strain energy on the epitaxial layer during growth. It leads to highly  
 11 defective heteroepitaxial films, such as antiphase boundaries and threading dislocations [24],  
 12 since the nucleation of a large number of interfacial dislocations is needed to relax the misfit  
 13 strain between the two semiconductors. However, to alleviate the problems associated with the  
 14 lattice mismatch, InGaAs/GaAs multilayers or superlattice defect filters are used [6, 24].

15 In this work, we report on the effect of the substrate material on the optical properties  
 16 of InAs QDs based laser structures. Two InAs QD laser structures with similar active regions  
 17 grown on GaAs and Si substrates using strain reducing layer (SRL) consisting of GaAs/InGaAs  
 18 have been investigated. We have observed that the type of substrate has important influence on  
 19 the strain lattice and structural associated defects, and consequently on the PL properties of  
 20 self-assembled InAs QDs.

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## Experimental

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The two InAs QD lasers studied in this work were grown on 2" (100) GaAs (Sample A: control sample) and 2" (100) Si (Sample B) substrates using a Veeco Gen20A Molecular Beam Epitaxy system (MBE) system equipped with a valved cracker to generate As<sub>2</sub>. The layer sequence of Sample A, grown on n-type GaAs substrate, is depicted in Figure 1(a) and consists of the following layers: a 50 nm n-type GaAs buffer layer, a 1500 nm n-type Al<sub>0.42</sub>Ga<sub>0.58</sub>As cladding layer, a 108 nm undoped GaAs spacer layer, 5× [2.5 monolayers (MLs) InAs QDs/10nm In<sub>0.15</sub>Ga<sub>0.85</sub>As (SRL)/ 40 nm GaAs], a 64 nm undoped GaAs spacer layer, a 1500 nm p-type Al<sub>0.42</sub>Ga<sub>0.58</sub>As cladding layer, and a 300 nm p-type GaAs layer.

The InAs QDs were grown at 500 °C and at a growth rate of 0.03 monolayer (ML)/s. This growth rate was chosen to obtain a uniform QD size distribution and reduce the PL linewidth [25]. A short growth interruption under As<sub>2</sub> flux was introduced before the growth

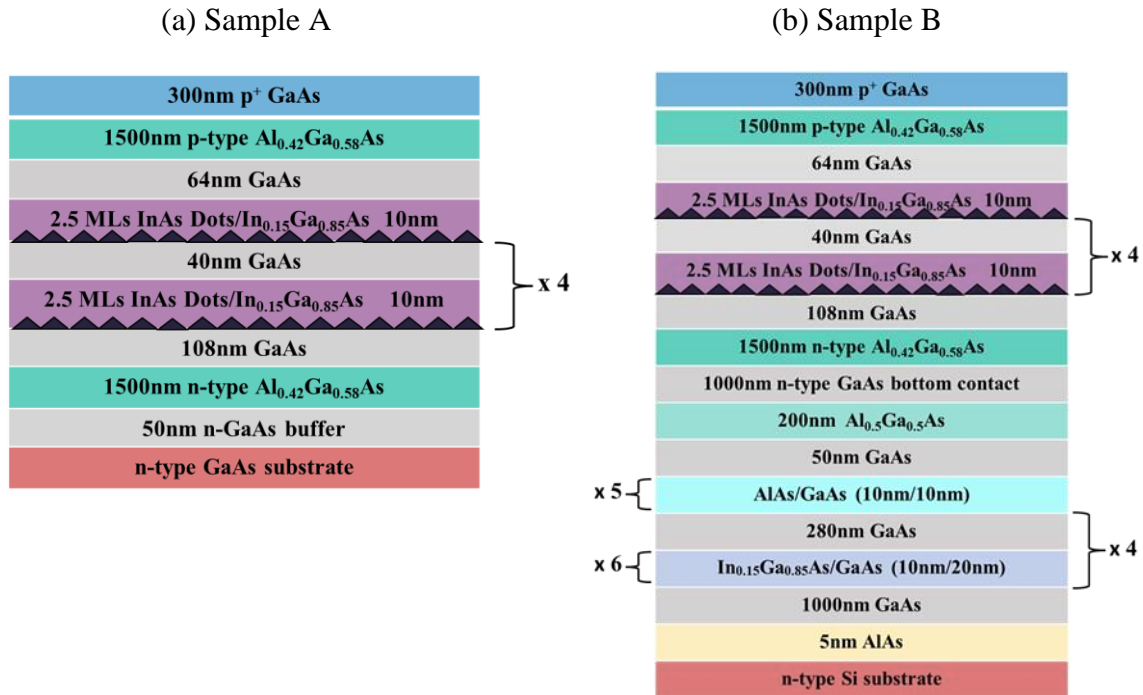
1 of the 6 nm-thick  $\text{In}_{0.15}\text{Ga}_{0.85}\text{As}$  Strain Reducing Layer followed by 10 nm-thick GaAs layer at  
2 the same temperature and using a growth rate of 0.5ML/s. The growth temperature was then  
3 ramped to 570 °C to grow the remaining GaAs cap layer. The spacers, claddings and contacts  
4 layers were grown at 570°C and using a growth rate of 1ML/s.

