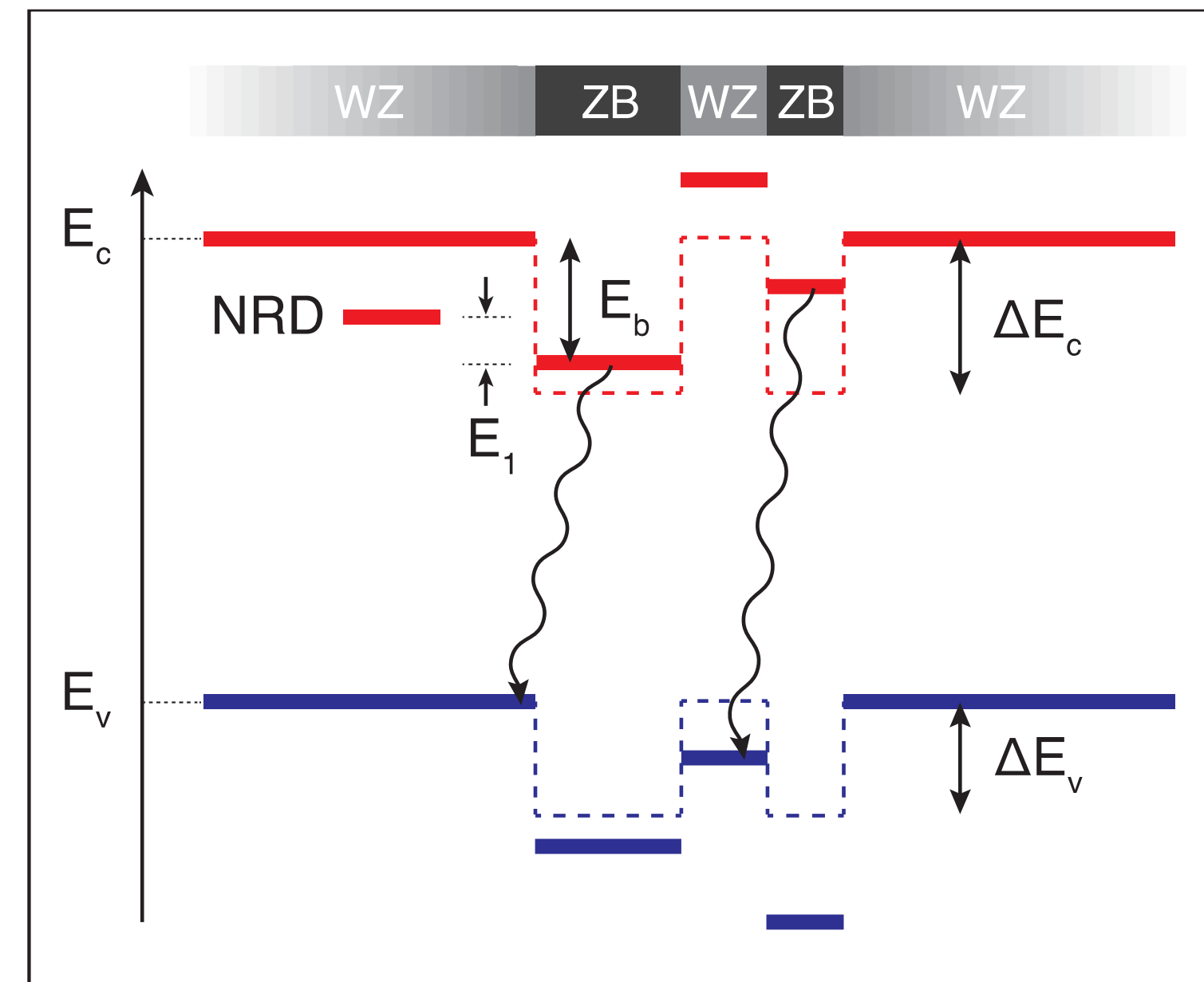
