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# Effect of inter-well coupling between 3C and 6H in-grown stacking faults in 4H-SiC epitaxial layers

T. Robert<sup>1,a</sup>, M. Marinova<sup>2,b</sup>, S. Juillaguet<sup>1,c</sup>, A. Henry<sup>3,d</sup>,  
E.K. Polychroniadis<sup>2,e</sup> and J. Camassel<sup>1,f</sup>

<sup>1</sup>Groupe d' Etude des Semiconducteurs, Université Montpellier 2 and CNRS, cc 074 GES, 34095 Montpellier Cedex 5, France.

<sup>2</sup>Physic Departement, Aristotle University of Thessaloniki , GR54124 Thessaloniki.

<sup>3</sup>Department of Physics, Chemistry and Biology, University of Linköping, Sweden.

<sup>a</sup>robertt@ges.univ-montp2.fr, <sup>b</sup>marinova@physics.auth.gr, <sup>c</sup>sandrine.juillaguet@univ-montp2.fr, <sup>d</sup>ahy@ifm.liu.se, <sup>e</sup>polychr@auth.gr, <sup>f</sup>camassel@ges.univ-montp2.fr

**Keywords:** Silicon carbide stacking faults, Quantum well approach, Inter-well coupling, Low temperature photoluminescence, High resolution transmission electron microscopy

**Abstract.** Both 3C and 6H stacking faults have been observed in a low doped 4H-SiC epitaxial layer grown in a hot-wall CVD reactor on a heavily doped (off-axis) 4H-SiC substrate. They appear differently on the different parts of sample, with energetic dispersion ranging from 3.01 eV to 2.52 eV. Since they behave as natural type-II quantum wells in the 4H-SiC matrix, the thickness dependence of the excitonic recombination is investigated using the standard effective mass approximation. The results are discussed in terms of built-in electric field and inter-wells coupling effects.

## Introduction

Stacking faults (SFs) are well known defects in 4H-SiC which degrade the performance and reliability of power devices [1]. They induce stable lamellae of a different polytype, with a finite thickness and a finite lateral extension between partial dislocations [2, 3]. Despite recent progress in growth technology, their formation is still an issue. The modified stacking sequence of the important lamellae is usually obtained from cross-sectional high resolution transmission electron microscopy (HRTEM) measurements. If the band gap energy of the SF polytype is smaller than the host material, they form new quantum well (QW)-like electron states [4] that can be observed in low temperature photoluminescence LTPL spectroscopy [3, 5-7]. In this case, using a type-II QW model, a good correlation is usually found between the SFs optical signature and the HRTEM thickness. In some cases two lamellae can be formed close enough to modify the single SF emission band. Such inter-well SFs coupling is investigated in this work.

## Experimental

We focus on a faulted part of 4H-SiC epitaxial layer grown on a 8° off-axis 4H-SiC substrate (Si-face) doped to  $\sim 10^{19} \text{ cm}^{-3}$ . The layer has a thickness of 33  $\mu\text{m}$  and was also N-doped, but only to  $10^{15} \text{ cm}^{-3}$ . LTPL investigations were done at 5K using 30 mW of the 244 nm wavelength of a frequency doubled Ar<sup>+</sup>-ion laser. A Triax Jobin Yvon-Horiba spectrometer is coupled with liquid nitrogen cooled CCD (Charge-Coupled Device) camera. HRTEM investigations were done on close areas using a JEOL 2011 microscope operated at 200 kV with a point resolution of  $\sim 1.94 \text{ nm}$ .

## Results and discussion

**LTPL.** On the main part of sample the typical near band edge optical signature of 4H-SiC, with well-resolved series of excitonic lines, could be easily observed. In some other parts, a series of stacking faults with optical signature ranging from 3.01 eV to 2.52 eV was also found [8]. Typical spectra are shown in Fig 1. with four main peaks corresponding to the energy of the four

momentum-conservative phonons replicas (TA  $\sim$  46 meV, LA  $\sim$  77 meV, TO  $\sim$  95 meV and LO  $\sim$  105 meV). The large energetic dispersion suggests that many different faults exist. With a spot diameter about 100  $\mu\text{m}$ , various SFs can be detected in the same area as for Fig.1 b) and d).