5 The laser structure grown on silicon substrate (Sample B), was grown by using the same  
6 process and growth conditions as the one used for Sample A grown on a GaAs substrate except  
7 for the buffer layer which is designed and used to reduce the defects resulting from lattice  
8 mismatch between Si and GaAs substrates. The defect filter undoped buffer layer consisted of  
9 5 nm AlAs, 1000 nm GaAs, 4 periods of [6× InGaAs (10nm)/GaAs (20nm)]/ 280nm GaAs], 5  
10 periods of AlAs (10nm)/GaAs (10nm), 50 nm GaAs and 200nm  $\text{Al}_{0.5}\text{Ga}_{0.5}\text{As}$  (Fig.1b). More  
11 details regarding the growth of the dislocation filter can be found in reference [6]. The purpose  
12 of this specific buffer layer was to reduce dislocations between silicon substrate and the active  
13 layers due to the large lattice mismatch between Si and GaAs. The rest of the structure is similar  
14 to Sample A. It is important to highlight that the formation of InAs QDs was verified by means  
15 of Reflection High Energy Electron Diffraction (RHEED) where a chevron patterns in the  
16 RHEED screen was clearly observed.

17 For atomic force microscopy (AFM) analysis, uncapped QDs grown on GaAs and Si  
18 (with dislocation filter) substrates were also grown. AFM was used to characterize the  
19 morphology of the uncapped QDs and the optical properties of the samples were characterized  
20 using temperature and power-dependent photoluminescence (PL). Transmission Electron  
21 Microscopy (TEM) was used for the structural analysis of InAs/InGaAs QDs grown on GaAs  
22 and Si substrates.

23 The PL signal of both samples were investigated as a function of laser power and  
24 temperature using a Janis closed-loop helium cryostat. The samples were excited with a 532  
25 nm solid state green laser. The PL spectra was collected in an Andor Shamrock 500i  
26 spectrometer coupled with a high sensitivity Andor iDus InGaAs CCD camera. The PL  
27 experimental conditions were the same for both samples in order to compare their PL spectra  
28 shape and intensities.

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1 **Figure 1.** Schematic structure of QDs laser samples grown on (a) GaAs substrate (Sample A)  
 2 and (b) on Si substrate (Sample B).