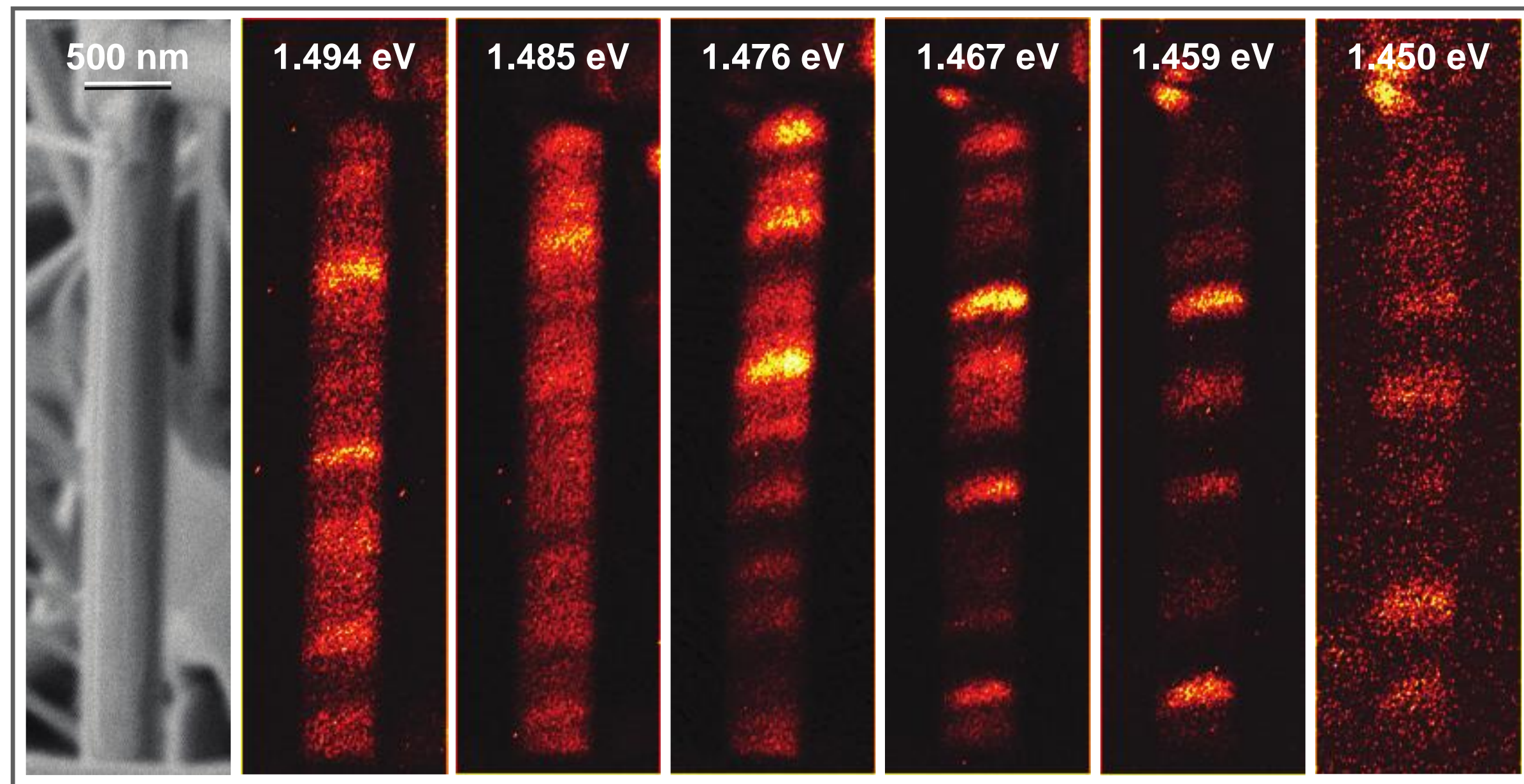


