Strain and composition effects on Raman vibrational modes of hexagonal GaP-Si-$Si_{1-x}Ge_x$ core shell nanowires

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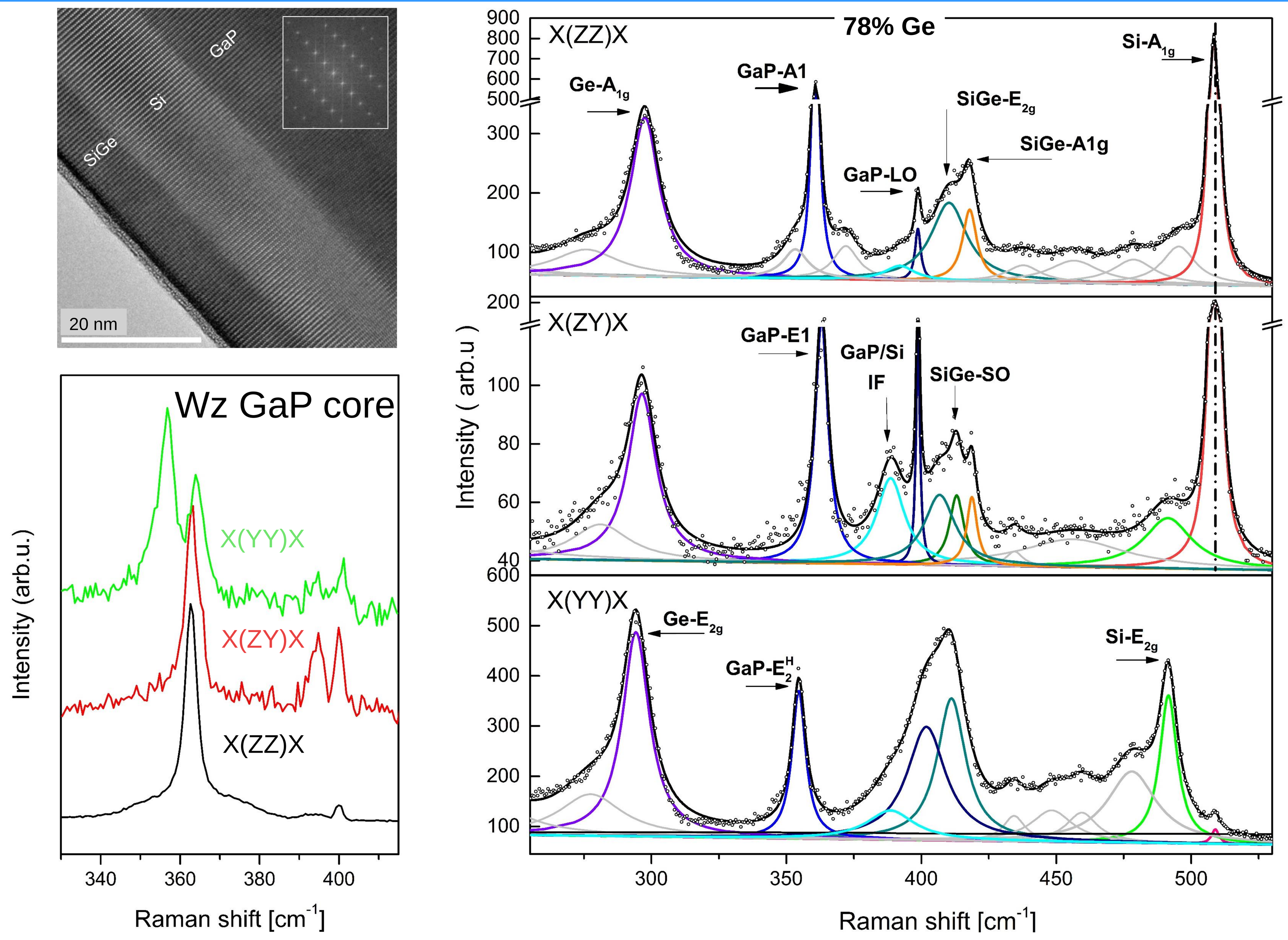
Motivation