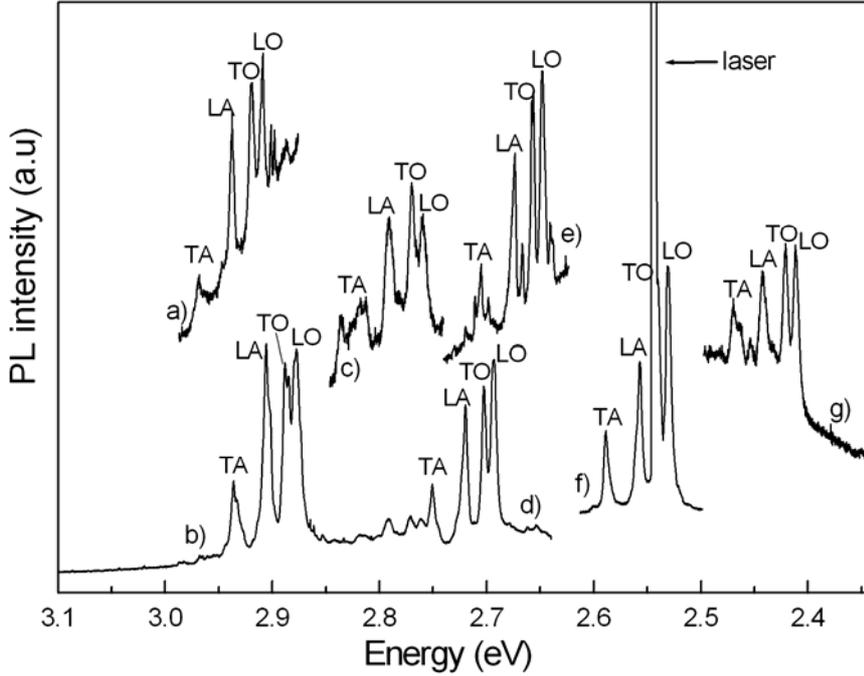
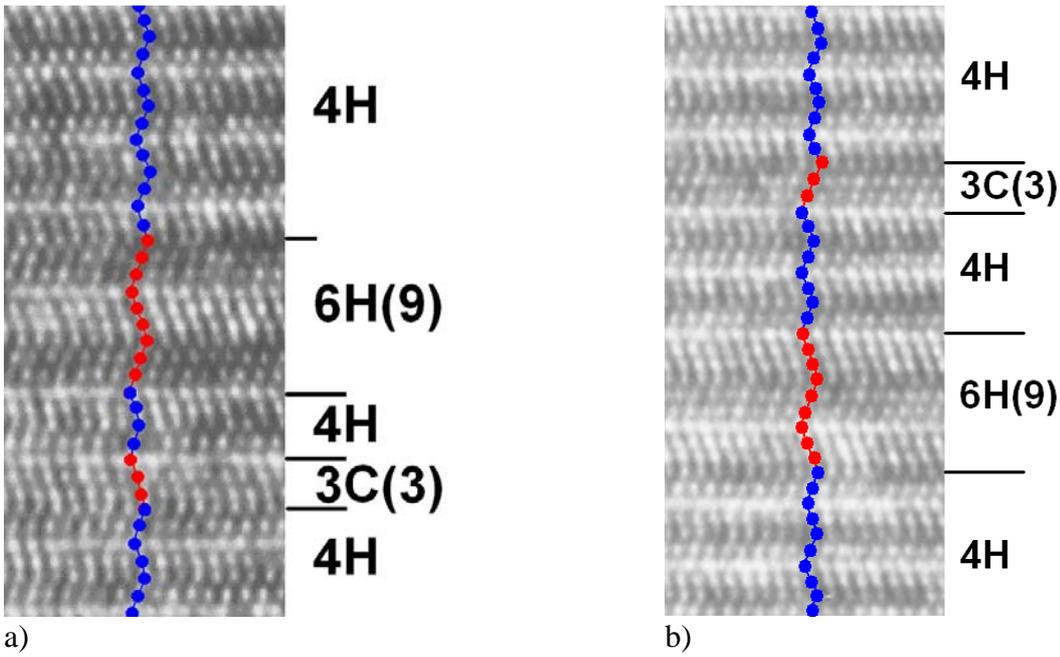


