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### D 1.2 Growth of nominally undoped hex-SiGe

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## Growth of nominally undoped hex-SiGe

To create devices from a semiconductor like LEDs, lasers and photodetectors, we need to carefully control the concentration of charged impurities in the hex-SiGe crystal. These charged impurities are referred to as dopants and are used to create electron- or hole-rich regions changing the material from intrinsic to n- and p-type respectively to create PN-junctions which are the basic building blocks of opto-electronics. However, to be able to fully engineer the doping of the material, we need to achieve a (near) intrinsic material to use as a basis.

During the growth of hex-SiGe, Arsenic n-doping is unintentionally incorporated into the material. The amount of Arsenic in the hex-SiGe nanowires is investigated using two methods. First, we discuss Atom Probe Tomography (APT) measurements that directly determine the doping concentration in the nanowires and then we investigate the activated doping density by fitting the Lasher-Stern-Würfel (LSW) model for direct bandgap band-to-band recombination to low temperature (4K) macro photoluminescence spectra.

### APT

In Atom Probe Tomography the doping background can be investigated by evaporating atoms from the nanowire using a laser pulse. These atoms are then measured on a detector which can determine which atom was measured and reconstruct where it came from on the sample. In Fig. 1a, Scanning Electron Microscope (SEM) image of the investigated nanowire is shown.

Recently we performed APT studies of new Hex-SiGe samples show that Gallium and Arsenic atoms are no longer detected during the measurement as shown in Fig. 1b. This shows that the hex-SiGe nanowires now have doping concentrations below the detection limit which is  $< 0.005\%$  which corresponds to a concentration of  $n_0 = 2.5 \times 10^{18} \text{ cm}^{-3}$ . If this doping density is compared to the APT values previously reported by Fadaly et al. [1] where an As concentration of  $n_0 = 9 \times 10^{18} \text{ cm}^{-3}$  was found, we can conclude that the As contamination is significantly reduced by almost an order of magnitude.

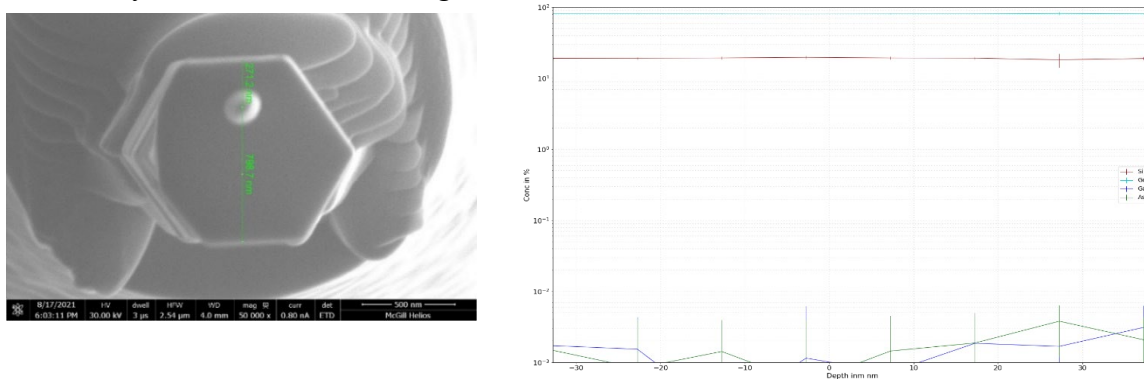


Figure 1: a) Scanning Electron Microscope (SEM) image of the investigated hex-SiGe nanowire. b) The concentration of measured elements Si, Ge, Ga and As, as a function of probing depth showing near constant values for Si and Ge while Ga and As are shown to have concentrations below the detection limit of 0.005%.

### PHOTOLUMINESCENCE USING THE LASHER-STERN-WURFEL MODEL

Because not all doping atoms are contributing to the carrier density, we also determine the active doping density. For this we use our second method, we perform low temperature (4K) macro photoluminescence measurements which are subsequently fitted by a Lasher-Stern-Würfel (LSW) model [2]. The LSW model is characterized by the generalized Planck's radiation law:

$$I_{PL} = \frac{2\pi}{h^3 c^2} \cdot \frac{(\hbar\omega)^2 a(\hbar\omega)}{\exp\left(\frac{\hbar\omega - \Delta\mu}{kT}\right) - 1}$$

With the absorptivity calculated from the absorption coefficient:

$$a(\hbar\omega) = 1 - \exp(-\alpha(\hbar\omega) \cdot d)$$

Where the absorption coefficient consists of the JDOS broadened by Urbach tail states and a Fermi-Dirac occupation correction:

$$\alpha(\hbar\omega) = \frac{A}{\hbar\omega} \left[ T(\hbar\omega) * \sqrt{\hbar\omega - E_g} \right] \times [f_V - f_C]$$

Here we investigate a recently produced hex-Ge sample by measuring the PL response as a function of excitation density as shown in Fig. 2a. The sample shows strong Burstein-Moss shift indicating bandfilling. The integrated PL intensity is also comparable to previously measured samples. We now calculate the LSW model fits for these spectra and find good agreement between the PL response and the fitted curves with the resulting parameters shown in Fig. 2b,c,d. From the quasi-Fermi level splitting we can now determine an estimate for the activated doping density of  $n_0 \approx 3 \times 10^{17} \text{ cm}^{-3}$ . If we again compare to the active doping density previously fitted for hex-Ge nanowires where a value of  $n_0 = 3 \times 10^{18} \text{ cm}^{-3}$  was found [1], we again obtain an order of magnitude reduction in the doping density which is consistent with the reduction from the APT results.

