Polarity determination in III-V nanowires using CBED and focal series reconstruction

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Nanowires made from III-V semiconductors are a possible platform for future electronic and photonic devices due to: their ability to combine lattice mismatched materials into defect free heterostructures, the possibility of using wrap-around gates for improved electrostatic control, and the possibility of controllably changing their crystal structure type [1].

Most III-V materials (except III-Ns) adopt the cubic zincblende structure type in bulk, but can when grown as nanowires also form the hexagonal wurtzite structure type. Both of these structure types are polar (i.e. not centrosymmetric). In GaN nanostructures polarity is known to affect both growth behaviour and their function as light emitting diodes [2]. III-V nanowires have commonly been grown on III-V substrates and in these cases the polarity of the nanowire crystal has been assumed to be the same as for the substrate. One advantage of the nanowire geometry is however that growth is also possible on non-polar group IV substrates and substrates with dissimilar crystal structures, such as graphene [3]. In these cases the polarity of the resulting nanowires needs to be investigated.

Nanowires span a wide range of diameters, and can be either phase pure or a random mixture of zincblende and wurtzite. For III-V materials there are examples both where the group III and group V have very similar Z (e.g. GaAs), and where they differ (e.g. InP). These factors make it necessary to employ several different methods for polarity determination.

For pure zincblende GaAs nanowires a convergent beam electron diffraction method has been applied to nanowires with diameters down to 40 nm. Due to the small difference in Z between Ga and As there is no asymmetric contrast in the zone axis CBED pattern. Instead the nanowire is tilted to simultaneously excite the 002 and the 1,1,11 and 119 type reflections. This result in either constructive or destructive interference in the 002 disc depending on which of the two sets of reflections was involved [4]. Figure 1 shows the resulting CBED pattern from two different GaAs nanowire samples, grown on a) (111)A and b) (111)B substrates respectively.

For InP there is enough difference between the two elements that a <112> CBED pattern shows considerable contrast difference between the 111 and -1-1-1 discs for nanowires more than 50 nm thick. In this projection however the different crystal structure polytypes and stacking faults are indistinguishable, making it very difficult to analyse the polarity for e.g. two adjacent twin segments. For this purpose zincblende InP nanowires with regular twinning and a 30 nm diameter were imaged in a <110> projection (figure 2a). Simulations of single HREM images found no combination of spherical aberration and defocus that could resolve the individual In and P columns at 17 nm projected thickness, corresponding to the thinnest parts of these nanowires. Using image series reconstruction from a 20 member focal series the In and P columns could however be resolved. From diffraction patterns calculated from the reconstructed exit wavefunction the local orientation of the bending and twisting nanowire could be estimated at the area of interest. At this particular thickness and small tilt away from the intended <110> direction the In positions appear darker than the P positions, making it possible to determine the polarity of the individual twin segments from the exit wavefunction [5].

These two examples illustrate how polarity in III-V nanowires can be determined for a wide range of thicknesses, different combinations of group III and V, and for both mixed and pure zincblende/wurtzite crystal structures.

All CBED patterns were recorded using a 300 kV JEOL 3000F. The focal series were recorded using a 200 kV aberration corrected JEOL 2200MCO [6].