Figure 1: Examples of LTPL spectra collected at 5K on a faulted part of 4H-SiC epitaxial layer. The optical signature of stacking faults is made of four phonons replicas (TA, LA, TO, LO) with zero-phonon values (optical energy gaps) of a) 3.015 eV, b) 2.983 eV, c) 2.869 eV, d) 2.792 eV, e) 2.751 eV, f) 2.635 eV, g) 2.516 eV.

**HRTEM.** From transmission electron microscopy, many different lamellas with thickness varying from 3 bilayers to 24 bilayers have been identified. They are made of an odd or even number of half unit cell of 6H-SiC that can be seen as 3C zigzag faults. In this case, every 3C-like sequence is made of 3 Si-C bilayers (BLs) alternatively stacked at the right and the left around the [0001] axis. In Fig. 2 we show two HRTEM cross-sectional images which represent two (different) local structures. One is made of 9 BLs of 6H. The other one is made of 3 BLs of 3C. They are embedded in the 4H-SiC matrix and are separated by a) 4 BLs of 4H and b) 8 BLs of 4H. All SFs have not such a close relationship and, in many cases, they appear as single isolated QW systems with 3, 6, 9, 12 and 24 BLs thickness. To clarify the origin of the energetic dispersion, we checked the dependence of the excitonic recombination energy vs QW thickness using a simple type II QW model.

**Single type II QW model.** We used a standard effective mass approximation [3], assuming only isolated 4H/3C/4H and 4H/6H/4H type-II QW systems. We take into account a built-in electric field of 0.8 MV/cm in the 6H QWs (deduced from the value of  $\sim$  1.2 MV/cm for 3C-SiC according to the hexagonality difference) and get for the transition energy versus QW thickness for 3C and 6H SFs in 4H-SiC the results shown in Fig 3.

To compare, we plot the experimental LTPL results as circles and show the HRTEM thicknesses as stars. Notice the good overall agreement. This suggests that both transition energies at  $\sim$  3 and 2.98 eV observed on the LTPL spectra correspond with 6 BLs of 6H-SiC in between two 4H barriers while, at lower energy (around 2.85 eV), it should be the structures for 9 BLs of 6H. Then, the energie at  $\sim$  2.8 eV, correspond with  $\sim$  15 BLs of 6H. All energies around 2.75 eV can be associated with 3 BLs of 3C (as shown in Fig.1), as well as a 6H structure with  $\sim$  18 BLs thickness even if these latter structures were not found from the HRTEM images, due to the very small area of observation. The HRTEM structures with optical signatures at about 2.6 eV and 2.5 eV have not also been identified. The optical signature corresponding to 24 bilayers of 6H was not seen.



a) b)  
 Figure 2: Cross-sectional HRTEM images collected in the [11-20] direction showing 3 bilayers of 3C close to 9 bilayers of 6H. They are separated by a) 4 bilayers of 4H-SiC and b) 8 bilayers of 4H-SiC.