We can conclude that both the physically present and the activated doping density is reduced by approximately 1 order of magnitude while maintaining the good optical quality of the Hex-SiGe nanowires.

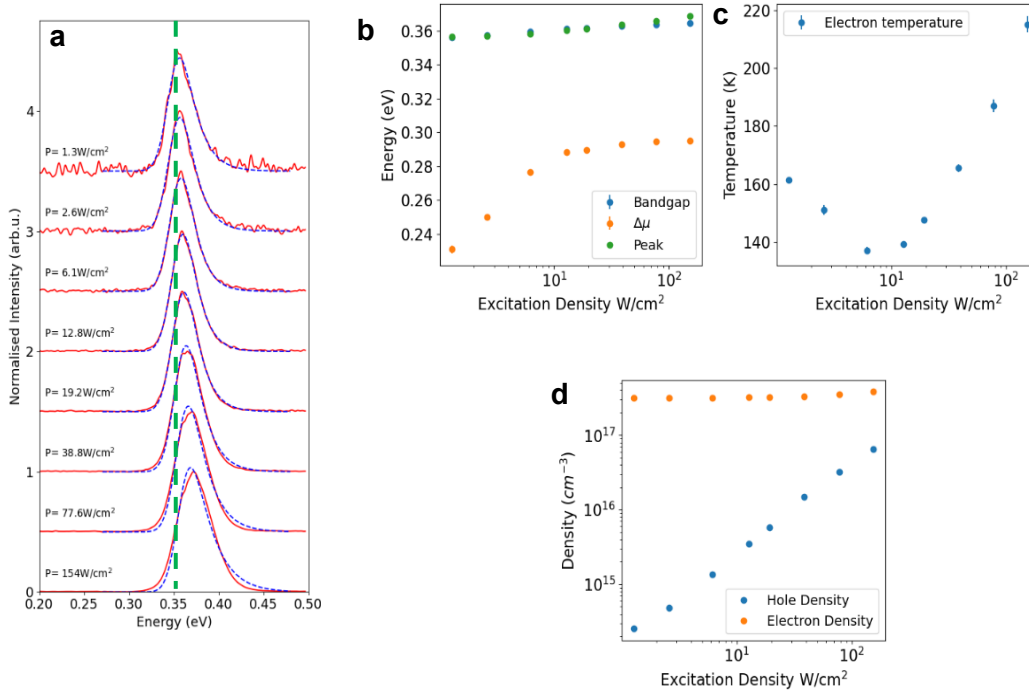
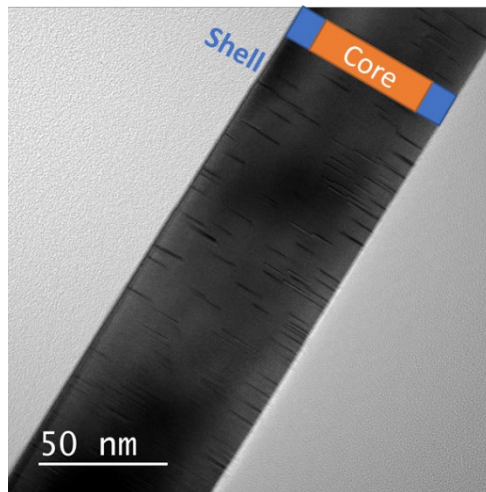


Figure 2: a) Normalized low temperature (4K) macro-photoluminescence response of Hex-Ge nanowires as a function of excitation density in red showing pronounced bandfilling and the fitted LSW model result in blue showing good agreement. b-c) The LSW fitting results showing the bandgap, the Quasi-Fermi level splitting  $\Delta\mu$ , the electron temperature and d) the fitted carrier densities showing a doping density of  $n_0 \approx 3 \times 10^{17} \text{ cm}^{-3}$

## MBE-GROWTH

Lower doping levels have thus already been achieved for hexagonal Germanium shells grown with MOVPE. A further reduction of the As doping density should be achievable if the shells are grown with Molecular Beam Epitaxy (MBE). A major advantage of MBE compared to MOVPE is the option to grow at lower substrate temperatures. The lower temperatures are possible because MBE uses no precursors that need to be thermally decomposed. The arsenic doping is expected to be reduced, since both the evaporation from the GaAs substrate and solid-state diffusion from core to shell are thermally activated processes.

Recently, an MBE system became operational for the deposition of Si and Ge through e-beam evaporation. The current status of MBE growth can be summarized in Fig. 3. The hexagonal phase is transferred from the GaAs to the Ge shell. However, the hexagonal Ge shell has many defects (~500 defects/ $\mu\text{m}$ ), most of which seem to start from the GaAs-Ge interface. The current hypothesis is that the interface is slightly oxidized. The oxidation might happen during the transfer between different reactors, since the GaAs cores are grown in a separate MOVPE reactor. Future research will explore how to improve the interface, for example by different pre-deposition annealing, or by tuning the growth conditions.



*Figure 3: BF-TEM image of a WZ GaAs – Hex Ge core-shell nanowire. Defects are visible as short dark lines. Most of the defects seem to start at the interface*

## REFERENCES

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- [2] J. K. Katahara and H. W. Hillhouse, “Quasi-Fermi level splitting and sub-bandgap absorptivity from semiconductor photoluminescence,” *J. Appl. Phys.*, vol. 116, no. 17, p. 173504, Nov. 2014, doi: 10.1063/1.4898346.