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D4.1 Growth of Hex-$Si_{1-x}Ge_x$ / $Si_{1-y}Ge_y$ (y>x) quantum wells

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DESCRIPTION OF DELIVERABLE

Description of work: *Document in which we detail the progress on the growth of Hex $Si_{1-x}Ge_x$ /$Si_{1-y}Ge_y$ (y>x) quantum wells*

1. INTRODUCTION

Hexagonal SiGe has been demonstrated to have a direct bandgap with a recombination efficiency comparable to III/V semiconductors. Until now, the composition of Hex SiGe was never varied inside a single crystal. Epitaxially connected SiGe layers with different compositions are necessary for most practical applications. This deliverable focuses specifically on the growth of Hex SiGe for quantum wells. Hex SiGe quantum wells are envisioned to be of critical importance for achieving low threshold Hex SiGe lasing.

2. THEORETICAL BAND ALIGNMENT OF HEX SIGE

Fig. 1 shows the calculated band offset for unstrained hex-SiGe alloys for different composition, calculated by FSU-Jena using ab-initio DFT calculations using both the MBJLDA and the HSE06 functional. Calculations taking into account the proper strain values for strained hex-SiGe quantum wells are presently underway. It can be seen that hex-Ge/hex-$Si_{0.25}Ge_{0.75}$ quantum wells feature sufficient conduction band offset, while it is not yet clear whether the valence band offset will make them type I or slightly type II.

Hex-$Si_{0.25}Ge_{0.75}$/ hex-$Si_{0.5}Ge_{0.5}$ quantum wells feature an indirect bandgap hex-$Si_{0.5}Ge_{0.5}$ barrier (in grey) with sufficient conduction band offset. The valence band offset is type I with the MBJLDA functional and type II with the HSE06 functional.

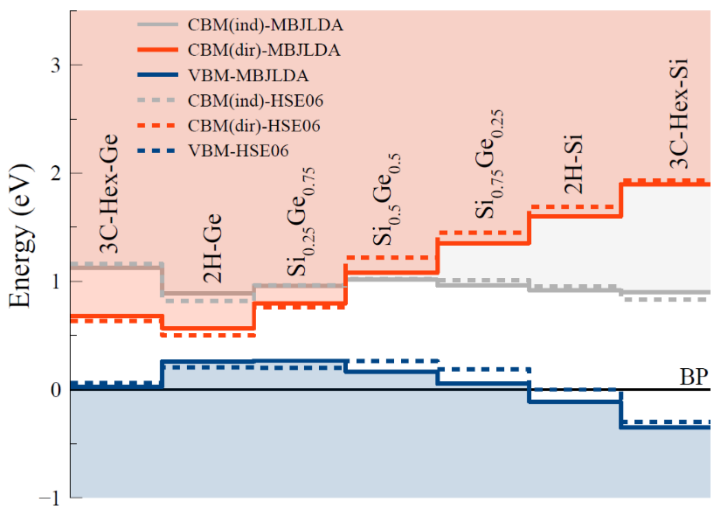

Figure 1: a) Calculated band alignment of hexagonal SiGe alloys. The different alloys have relaxed lattice constants, and strain has not been taken into account.

3. NUCLEATION STUDY OF SIGE SHELLS ON GAAS

The hexagonal SiGe is grown using the crystal transfer method by copying the crystal structure from wurtzite GaAs NWs. The GaAs NWs are grown with gold catalysts on GaAs (111)B substrates. The Vapor-Liquid-Solid (VLS) mechanism drives axial growth of the GaAs. Recent innovations did lead to the development of wurtzite GaAs NWs on masked GaAs (111)B substrates. The thin mask of SiO_x increases the diffusion length of Gallium, and therefore the material supply for each NW is different than before. As a result, some vapor-solid (VS) growth occurs radially on the GaAs NWs due to excessive material supply.

In absence of radial growth, the GaAs NWs have 6 {1-100} facets. The radial growth forms 6 additional {11-20} facets, and the GaAs NWs thus have a total of 12 sidewalls (Fig 2a).

The crystal transfer method has not been applied before to these 12-facetted wurtzite GaAs cores. Therefore, the nucleation of Hex Ge and SiGe shells has been studied in more detail. During the initial stages of growth, the SiGe forms long stripes along the length of the NW (Fig 2b). In a cross-sectional view, it is clear that the SiGe grows selectively on the {11-20} facets of GaAs (Fig 2c). Not even a single monolayer of SiGe has been grown on the {1-100} facets of GaAs

On the contrary, nucleation of a thin Hex Ge layer does not seem to have an as-pronounced facet selectivity.

The facet-selective growth of SiGe is a phenomenon that has not been observed before. Potentially, it could be exploited to grow structures with confinement in two directions. If the initial SiGe is overgrown with a Si-rich alloy, the confinement can occur both radially and azimuthally, creating six 1D channels along the length of the NW. The growth of structures with a higher degree of confinement is interesting for reducing lasing thresholds in the future.