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## Results and discussion

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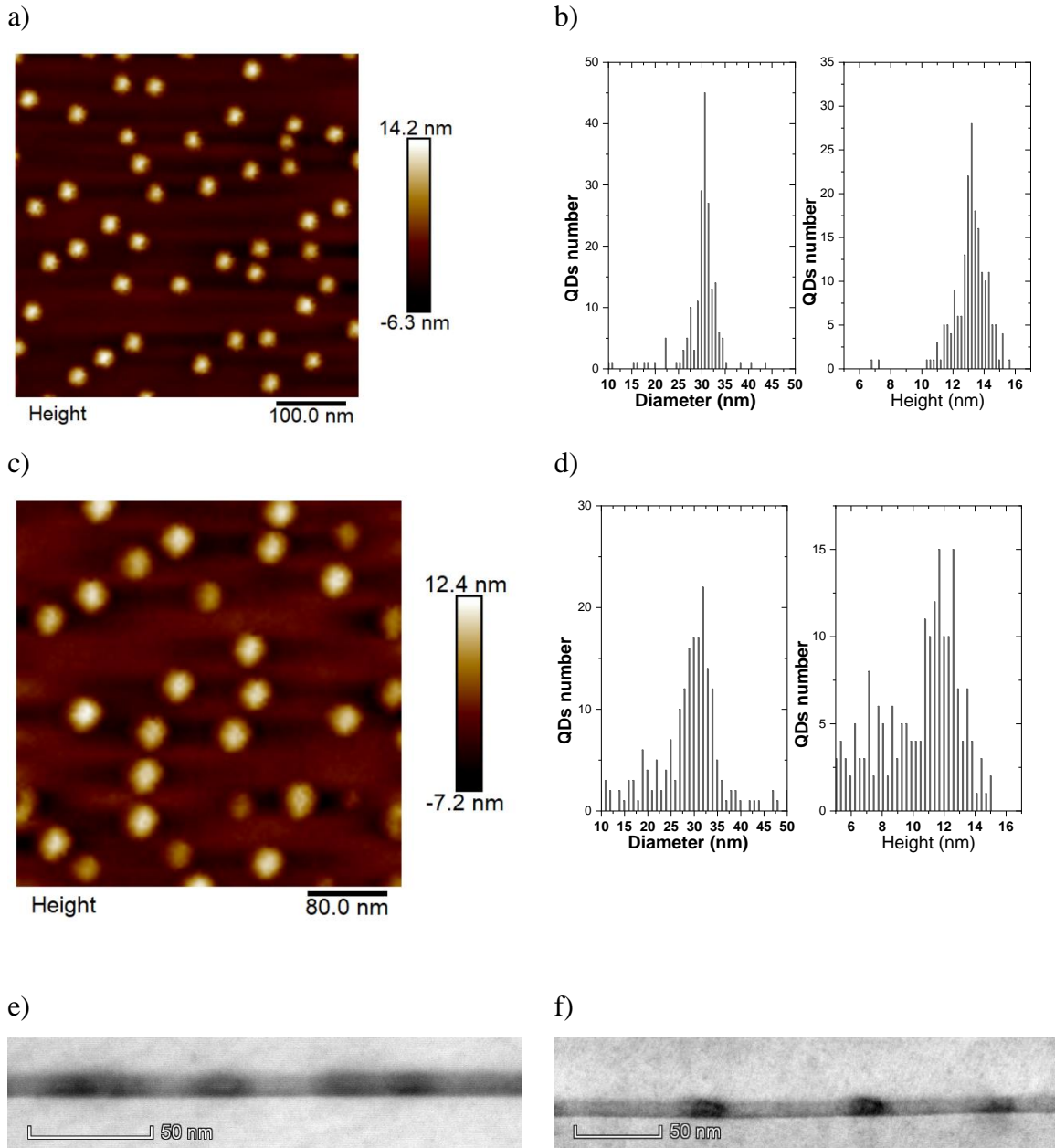
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AFM was used to characterize the morphology of the uncapped QDs and the results are shown in Figure 2 (a-d). The obtained values of the QDs' density is  $\sim 1.8 \times 10^{10} \text{ cm}^{-2}$  for both samples grown on GaAs and Si substrates. However, we noticed a reduction of the QDs aspect ratio for the sample grown on Si. The average diameter and height of the QDs grown on GaAs and Si substrates were  $30.8 \pm 2.1 \text{ nm}$  and  $13.3 \pm 0.9 \text{ nm}$ , and  $30.7 \pm 4.2 \text{ nm}$  and  $11.8 \pm 1.9 \text{ nm}$ , respectively. During the capping process, the QDs size was reduced in both samples as shown in the bright field transmission electron microscopy (TEM) images (Figure 2 (c,d)). In particular, the diameter of the QDs in both samples ranges between 20 and 25nm and the height is reduced to 10nm which is the same as the width of the  $\text{In}_{0.15}\text{Ga}_{0.85}\text{As}$  QWs (Figure 2c and Figure 2d). We note that it is not easy to do a direct comparison of TEM and AFM data as the number of QDs measured with TEM (10 QDs) is far below the number of QDs measured by AFM ( $\sim 200$  QDs).

