Determination of the Band-Offset between wurtzite and zinc-blende InP using photoluminescence

Carl Henrik Dahmén
Sebastiano Scrofani

December 17, 2019

1 Introduction

The main objective of this project is to study the bandstructure of zb- and wz-InP nanowires and how they differs using power-dependent photoluminescence. The normal crystal structure for grown 2D InP is zb but grown as nanowires (NW) they can form wz structures under right conditions. The zb and wz InP will then create a atomically sharp interface with minimal strain, which is crucial in good high electron mobility transistors (HEMT). wz InP has a larger band gap than zb and different electron affinity, resulting in a band-offset which we are going to study.

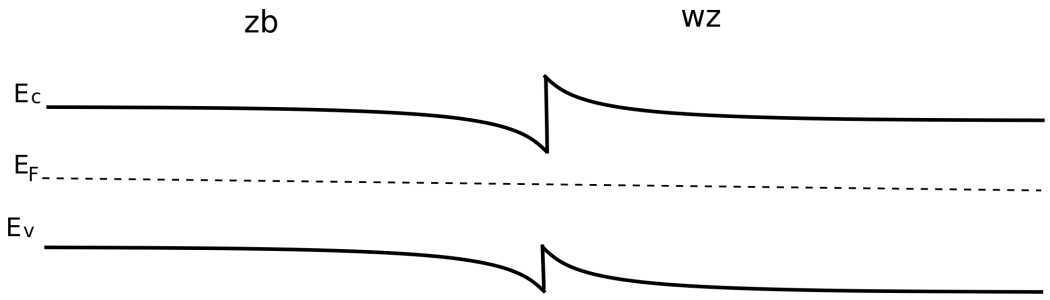

Figure (1) zb-wz InP band structure.

In figure 1 the junction of zb and wz InP is drawn. At low temperature the band gap of zb InP is 1.42 eV and wz InP is 1.49eV, and the heterojunction is of type II (E_C(wz) > E_C(zb) and E_V(wz) < E_V(zb)). We will first study the wz-structure of InP NW by photoluminescence (PL) and photoluminescence excitation (PLE) and then the wz-zb junction by PL. All the measurement were made at low Temperature (between 4K and 5K) using a system which involves the use of lasers, helium to keep the low temperature, a spectrometer and a computer with an analyzing software.

2 Theory and measurements

Photoluminescence is the process of a material emitting photons due to being stimulated by light. The incident photon is absorbed over the band gap and excites an electron to the conduction band. This electron will then find the lowest possible energy and after a certain time recombine with a hole in the valence band emitting a photon with the band gap energy in the process. Photoluminescence excitation is a way to study the density of states of a semiconductor. By irradiating the sample in steps of energy, the photons will be absorbed as you match energy states. By measuring the emission you will get a picture of the density of states, a higher intensity corresponds to a larger density of states. For a 3D structure the density of states follows $E^{1/2}$.

3 Photoluminescence of wurtzite InP

The first samples analyzed were pure wz-InP nanowires. The samples were mounted on a cryostate and the nanowires (of the order of micrometers) were focused on by a camera. A system of flipping mirrors and a spectrometer was used and the laser power was set by the computer software. The tunable laser was set to 1.75 eV (λ=710nm) to study the PL. We measured PL for different laser powers in steps of half an order of magnitude to the previous one, in order to study the power dependency of the wz-InP band gap, resulting in different PL spectra. While decreasing the power, we increased the exposure time to avoid noise in the measurement. The power dependency effect, the shift of the PL-peak to higher energies while increasing the laser power is called the Burstein Moss Shift. This happen when there are so many charge carriers that instead of recombining from the bottom of the CB to the top of

the VB, the recombination occurs from higher energy levels in the CB to the VB resulting in higher energy of the peaks. The first PL spectrum measured was at room temperature, when the wz InP bandgap is equal to 1.42eV. Two peaks are observed: one at around 1.42eV (as expected) and one at an higher energy. The first is the bandgap of wz-InP and the second one is at about at 1.46eV and we don't know exactly what it is but it is still present at cold temperature in all samples, and we can only say that there are some impurities that does not change with temperature. The peak of interest in this lab is the first one at cold temperatures. Knowing that InP in the wz form (wz-InP) has a bandgap of 1.49 eV at low temperatures, we measured the PL spectrum at the temperature of 4.8K and the result is shown in figure (2):