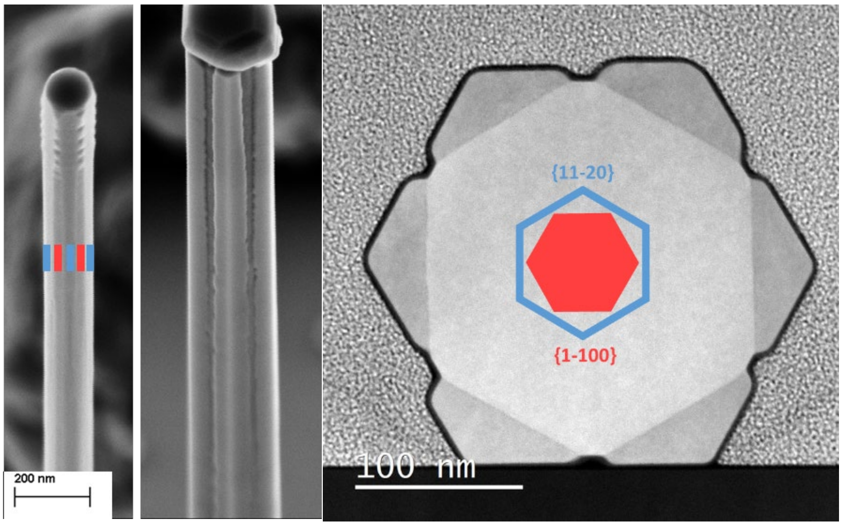

Figure 2: Nucleation of SiGe on 12-facetted GaAs. a) SEM image of a wurtzite GaAs NW. The {1-100}/{11-20} facets are colored red/blue respectively. b) SEM image of a similar wurtzite GaAs NW after a short growth of SiGe. The SiGe forms long stripes along the length of the NW. c) Cross-section of a Wurtzite GaAs – Hexagonal SiGe core-shell nanowire, imaged in HAADF-TEM. The SiGe shell is grown selectively on the 6 {11-20} facets of the GaAs core, resulting in separate islands.

4. GROWTH AND OPTICAL STUDY OF SIGE HETEROSTRUCTURES

Growth of Hex $Si_{1-x}Ge_x$ – $Si_{1-y}Ge_y$ heterostructures has been demonstrated on wurtzite GaAs nanowires. The Ge-rich $Si_{1-y}Ge_y$ layer has been chosen to be Hex Ge, in order to avoid alloy fluctuations in the layer with the smallest bandgap. Specifically, the heterostructures studied are a Hex Ge-SiGe-Ge multishell structure (Fig 3a-b). The thickness of each layer has been estimated by removing samples from the reactor after each step (Fig 3c). The layer with the lowest bandgap, e.g. the optically active layer in a quantum well structure, is the Hex Ge between the GaAs core and SiGe shell. Thus, this layer benefits from the large band offset with the GaAs core. However, the thickness of roughly 30nm is too much to observe any confinement effects.

The outer shell of Germanium seems to be very thin, possibly indicating a delay of nucleation. However, such incubation time is only expected when growing Ge on GaAs, and not if the Ge is grown on SiGe. In the future, such a nucleation delay may have to be taken into account for growing quantum wells.

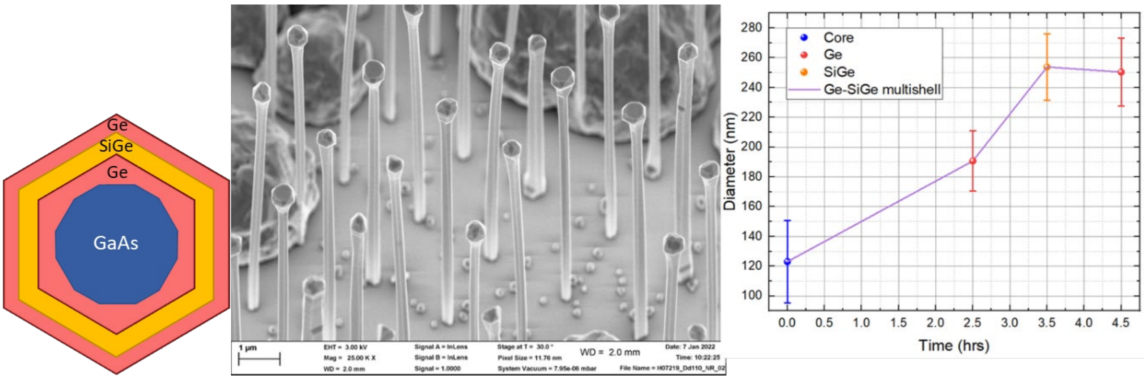

Figure 3: a) Schematic cross-section of the Ge-SiGe-Ge multishell structure b) SEM image of NWs with a hexagonal Ge-SiGe-Ge multishell. c) estimated diameter of each subsequent shell in the multishell structure.