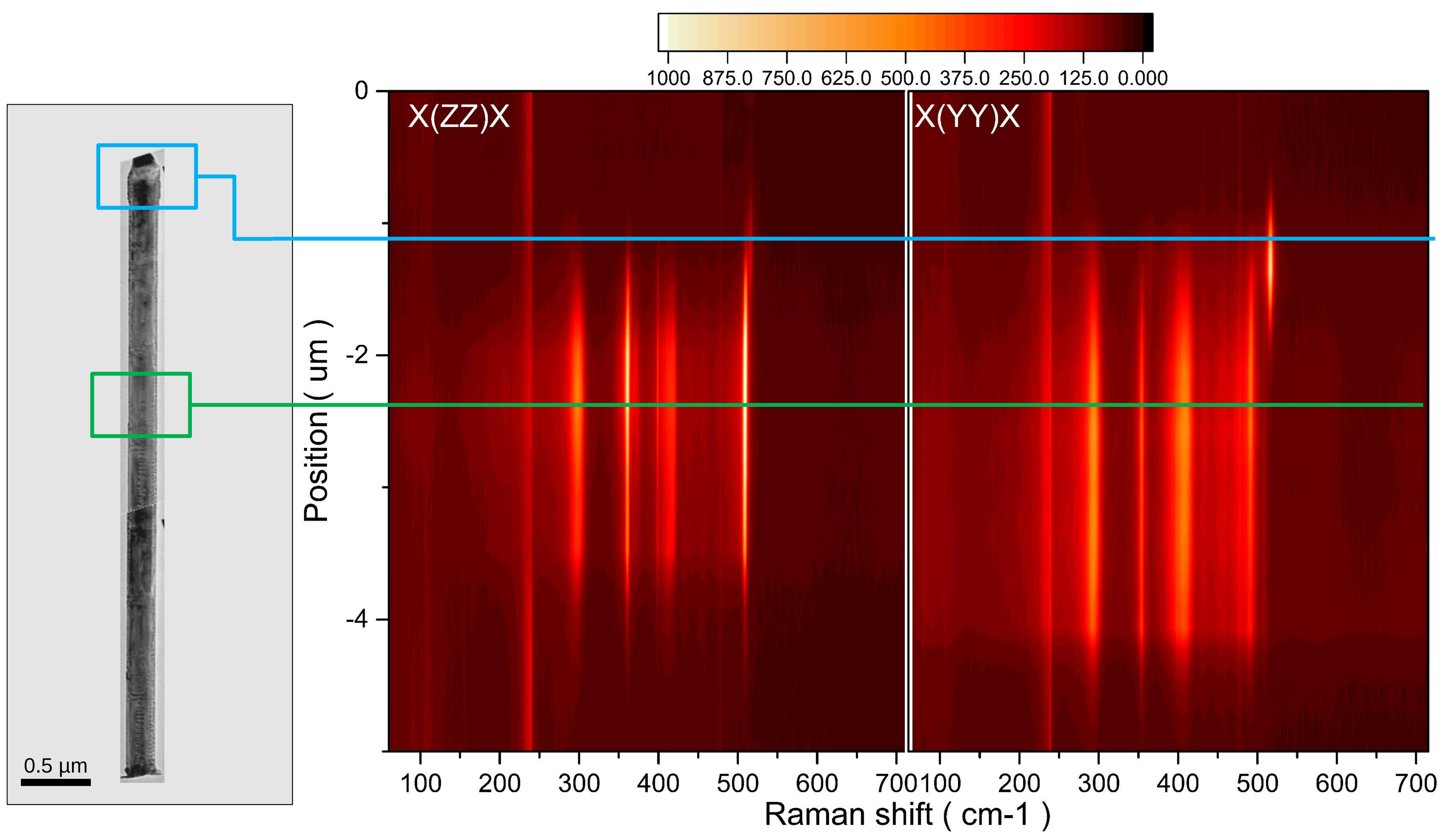
- Hexagonal Ge is predicted to have a direct bandgap. Combining Si and Ge in the hexagonal structure to form hexagonal SiGe alloys is expected to provide a direct bandgap semiconductor for sufficiently high Ge content.
- µ-Raman spectroscopy can provide information on the crystalline quality, strain field, and alloy composition of single GaP-Si-$Si_{1-x}Ge_x$ core shell Nanowires (NW) in a spatially resolved manner.