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3 **Figure 2.** AFM images ( $0.4\mu\text{m}\times 0.4\mu\text{m}$ ) and histograms distribution of 2.5 MLs uncapped InAs  
 4 QDs grown on (a-b) GaAs substrate and (c-d) Si substrate. Bright field TEM images of  
 5 InAs/InGaAs QDs grown on GaAs substrate (e) and Si substrate (f).

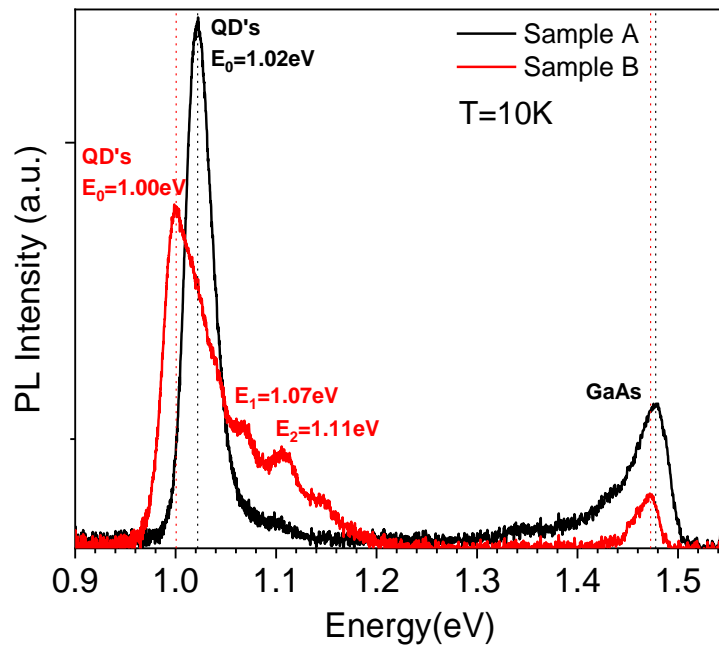
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7 The use of the dislocation filter and the GaAs buffer layer for the growth on silicon  
 8 substrate is equivalent to a virtual GaAs substrate and allowed to achieve the same QD density  
 9 and nearly the same dimensions compared to the ones grown on GaAs substrate as confirmed

1 by AFM measurement. The growth of InAs QDs grown directly on silicon substrate would  
 2 have a significantly different QD distribution and density because of the large lattice mismatch.

### 3 4 Photoluminescence

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 6 Figure 3 shows typical PL spectra of (InGaAs/GaAs) QDs for Sample A (GaAs substrate)  
 7 and Sample B (Si substrate), at 10 K and laser excitation power  $P_{\text{EXC}}=40\text{mW}$  **corresponding to**  
 8 **a laser power density of  $2.0\text{ W/cm}^2$  (laser spot diameter  $\sim 0.8\text{ mm}$ ).** The dominant peak at 1.02  
 9 eV in Sample A is ascribed to interband transition occurring from the electron ground state  $E_0$   
 10 to the heavy hole ground state  $\text{HH}_0$  of the InAs dot ( $E_0\text{-HH}_0$ ). This PL band also exhibits some  
 11 asymmetry in the high-energy side that could be ascribed to reduced filling of QDs excited  
 12 states, not well distinguishable and resolved in PL spectra. In addition, a small peak at 1.477  
 13 eV is attributed to the GaAs capping layer. For Sample B, the observed  $E_0$  (1.00 eV),  $E_1$  (1.11  
 14 eV) and  $E_2$  (1.07eV) PL peaks are well resolved and correspond to ground state transition, first  
 15 and second excited states, respectively. It is plausible to suggest the presence of these same  
 16 excited states peaks on the high energy shoulder of the PL spectra of Sample A, although they  
 17 are not well pronounced and well resolved as in Sample B.



