

Wurtzite GaAs_xP_{1-x} Nanowires: micro-Raman and micro-Photoluminescence Studies

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III–V semiconductor alloys provide a versatile platform for band-structure and materials engineering. While cubic zincblende alloys have been extensively studied, their wurtzite (WZ) counterparts remain comparatively unexplored due to the limited stability of this crystal phase under bulk growth conditions. Semiconductor nanowires (NWs) can overcome this limitation and enable the controlled realization of phase-pure WZ nanostructures.[1]

Here, we present a comprehensive experimental and theoretical investigation of the structural, electronic, optical, and vibrational properties of GaAs_xP_{1-x} NWs in the novel hexagonal WZ phase, as a function of As composition.

By combining optical nanospectroscopy and *ab initio* density functional theory (DFT), we characterize the evolution of the electronic band structure across the alloy. The bandgap is continuously tuned from 2.01 to 1.57 eV at 5.5 K and exhibits a moderate compositional bowing of (0.19 ± 0.02) eV, in excellent agreement with theoretical predictions. Band-unfolding calculations, supported by time-resolved photoluminescence measurements, indicate that the alloy retains a direct or pseudo-direct bandgap character throughout the investigated compositional range.[2]

We complement this electronic and optical picture by investigating the composition-dependent lattice dynamics by means of micro-Raman spectroscopy. Raman measurements reveal the systematic evolution of the characteristic vibrational modes between the GaP- and GaAs-rich limits following the typical two-modes behaviour, providing insight into the interplay between alloy composition, crystal symmetry, and phonon dynamics in the WZ phase. The experimental results are further supported by DFT calculations, which show good agreement with the measured data.[3]

Together, these results establish a unified description of the composition-dependent electronic and vibrational properties of WZ GaAs_xP_{1-x} and provide an experimental and theoretical benchmark for this emerging III–V alloy system. Its wide bandgap tunability in the visible spectral range, direct-like optical transitions, and composition-engineered lattice dynamics highlight WZ GaAs_xP_{1-x} NWs as a promising platform for optoelectronic and phononic applications.

[1]: F. Glas, J.-C. Harmand and G. Patriarche, Phys. Rev. Lett., 2007, 99, 146101.

[2]: P. De Vincenzi, I. Santanchè, R. Rurali, R. A. Sorodoc, A. A. Sharma, H. Gopalakrishnan, M. Roggi, E. Mugnaioli, F. Mura, F. Beltram, L. Sorba, V. Zannier, M. De Luca, Direct Band Gap Wurtzite GaAs_xP_{1-x} Nanowires (under submission)

[3]: I. Santanchè *et al.* (under preparation)