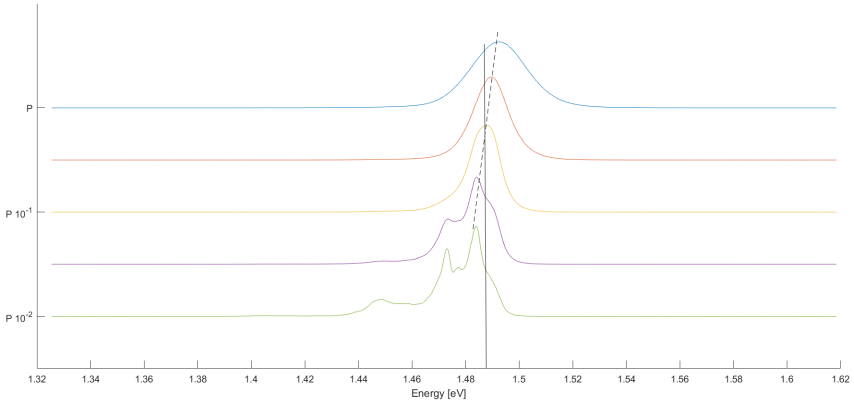

Figure (2) Power-dependent PL-spectra of wz-InP nanowire. The peak intensities are normalized and in arbitrary units, the y-axis shows the excitation power density of each of the spectra. The dotted line is to highlight the power dependency and the other line is showing 1.49 eV.

The big peak is from the wz-InP bandgap at 1.49 eV and the extra peak at approximately 1.46eV is something we are not sure of its origin. We repeated the measurements at different powers and changed the exposure time, and we found that decreasing power, the shape changes a little bit. At high power the peak looks very symmetrical and decreasing the power, the peak gets thinner and more noise can be seen due to impurities in the nanowire just below the CB or above the VB. A small shift of the peak to lower energy is present while decreasing the power due to the Burstein Moss Shift. This

small shift changes the measured bandgap from the real value of 1.490 eV to the one of 1.491eV. To be sure that the spectrum is correct, we took the PL spectrum of another nanowire of pure wz InP in the same sample and we found the same spectrum.

4 Photoluminescence excitation of wz-InP

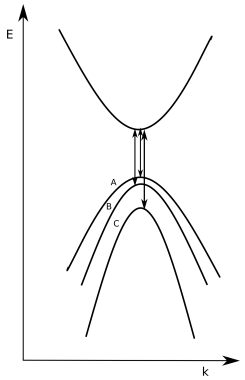

Figure (3) Schematic picture of the wz-InP dispersion diagram.

The valence band structure of the wz-InP, shown in figure 3, consist of one electron-conduction band and three different hole-valence band states labeled A,B and C in the figure 3 and through photoluminescence excitation measurement we verified this valence band structure. In particular the nanowires were photoexcited using a red laser which was tuned for scanning from 838nm to 707nm (or alternatively to 1.48eV to 1.75eV with an increasing energy) in 132 steps and for every step the intensity of light emitted was measured. A detection low-pass filter at λ=845nm was used in order to filter out all the energies bigger than the one corresponding to 845nm (as the laser one). The PLE was made keeping the power that heat the sample to a constant value. What we detect in a PLE experiment is the intensity of the emitted light that is related to the number of electrons that can be absorbed in the system and thus to the density of state. From the theory we expect to see in our spectrum see the density of states increase like $\sqrt{E - E_v}$ for every energy transition between the conduction band and valence band A, B and C.

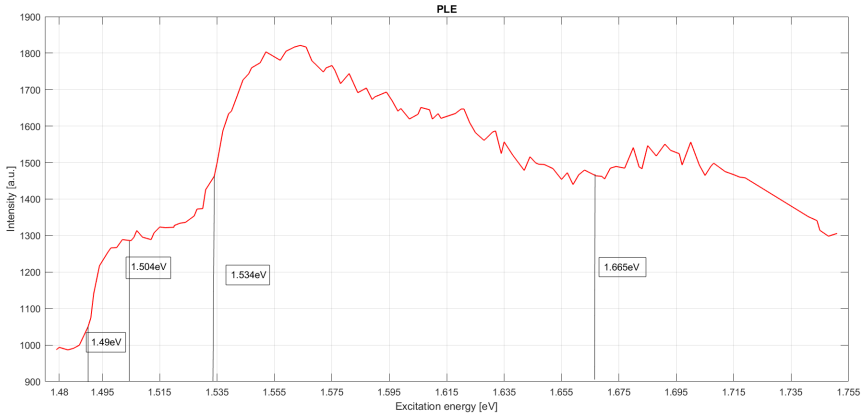

Figure (4) PLE spectrum of wz InP with highlighted the three steps related to the three different recombination CB-A, CB-B and CB-C. The 1.505 eV "bumb" are from an exciton.