18 **Figure 3:** PL spectra of InGaAs/GaAs QDs grown on GaAs (Sample A) and silicon (Sample  
 19 B) substrates at laser power  $P_{\text{EXC}}=40\text{mW}$  and 10K. The PL bands attributed to InAs QDs and  
 20 GaAs capping layer are indicated.

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2 Figure 4 (a) presents the PL spectra for Sample A measured under different excitation  
 3 power intensities at 10 K. At low excitation power (3 mW) only one symmetric peak is present  
 4 at 1.02 eV (ground state transition  $E_0$  to  $HH_0$ ) and it remains nearly symmetric and unchanged  
 5 up to an excitation power  $< 10$  mW. With increasing excitation power, one additional peak is  
 6 evidenced on the high-energy side of the PL spectra (1.1 eV, see inset), which corresponds to  
 7 the filling of the first excited state  $E_1$ .

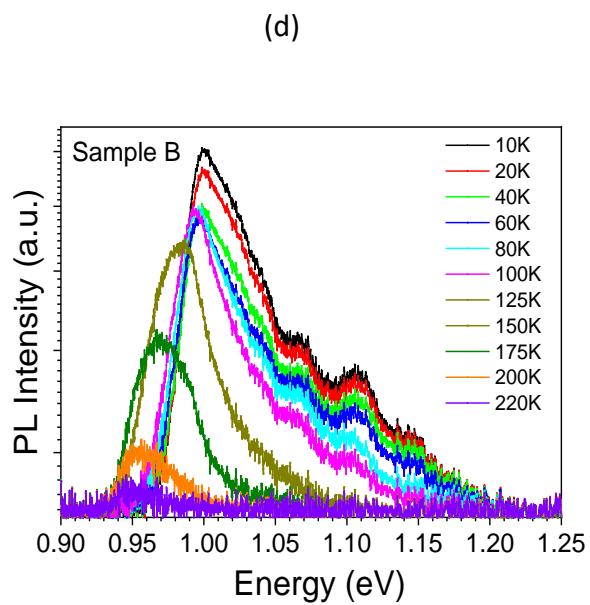
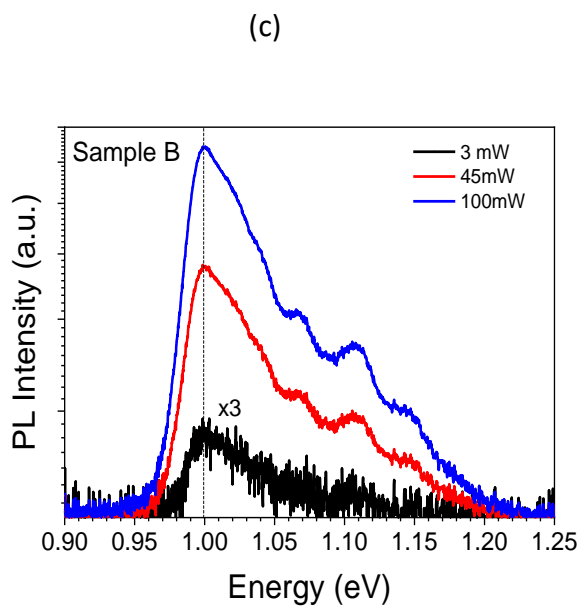
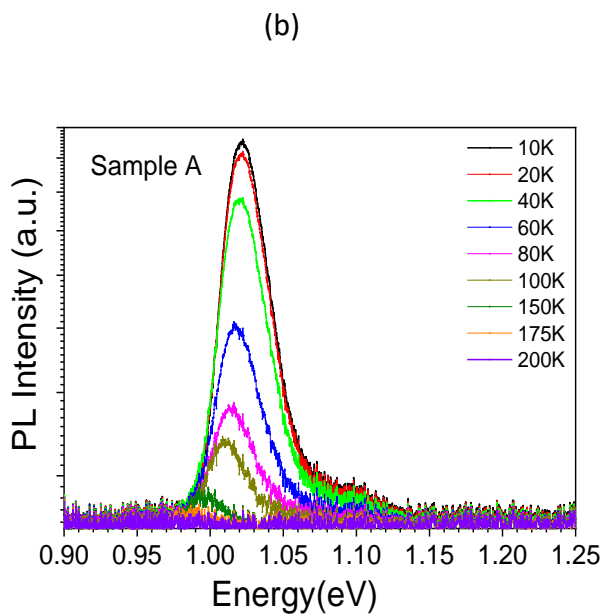
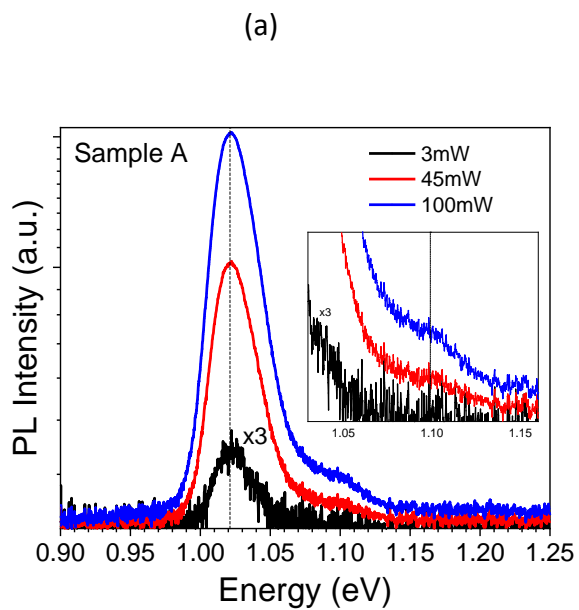
8 Figure 4(c) shows the  $E_0$  PL peak (1.00 eV) observed in Sample B, and it is clearly  
 9 asymmetric and broader than the one detected in Sample A. The peak energy also remains  
 10 nearly unchanged with increasing excitation power. Therefore, the broad and asymmetric PL  
 11 peak at 1.00 eV may reflect an inhomogeneous size distribution of the QDs, associated with  $E_0$   
 12 transition induced from the finite-size distribution of the QDs as a consequence of carrier's  
 13 random distribution at low temperatures. As the laser power increases, additional peaks are  
 14 revealed. These peaks are probably due to excited states of the self-assembly QDs as discussed  
 15 before. Figure 4 (b,d) shows that the QD PL intensity decreases for Sample A in the temperature  
 16 range of 30-120 K, and quenches completely at temperatures above  $\sim 180$  K, while for Sample  
 17 B although the PL intensity at 10K is smaller than Sample A, it decreases and quenches  
 18 completely at a higher temperature of  $\sim 220$  K than Sample A. This decrease of the PL intensity  
 19 as function of temperature is usually attributed to thermal escape of carriers from the QD  
 20 ground states into the continuum followed by nonradiative recombination in the InGaAs and  
 21 GaAs barriers (SRL and capping layer) at higher temperatures, when the thermal escape  
 22 becomes dominant [25-27]. As will be discussed below, the difference in the PL intensity  
 23 between the two samples shown in Fig. 3 is attributed to the different surface growth condition  
 24 that could change the QD emission efficiency.