# Structural and optical properties of Mg-doped wurtzite-rich GaAs nanowires



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## Objectives

The core idea of this work lies on the application of GaAs nanowires on third-generation photovoltaic technologies. To this end, we are carrying out an experimental research effort in order to:

- Investigate the influence of substrates (GaAs and Si) and occurrence of transversal stacking defects on the optical properties of the nanowires.
- Determine the electronic band gap of wurtzite GaAs.
- Evaluate the intentional introduction of Mg impurities and the effective role of doping on the electrical properties of the nanowires.

## Methods and techniques

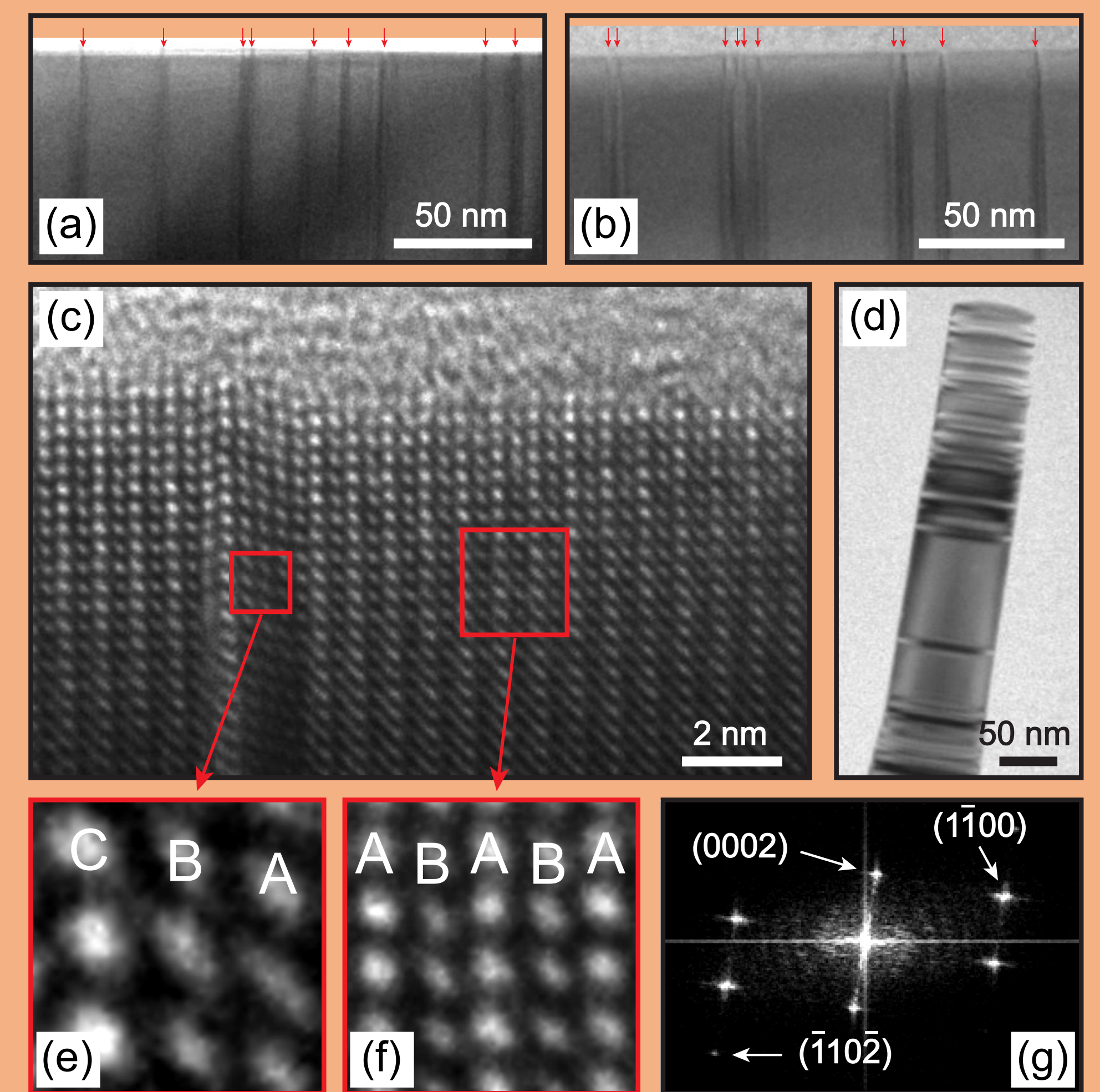
- Mg-doped GaAs nanowires are grown by molecular beam epitaxy via Au-assisted vapor-liquid-solid mechanism on GaAs and Si substrates.
- The structural properties are evaluated through scanning electron microscopy (SEM), high-resolution transmission electron microscopy (HRTEM), as well as Raman spectroscopy and X-ray diffraction.
- The optical characterization is performed by means of temperature and excitation power dependent photoluminescence (PL) and cathodoluminescence (CL) experiments on individual nanowires and on bunches of nanowires.

