Direct bandgap hexagonal SiGe: A light emitter for Si-photonics?

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ABSTRACT
Hexagonal crystal phase $Si_{1-x}Ge_x$ is a direct bandgap semiconductor for x>70%. We observe tunable light emission from 1.9 up to 3.5 µm at 4K as well as amplified spontaneous emission for Hex-Ge. Applications for Si-photonics will be discussed.

Keywords: SiGe light source, direct bandgap, Silicon photonics, hexagonal crystal structure.

1. INTRODUCTION

It is a major drawback of Silicon Photonics that it is currently lacking a lightsource which can be monolithically integrated. The main problem is that group IV semiconductors like Si and Ge naturally crystallize within a cubic lattice and feature an indirect bandgap. Both Si and SiGe can however be forced to grow in the hexagonal crystal structure as has been shown by IMEC in a conventional CMOS process[1] as well as by crystal phase transfer by using a wurtzite III-V nanowire core to force the $Si_{1-x}Ge_x$ shell into the hexagonal crystal phase[2,3].

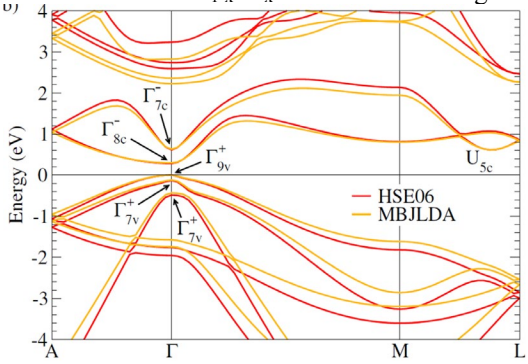

Fig. 1: Bandstructure of hexagonal Ge calculated by ab initio density-functional theory[4].

This contribution is intended to be an update of the H2020 SiLAS project which is aiming towards a hexagonal $Si_{1-x}Ge_x$ nanolaser. Within the project, evidence is currently accumulating that hexagonal $Si_{1-x}Ge_x$ is a direct bandgap semiconductor (see Fig. 1) which is capable to efficiently emit light in the wavelength region between 1.9 and 3.5µm at 4K. Slightly shorter wavelengths might be possible when we would be able to more closely approach the direct-to-indirect transition by increasing the crystal perfection.

2. WAVELENGHT TUNABILITY

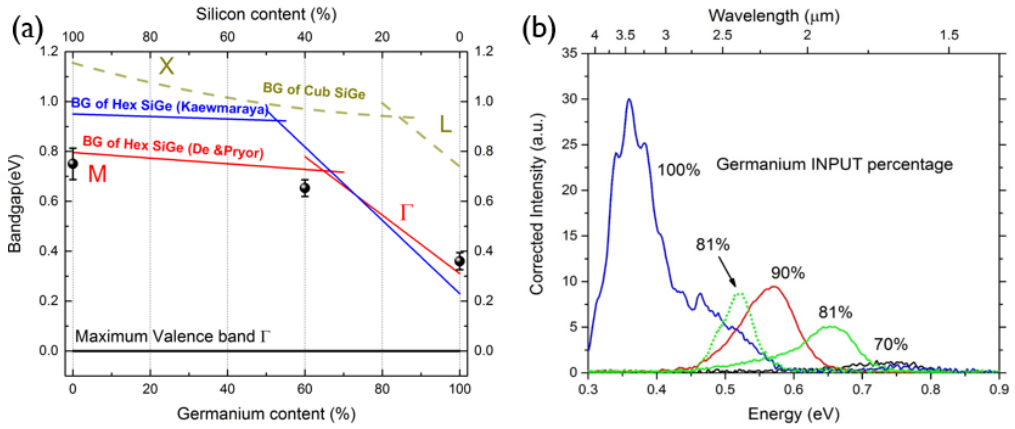

Fig. 2: (a) Linear interpolation of the band edges in Hex-SiGe based on references 7 and 8, together with our preliminary experimental data showing that Hex-SiGe becomes a direct semiconductor above 60-70% Ge. (b) Photoluminescence spectra of Hex-SiGe versus the input percentage of Ge during growth.

Both hexagonal Si and Hexagonal Ge have been predicted[4,5] to have a minimum in the conduction band at the Γ-point. However, Hex-Si is still indirect, while Hex-Ge has been predicted[4,6-8] to be a direct semiconductor (Fig. 1). By using a linear interpolation[7,8] (Fig. 2a) based on Vegard's law, which works well for SiGe alloys[6], it is suggested that Hex-SiGe becomes a direct semiconductor for Ge-compositions above 60-70%.