References

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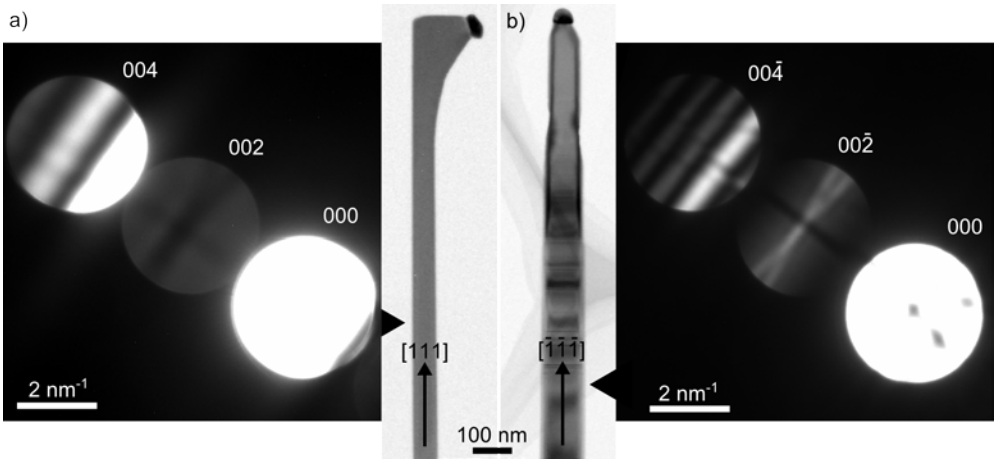

Figure 1. *Detail of CBED pattern and TEM overview of nanowires grown on a) (111)A substrate growing in [111]A, and b) (-1-1-1)B substrate growing in [-1-1-1]B. The thickness of the analysed area in a) is only roughly 40 nm (compared to 80 nm in b), which explains the weak contrast.*

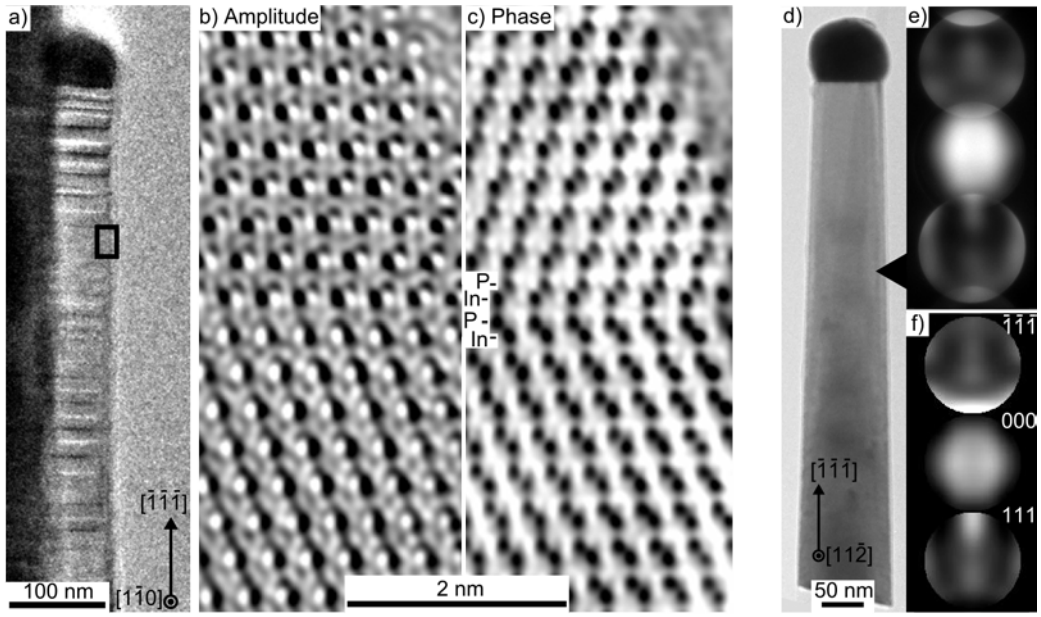

Figure 2. *a) Overview image of an InP nanowire with a diameter of about 30 nm. Reconstructed exit wavefunction amplitude b) and phase c) from a 20 member focal series recorded in [1-10]. Polarity can be determined from the contrast difference between the In and P columns. d) For a thicker, 80 nm, nanowire matching between e) experimental and f) simulated <112> CBED patterns is used instead. Note that in this projection the twins readily visible in a)-c) cannot be seen. Both nanowires grew in the [-1-1-1]B direction.*