Looking at the spectrum obtained from PLE in figure 4, when the laser scanner moves to higher energies, as expected, two really clear different steps will be observed at 1.49eV, 1.534eV and another one can be identified where, after a first decrease of intensity, it start again to increase at approximately 1.665eV. The noise in the spectrum is probably due to the spot moving a little bit with the increasing temperature. The first result to be related with the transition A, the second one is related with transition B and the third one correspond to transition C in figure 3 and the energies at with we have the three steps are respectively Eg_A, Eg_B and Eg_C. From the difference between the value of Eg_B and Eg_A we can find that the energy splitting between the A and B hole bands is equal to 44meV.

The 1.505 eV "bump" is no transition but an exciton, a coupled electron and hole pair between the conduction and valence band A.

5 The wz- and zb-InP junction

At a high excitation power density (epd) of the laser a big number of electrons will be excited from the valence band to the conduction band. In the QW the density of states is limited and the electrons will populate the lower energy states pushing the apparent band gap to a higher energy by the Pauli exclusion principle. See figure 5. As seen in figure 1 this is not a direct band

gap, unlike the Burstein Moss shift. We have tunnel assisted recombination, the electrons and the holes in the wells tunnel into their respective barrier making their wavefunctions to overlap and recombine.

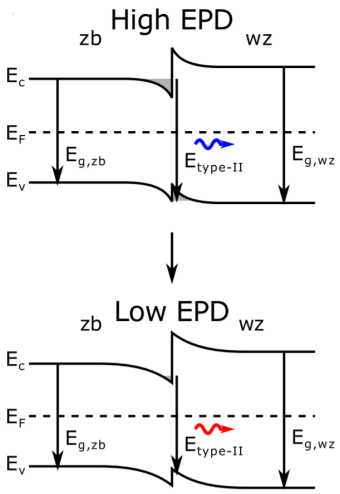

Figure (5) Band gap junction of wz and zb. High energy power density vs. low energy power density. Picture taken from the paper: "Two-dimensional electron gas at Wurtzite-Zinc-blende InP interfaces induced by modulation doping" Irene Geijselaers et al.

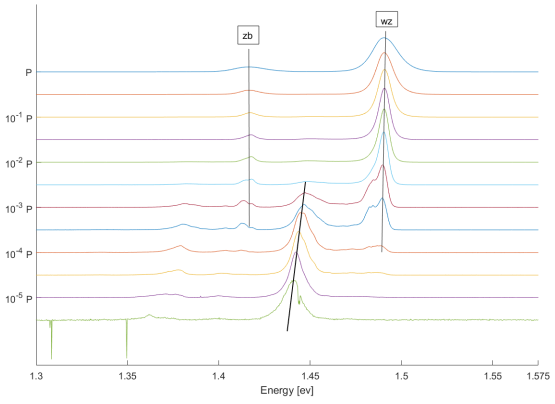

Figure (6) Power-dependent PL-spectra of wz-zb-InP nanowire. The peak intensities are normalized and in arbitrary units, the y-axis shows the excitation power density of each of the spectra.

In figure 6 we have plotted our measured PL-spectra for different powers. The peaks at 1.49 eV are from wz and the peak at 1.42 eV are from the zb. The decreasing peaks around 1.45 eV are from the well. All other peaks are from impurities. We were interested in studying the spectra for even lower epd but we were limited by the increasing exposure times needed for low epd that extended 1 hour for the smallest power. If we would be able to decrease the power even more we might have observe the E_{typeII} to decrease even faster due to the triangular shape of the well giving rise more and more sparse energy states. As seen in figure 5 the band gap of the junction is actually smaller than $E_{g,zb}$ but we're never reaching that low laser power needed.

6 Conclusion

We verified the band gap energy of wz-InP to be 1.49eV at low temperature and we found the spacing between the first and the second valence band in wz-InP nanowires to be equal to 0.44eV and we did't determine the exact band-offset between wurtzite(wz) and zinc-blende(zb) InP nanowires using power-dependent photoluminescence because of the long time needed to do that, but we are satisfied to to have highlighted how the energy of the peak to decrease with power and we can expect that if we would continue to decrease the power and waiting enough time, the bandgap of the junction will be lower that $E_{g,zb}$.