At the conference, we will present strongly improved data showing photoluminescence spectra which precisely coincide with *ab initio* density-functional theory as calculated by the Jena group. Preliminary photoluminescence data are presented in Fig 2b showing bandgap tunability between 1.9 and 3.5 µm. We observe that the emission intensity strongly decreases near the direct-to-indirect transition around a Ge-composition of 70% which is an experimental indication for the direct bandgap of Hex- $Si_{1-x}Ge_x$ for x>70%.

3. EVIDENCE FOR DIRECT BANDGAP EMISSION.

We present excitation power dependent photoluminescence at 4K in Fig. 3. The spectra show a single peak which is probably a consequence of high As-doping as evidenced by atom probe tomography measurements (not shown). The As-doping is due to As evaporation from the GaAs substrate as well as from the walls of the MOVPE during growth while growing hexagonal GaAs/SiGe core/shell nanowires. The spectra show a clear broadening towards higher energy at high excitation density. This phenomenon is attributed to bandfilling due to the Burnstein-Moss effect. The observation of bandfilling is a strong indication that we are observing band-to-band emission.

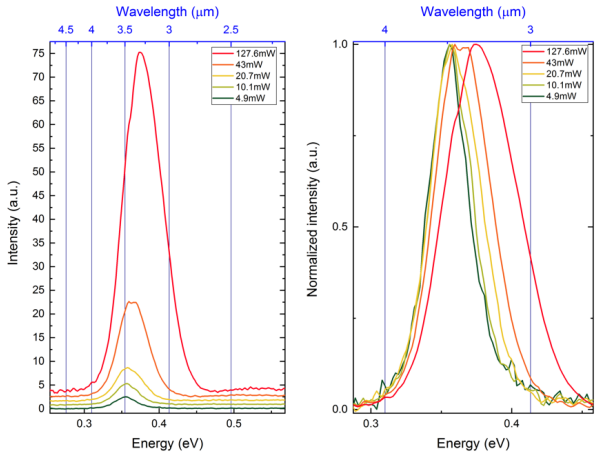

Fig. 3: Excitation dependence of the photoluminescence at 4K of hexagonal Ge shells grown around a wurtzite GaAs nanowire core showing the bandfilling behavior.

Another important observation is that we observe relatively strong room temperature emission. The ratio of the emission intensity at 4K and 300K is less than a factor 50 without apply any kind of intentional surface passivation.

4. OBSERVATION OF STIMULATED EMISSION.

Subsequently, measurements were performed at the Walter Schottky Institute on single Hex-Ge nanowire at high excitation density. The majority of the nanowires (NW0, green) show weak photoluminescence with a sub-linear power-dependence with an exponent of 0.83. Few nanowires (NW1, red) exhibit a much larger signal and show a strong super-linearity with an exponent of 8.17, which is interpreted as being light amplification via stimulated emission. A single nanowire (NW2, blue) exhibits a very strong PL signal with a slightly super-linear power dependence of 2.39 that decreases to an almost linear regime with a slope of 1.35 at ~0.1kW/cm^2. We tentatively interpret the transition to the linear regime as being due to optical feedback from the nanowire end-facets. This interpretation is further supported by Michelson interference measurements at 7K showing a 124 fs coherence time in NW2 as compared to a 27fs coherence time in NW0, indicating amplified spontaneous emission in NW2.

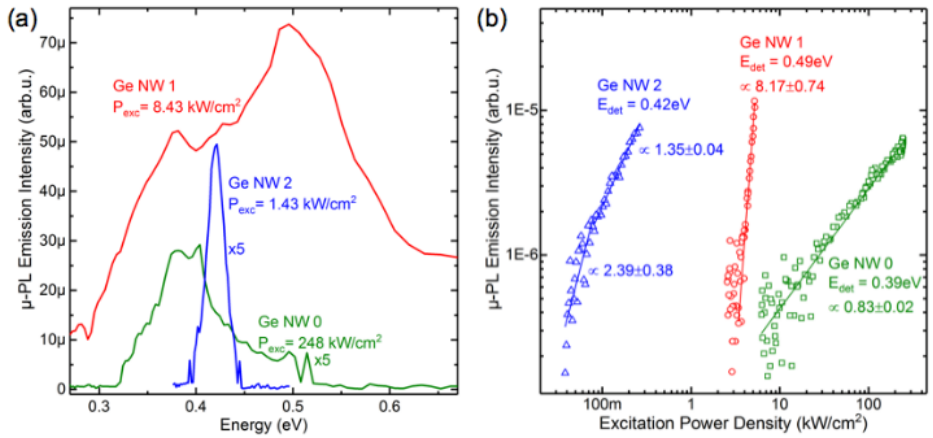

Fig. 4: : *(a) Typical micro-photoluminescence (PL) spectrum of a disordered nanowire (NW0), a wire with very few dislocation (NW1) and a wire of high crystal quality (NW2). (b) Excitation power dependence for Hex-SiGe nanowire shells with three different morphology classes.*

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