## Results

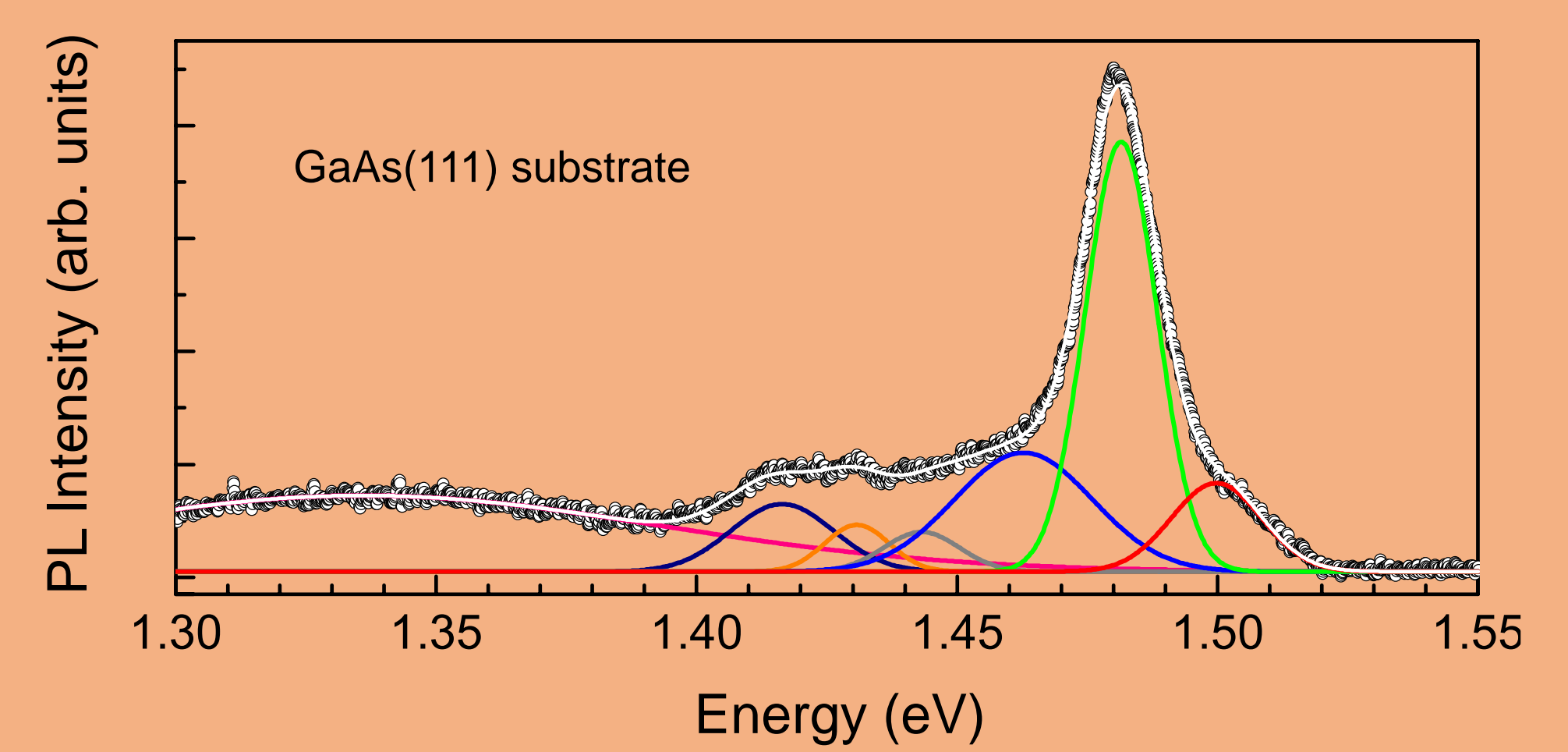
- Very large wurtzite-rich GaAs nanowires with some stacking defects (zinc-blende) along its axis can be grown by MBE on GaAs and Si substrates, with a slightly higher mean linear density of such segments for the later.
- The polytypic crystalline structure leads to a staggered band alignment that is detrimental to the mobility of charge carriers, but favours the charge separation at the two-phase boundaries as required for photovoltaic applications.
- The high aspect ratios of the nanowires cause additional difficulties in the incorporation of dopant impurities, namely Mg, as well as in the evaluation of their properties; indeed, the optical activity in the nanowires lacks a distinct acceptor-impurity behaviour primarily due to the polytypic structure.

