

Electronic Supplementary Information (ESI)

Procedures to evaluate data of selected area electron diffraction (SAED)

Due to the small electron wavelength, the Bragg angles in electron diffraction are usually smaller than one degree and the diffracted beams are almost parallel to the direct beam. Therefore, approximating $\tan \theta \cong \sin \theta$ for small angles yields a simple correlation as

$$\lambda L = R d_{hkl} \quad (1)$$

between the reflection distances on the screen, R and the corresponding lattice plane spacing, d_{hkl} , using the camera length, L , and the electron wavelength, determined by the acceleration voltage (200 kV), λ (2.51 pm). The camera length is a tool specific parameter and determined by using reference samples with known lattice parameter.

Different crystal lattices lead to distinct diffraction patterns, due to their different extinction rules and lattice plane spacings. Especially for ring diffraction patterns of polycrystalline samples these differences are often clearly visible in the SAED pattern. There, the relation of the ring diameters to each other are unique and allow the easy determination of the underlying crystal lattice. Thus, SAED is a perfect characterization technique for the identification of the individual phases within heterostructured nanowires. In this work, a computer software has been developed for the easy comparison of X-ray (XRD) or neutron diffraction data with the SAED diffraction patterns of polycrystalline samples. This allows the easy and fast identification of phases through SAED by relying on the huge amount of available experimental data from X-ray and neutron diffraction.

The developed software uses Eq. 1 to calculate the on-screen distances of the reflections R with the lattice plane spacings d_{hkl} from literature data. For polycrystalline samples the on-screen distance correlates to the radius of the diffraction ring. For easy comparison, the calculated diffraction rings are projected onto the SAED diffraction pattern. Even without considering the peak intensities, this allows the fast screening of possible crystal structures to identify the nanowire phases.

In addition, the developed software allows another simple way to identify the phases in the SAED pattern. In this approach, a certain crystal structure is assumed first. Then, multiple lattice plane spacings d_{hkl} , which are allowed by the corresponding extinction rules, are calculated using an arbitrary lattice parameter. The lattice plane spacings are used to calculate the on-screen radii of the diffraction rings by using Eq. 1 and the rings are again projected onto the SAED pattern. Next, all diffraction rings are scaled by the same factor until all rings match the actual pattern. Scaling the rings correlates to changing the initial arbitrary lattice parameter. If the projected rings match with the actual diffraction rings the corresponding lattice parameter can be calculated by using Eq. 1 by measuring their on-screen distance. If the projected rings cannot be matched with the actual pattern, the assumed crystal structure is not present in the diffraction pattern.

At first, this approach may appear useless, because the diffraction rings itself can be used to calculate the lattice parameter in the first place. However, if the diffraction pattern is comprised of multiple structures, it is very hard to correlate each diffraction ring to its structure. Then, aligning many rings at the same time, helps the human eye to differ among the structures.