Assessment of vibrational modes



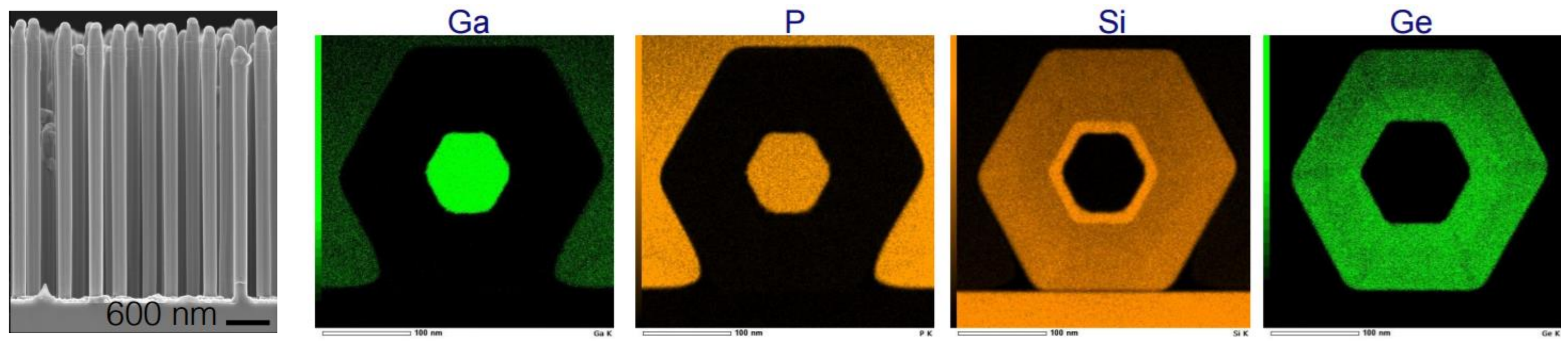
- Polarization dependent measurements have revealed the characteristic modes of hexagonal phase (E_2^H, E_{2g}) for all the layers.
- We observed some additional modes in the X(YZ)X configuration located at 388 and 412 cm-1 that have been possibly assigned to GaP/Si interface mode and SiGe surface mode.
- We report for the first time the E_{2g} mode of Germanium, located at 294.5 cm-1 for 78% Ge.

Investigation of growth homogeneity



- Spatially resolved µ-Raman measurement revealed the existence of defected region which extend up to 0.5 µm from the gold droplet. These defects are manifested in the form of a mix domain where both hexagonal and cubic Si modes are observed.
- The NW's feature then high crystal quality, which is homogenous along the wire as witnessed by the constant intensity of GaP, Si , SiGe and Ge phonon modes.