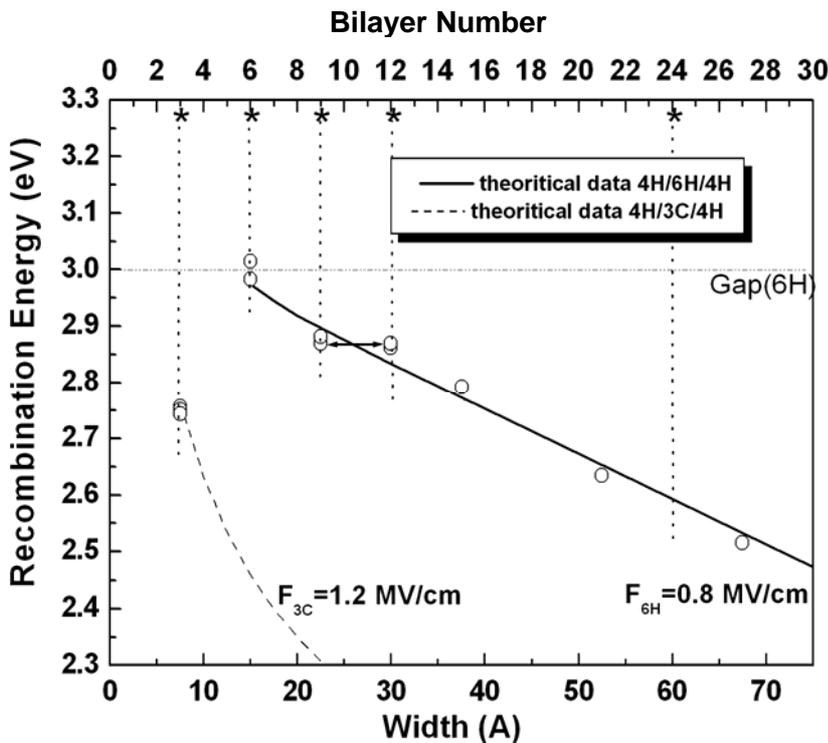


Figure 3: Recombination energies computed as a function of the thickness of the 3C and the 6H QWs in a 4H matrix. LTPL experimental data, shown in Fig 1., are represented in open circle. The structures observed in HRTEM are indicated by stars. The arrow connects the same experimental data to different widths.

**Coupled QWs.** The single QW model works well to assign the different optical stacking faults signatures but it does not explain the close series of energies with 5-10 meV difference that we observe around 2.75 eV. To clarify this, we have considered one unit cell of 3C QW that becomes more and more coupled with a 6H-type QW within the 4H matrix. This assumption is justified by the experimental results found in HR-TEM (see Fig.2). Results are shown in Fig.4. They show that the minimum distance for an effective inter-well coupling between the isolated (3C) QW and the 6H-type one is  $\sim 8$  BLs. Below this limit the fundamental transition energy red shift increases when the 4H barrier thickness decreases and reaches 5-10 meV for  $\sim 3$ -4 BLs inter-well distance.

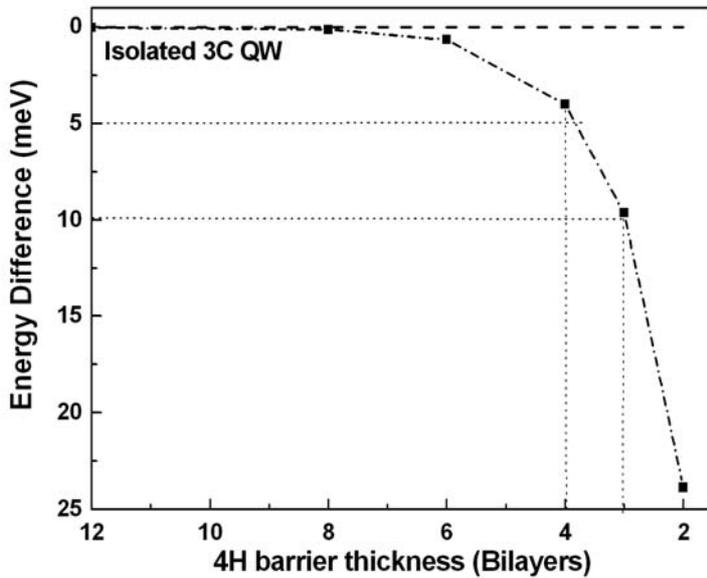


Figure 4: Fundamental energies difference between the isolated and the coupled 3C QW for different 4H barrier thickness.

## Summary

Using LTPL measurements and HRTEM observations, we have investigated 3C and 6H SFs lamellas in a low doped 4H-SiC homoepitaxial layer. The corresponding change in excitonic energy gap ranges from 3.01 eV to 2.52 eV for thicknesses varying from 3 bilayers to 27 bilayers. According to their respective position along the [0001] direction, these 3C and 6H local sequences embedded in the 4H-SiC matrix can be coupled. In this case, our computational results show that the effect of inter-well coupling must be taken into account when the 4H-SiC barrier thickness is lower than 8 BLs. Then, it red shifts the fundamental recombination energy of the 3C-like SFs

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