## Publications

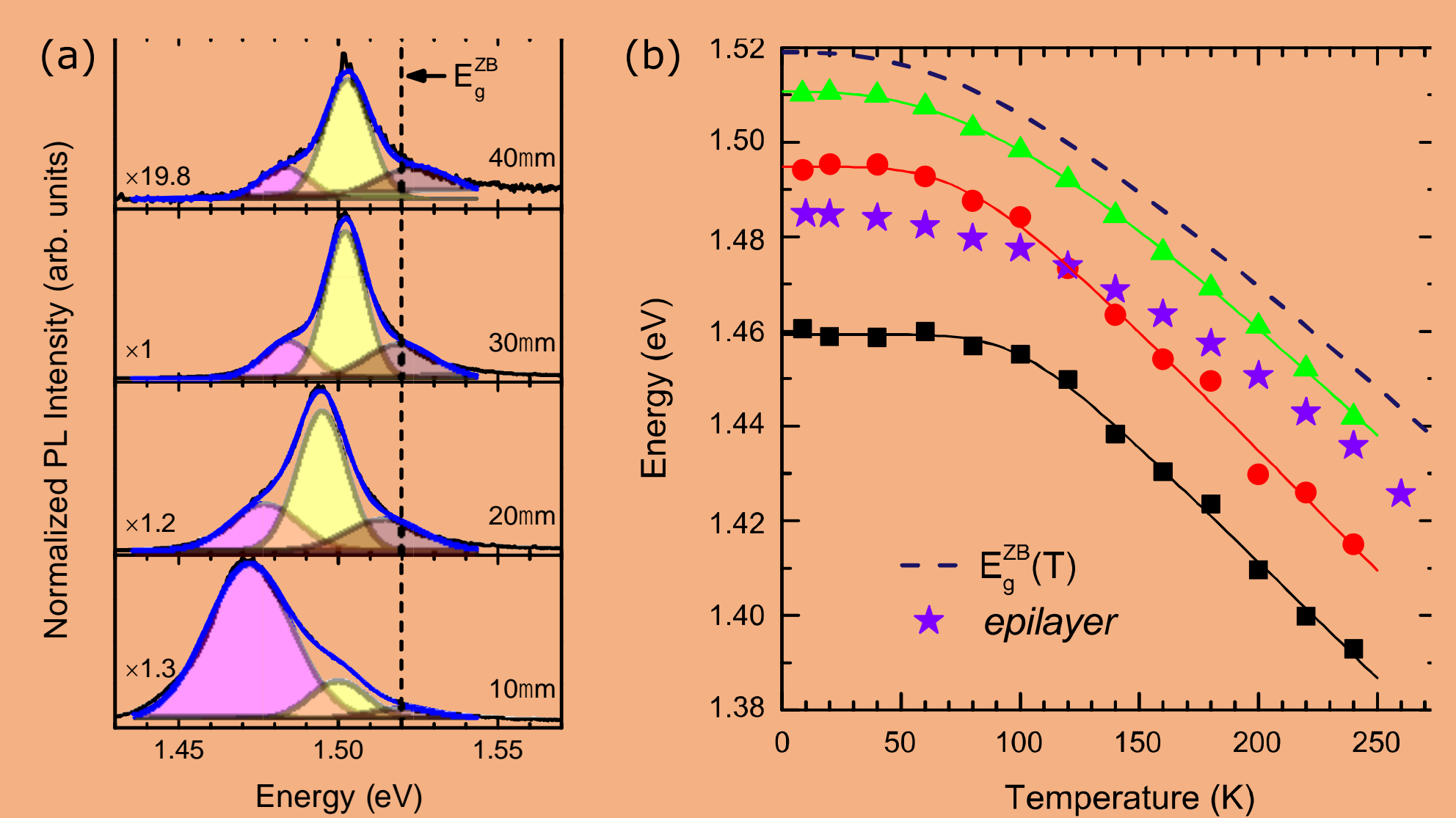
- B.P. Falcão *et al.*, *New insights on the temperature-dependent photoluminescence of Mg-doped GaAs nanowires and epilayers*, Journal of Materials Chemistry C 2, 7104 (2014).
- B.P. Falcão *et al.*, *Structural and optical characterization of Mg-doped GaAs nanowires grown on GaAs and Si substrates*, Journal of Applied Physics 114, 183508 (2013).
- B.P. Falcão *et al.*, *Photoluminescence study of GaAs thin films and nanowires grown on Si(111)*, Journal of Materials Science 48, 1794 (2013).



HRTEM images showing the wurtzite crystalline structure and the existence of transversal stacking defects with a zinc-blende lattice.



PL at 5K from Mg-doped GaAs nanowires shows near band edge emission related with spatially indirect transitions (type II).



(a) PL spectra along the axis of an individual nanowire, and (b) temperature dependency of the identified radiative transitions from a bunch of nanowires.