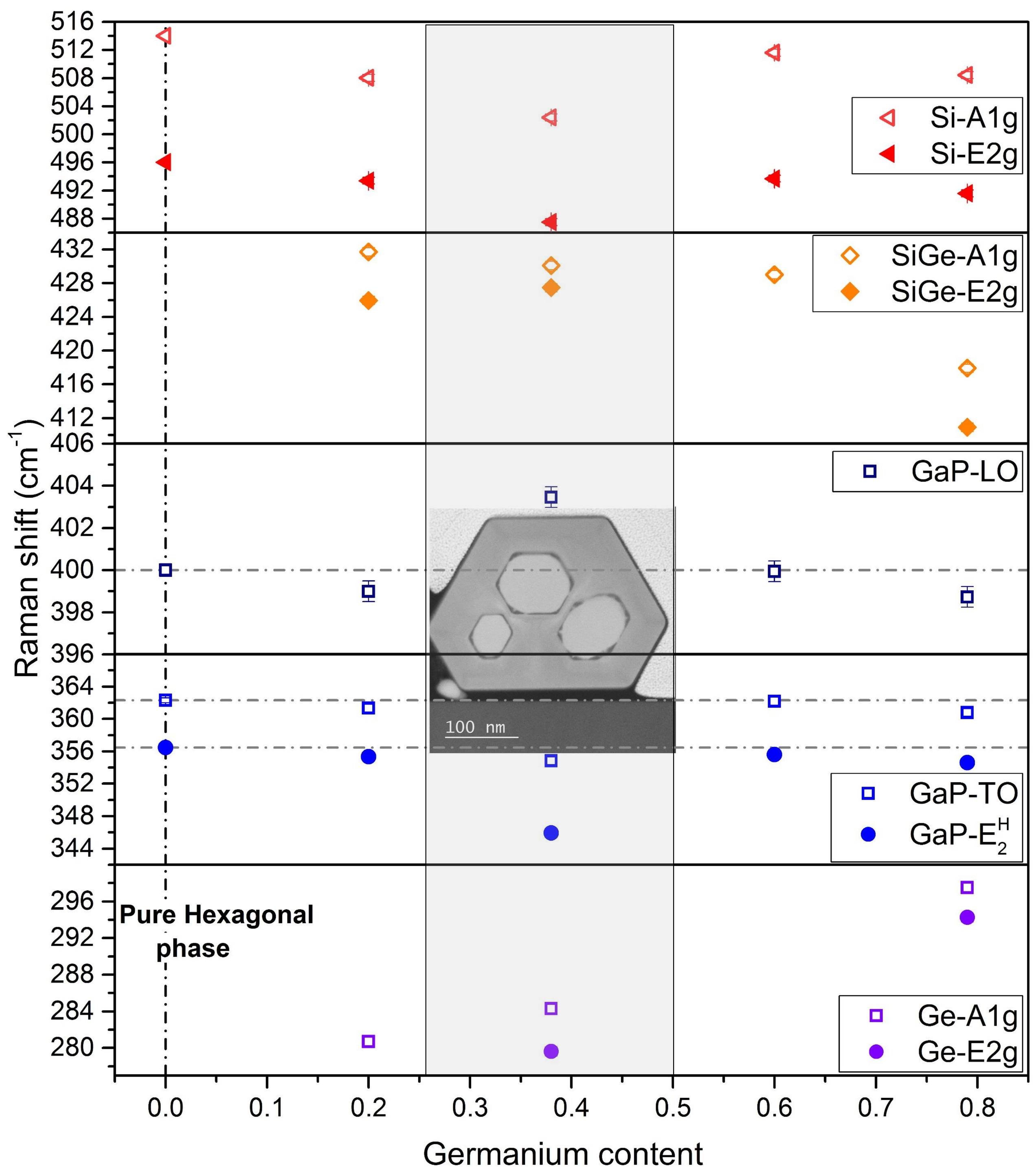
Sample description



Hexagonal GaP-Si-Si_{1-x}-$SiGe_x$ core shell NW's were grown using metal−organic vapor phase epitaxy (MOVPE) [1] :

- First: A high quality GaP hexagonal core was grown.
- Second : A perfect hexagonal Si shell was epitaxially grown around the wire.
- Third: A second shell is then grown varying the Ge content.

Assessment of composition and strain



- Varying Ge in Si matrix influences the vibrational frequency of Si-Si, Si-Ge and Ge-Ge modes.
- Both Ge-Ge A_{1g} and E_{2g} modes show a linear trend with a positive slope with increasing Ge content.
- For Si modes, the trend is more complex probably because of the contribution of the Si-Si modes stemming from the Si inner shell and SiGe outer shell.
- The presence of strain can be assessed more reliably from the GaP core since there is no contribution from the compositional variation to the shift of the mode frequency.
- We observed a negligible shift in the frequency of GaP modes up to 60% Ge. Increasing the Ge% to 80%, we observe a down shift of all GaP optical modes of 1.3 cm-1 in agreement with the presence of tensile strain.
- For 38% Ge content we observed a sudden red shift in the LO, TO and E_2^H modes of GaP. Correlation with cross sectional TEM suggests that this behavior might be related to the presence of multi core structure, with cores of different dimensions, and a highly defected SiGe shell.

Conclusions

- µ-Raman spectroscopy was used to investigate the phonon modes of single GaP-Si-$Si_{1-x}Ge_x$ core-shell NWs.
- Polarization dependent measurements were employed in a spatially resolved manner to assess the NW crystal phases.
- We investigate the crystalline quality, the strain field, and the alloy composition along these technologically relevant NWs.

Acknowledgements

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References

[1] Håkon Ikaros T. Hauge, Sonia Conesa-Boj et al. Nano Lett. **17** (1), 85 (2017)
[2] Zheng Wenli, and Li Tinghui, Journal of Semiconductors, **33**(11), 112001 (2012)

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