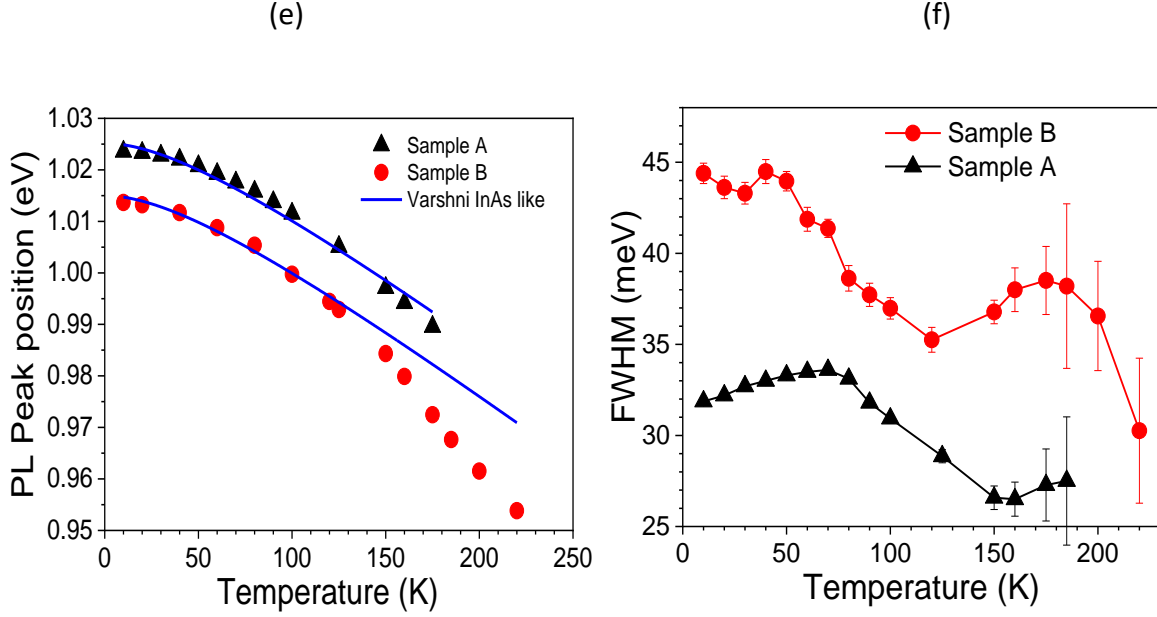
25 The effect of the silicon substrate on the QDs' PL emission is clearly demonstrated by  
 26 the following observations (from Sample A to Sample B): (i) the QD PL peak red-shifted from  
 27 1.02 eV to 1.00 eV; (ii) the PL intensity decreased by a factor of  $\sim 1.75$ ; and (iii) the Full Width  
 28 at Half Maximum (FWHM) increased from 31 meV to 46 meV (at a laser excitation power of  
 29 3mW). In our previous discussion we showed that the size of the QDs is similar for both  
 30 samples, with a slight reduction of the aspect ratio from Sample A to Sample B, which is a  
 31 negligible effect in terms of quantum confinement between the two samples. Although the  
 32 redshift in the PL energy has been reported and explained by different mechanisms along with  
 33 strain and carrier confinement, in this case it is probably [due to dislocations coming from the](#)