The optical properties of the multishell structures have been probed in photoluminescence (Fig. 4). Three peaks are measured which are associated with the sample. The first peak (1) is attributed to Hex Ge. Remarkably, the onset of this peak is comparable to earlier measurements of Hex Ge in single shell structures. This is despite some compressive strain that is present in the NWs due to the SiGe layer with a smaller lattice constant.

The second peak (2) comes from the Hex SiGe layer. The Ge-fraction of the alloy is ~80-86%, which is consistent with the growth conditions used.

The third peak (3) is associated with emission from cubic SiGe or the GaAs substrate. Additionally, the fourth peak comes from a nearby InGaAsP alignment sample. Both are thus not related to the hexagonal multishell structure.

The spectral shape of the Germanium peak is compared to samples with only a single Hex Ge shell (fig. 4b). The spectra of the single Ge shell have been volume-corrected in two different ways. The volume of either the complete multishell or only the Ge segment of the multishell has been set equal to the volume of the single shell spectrum. There are three important observations that can be made from this comparison.

To start, it is clear that the multishell sample has a higher intensity of Germanium photoluminescence as compared to a single shell. It highlights the crystal quality of the multishell. Moreover, it could suggest that the SiGe acts like a passivation layer on the inner Ge shell.

Secondly, the low-energy onset of all peaks is at a similar energy. This indicates a similar bandgap, and highlights that no quantum confinement effect has been observed in the multishell. However, the peak energy of the multishell is significantly blueshifted. The shift is attributed to additional bandfilling. Thus, more carriers are localized in the Hex Ge segment under similar excitation conditions.

Lastly, there is also no emission below the bandgap of Hex Ge. Emission at lower energies would have been expected if the band alignment between Hex Ge and Hex SiGe was of type II.

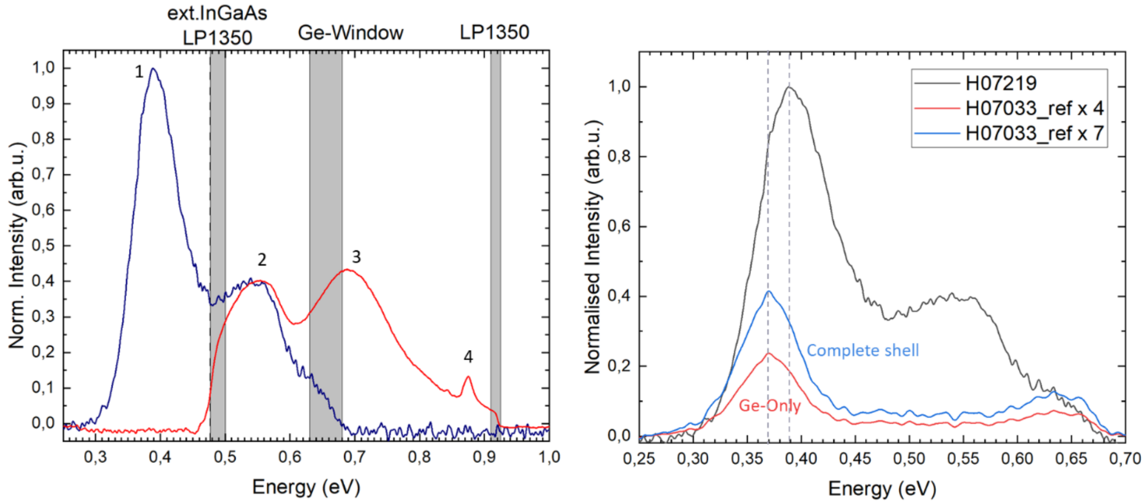

Figure 4: a) Photoluminescence spectrum of the Hex Ge-SiGe-Ge multishell. The blue- and red-curves are measured with an MCT and extended InGaAs detector respectively. The intensity of the red curve is adjusted to match the spectral shape of the MCT measurement. b) Comparison of the multishell spectrum (H07219) to a single Ge shell (H07033). The spectrum of the single shell is volume-corrected to have an equal volume of Ge (red) or total shell (blue).

5. CONCLUSION AND OUTLOOK

Hexagonal Ge-SiGe-Ge heterostructures have been grown. Light emission has been observed from both Ge and SiGe. Thus, both layers have a crystal quality sufficient for probing optical properties.

The photoluminescence experiments suggest the localization of charge carriers in the lower bandgap Hex Ge region. Strong evidence of either type-I or type-II band alignment is still lacking, since neither quantum confinement nor emission below bandgap has been observed respectively.

In the next steps, the thickness of the smallest bandgap region will be decreased. Quantum confinement effects should be more pronounced if alignment is of type I. Additionally, facet-selective growth of Hex SiGe will be explored to grow structures with a higher degree of confinement.