1 Si/GaAs interface and reaching the QD region that could affect the surface conditions for the  
2 growth of the QDs, and thus reducing their emission efficiency. The residual strain of the  
3 GaAs/Si heterointerface is not expected to have a very significant influence in these samples  
4 since there is a GaAs layer with a thickness of more than 3 microns before the QDs layer and,  
5 therefore, the strain should be fully relaxed [28-30]. Additionally, the decrease of the PL  
6 intensity of Sample B as compared to Sample A indicates that the growth condition of QDs  
7 was significantly changed in the InAs QDs active region when Si substrate is used, reducing  
8 the optical emission efficiency [31-34].

9 Furthermore, the QDs PL peak of Sample A (FWHM= 31 meV) at 10K and 3mW laser power  
10 excitation is narrower than that for Sample B (FWHM= 46 meV) by considering only the  
11 deconvoluted transition associated with  $E_0$ . As discussed before, the distribution of the InAs  
12 QD size in the samples grown on GaAs and Si substrates is possibly affecting the changes  
13 observed in the PL results. The observed narrower FWHM for samples grown on the GaAs  
14 substrate sample indicates that the QD size distribution is better in Sample A than in Sample B  
15 (as shown in Figure 2b and Figure 2d), meaning that the QDs distribution is more  
16 inhomogeneous for Sample B than in Sample A, since the FWHM is inversely correlated with  
17 QD size and shape uniformity. It is important to note that the emission efficiency can also be  
18 reduced due to the introduction of different surface growth conditions for the QDs, resulting in  
19 more inhomogeneous size and shape distributions. These aspects may have been caused by the  
20 relatively higher number of threading dislocations in the active region, while the increase of  
21 the FWHM confirms a less uniform QD size distribution for this sample. Therefore, the use of  
22 Si substrates can have a profound impact on the optical properties of InAs QDs.





1 **Figure 4:** 10K PL spectra as function of laser power (a: Sample A, c: Sample B). PL spectra  
 2 as function of temperature for a laser excitation power  $P_{\text{EXC}}=40\text{mW}$  (b: Sample A, d: Sample  
 3 B). (e) PL peak energy and (f) PL FWHM of  $E_0$  transition as a function of temperature for  
 4 InAs/GaAs QDs grown on GaAs (Sample A) and Silicon (Sample B) substrates at a laser  
 5 excitation power  $P_{\text{EXC}}=25\text{mW}$  and respective error bars. Solid lines in (e) are the InAs band  
 6 gap shrinkage obtained from Varnish law. The results of  $E_0$  transition from PL data was  
 7 obtained from the deconvoluted PL spectra (excluding effects of QD excited states).

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9 Figure 4 (e) shows the  $E_0$  PL peak as function of temperature as well as the InAs-like  
 10 band gap decrease by using the Varshni approximation fitting [35]. The PL peaks match well  
 11 with the band gap variation up to 150 K. However, the QD PL peak redshifts faster when further  
 12 increasing the temperature. The competing mechanisms of the carrier's thermal escape and  
 13 recapture between the QDs, results in the redshift of the PL peak energy and the narrowing of  
 14 the FWHM as the temperature increases [27]. This behaviour indicates that the carriers  
 15 experience a transfer from the smaller QDs with deeper energy levels to the larger QDs with  
 16 shallower energy confinement under thermal excitation, which results in a lower interband  
 17 emission energy and a red-shift of the PL peak position [36]. This same carrier transfer process  
 18 could also be evidenced by the temperature dependence of the PL FWHM for  $E_0$  transition for  
 19 both samples as shown in Fig. 4 (f), and will be discussed below.

20 The PL FWHM presents a similar trend for both samples, with a decrease of the FWHM  
 21 as the sample's temperature increases. The PL FWHM variation with temperature is generally  
 22 attributed to the carrier thermal redistribution amongst QDs with different sizes. A decrease of

1 the FWHM together with a red shift of the PL emission, when the temperature rises up to 150  
2 K, are usually observed in the mid temperature range and explained by thermal escape of  
3 carriers occurring at lower temperatures for high-energy dots and carriers being recaptured by  
4 dots emitting on the low-energy side of the distribution [37]. Sample B also shows the largest  
5 FWHM variation and has the highest FWHM for all temperature ranges. With a further increase  
6 of the temperature above 150 K, the broadening of PL FWHM is likely attributed to the  
7 electron-phonon scatter over QDs with different sizes [36,38].

8 In general, our results indicate that the use of Si substrate combined with a SRL to grow  
9 InAs QDs is a promising approach to integrate them with Si technology what is demonstrated  
10 by QD morphology data and a significant efficiency of the optical emission. However, there  
11 are still some important issues for obtaining the appropriate design and [materials for the  
12 dislocation filter at the Si/GaAs heterointerface in order to reduce the dislocations coming from  
13 the Si/GaAs interface that reach the QD region, consequently improving](#) the optical properties  
14 of the QDs.

## 15 Conclusion

16 In summary, the structural, morphological and optical properties of two InAs QD laser  
17 structures with similar active regions grown on GaAs and Si substrates using strain reducing  
18 layer (SRL) have been investigated using AFM, TEM and PL techniques. Our results evidenced  
19 the formation of quite similar QDs in both structures, with higher strain for QDs in sample  
20 grown on Si substrate. It was observed that the PL intensity from QDs grown on Si substrate  
21 decreased by a factor of  $\sim 1.7$  when compared with those grown on GaAs substrate control  
22 [sample. However, despite this reduction, our results demonstrate the possibility of growing  
23 InAs QDs on Si substrates with good emission efficiency for laser applications.](#) In addition,  
24 was also observed in the InAs QDs grown on Si substrate a broadening of the PL spectrum  
25 from  $\sim 30$  meV to a value of  $\sim 52$  meV for an excitation power of 3 mW. This broadening is  
26 attributed to the QD size inhomogeneity increase during the growth on Si substrate. This opens  
27 up new possibilities for controlling the density and size of QDs when using specific type of  
28 SRL/substrate.

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