Supplementary Information for

Effect of Nitrogen Incorporation and Surface Passivation on Photoluminescence Properties of InAs-Based Nanowires

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The structural studies of the InAsN / InP core / shell NW sample was performed via the X-ray diffraction reciprocal space mapping (XRD-RSM) technique. XRD studies were carried out using a 4-circle Bruker Kappa Apex II diffractometer equipped with a microfocus Incoatec IμS 1.0 Cu-Kα X-ray source and 2D charge-coupled detector (Apex CCD). NW samples were mounted with the surface normally oriented along the diffractometer φ-axis. First, NW lattice orientation with respect to the orientation of the diffractometer axes was determined. Then, a three-dimensional (3D) RSMs were acquired by performing omega rocking (±5) scans with a 0.1 angular step and 10 s exposure time in the vicinity of both symmetric (0006) and asymmetric (21-31 and 1-101) Bragg reflections of the wurtzite InAs structure. RSMs in the vicinity of asymmetric Bragg reflections were obtained in noncoplanar diffraction geometry. Two-dimensional (2D) cross-sections of the obtained XRD-RSM were analyzed. The more details on the XRD-RSM experiment can be found in Refs. [10.1021/acsanm.3c06295] and [10.1039/D4TC04227A].

Figure S **XRD** (a) presents 2D XRD-RSM taken in the vicinity of the <-1-100> Bragg reflection of the wz-phase of InAs(N) from the InAsN / InP NW sample. Besides the wurtzite phase reflection of InAs(N), bright 002 and 11-1 Bragg reflections of the zinc-blende phase and its rotational twin are visible. Furthermore, additional weak reflections with larger diffraction vectors corresponding to wz- and zb- phases of InP are observed next to InAs ones. White arrows in Figure S **XRD** (a) indicate the corresponding Bragg reflections. The InP reflections are positioned along the relaxation line (both zb and wz-phase reflections of InAsN and InP share the same orientation of diffraction vector), which indicates the absence of distortions in the crystalline lattice of the InP shell. Thus, we suggest that there are no elastic strains in the core / shell nanostructures.

To estimate the lattice parameters for InAsN / InP NW samples we plot the XRD intensity profiles in the out-of-plane and in-plane directions for symmetric and asymmetric Bragg reflections, respectively, presented in Figures S **XRD** (b) and (c). The symmetric zb and wz-phase reflections are overlapped in the out-of-plane XRD intensity profiles, as the interplanar spacing in close-packed direction differs only slightly. In contrast, to estimate the in-plane lattice parameter, a wz-phase reflections, non overlapping with zb-phase reflections, were chosen. It should be noted that in a single crystal XRD experiment each set of crystallographic planes should produce a pair of reflections corresponding to the Cu $K\alpha_1$ and $K\alpha_2$ X-ray emission doublet. The estimated position of Cu Kα-doublet diffraction reflections for InP and InAs is marked by solid and dashed rugs in Figures S **XRD** (b) and (c).

The corresponding pair of reflections is well-resolved for the InAs NW sample. On the other hand, for the InAsN / InP core / shell NW sample, the reflections are significantly broadened. We attribute this to the composition inhomogeneity of the NW array. Since the incorporation of nitrogen is accompanied by a decrease in the lattice parameter, the Bragg reflections of InAs in the InAsN / InP core / shell NW sample are shifted to larger diffraction vector values compared to the pristine InAs NW sample. For the InAsN / InP core / shell NW sample, in addition to the Bragg reflections of InAsN, diffraction reflections located at larger diffraction vector values corresponding to the InP shell are also present. The position of the observed Bragg reflections of InP corresponds to a relaxed lattice.

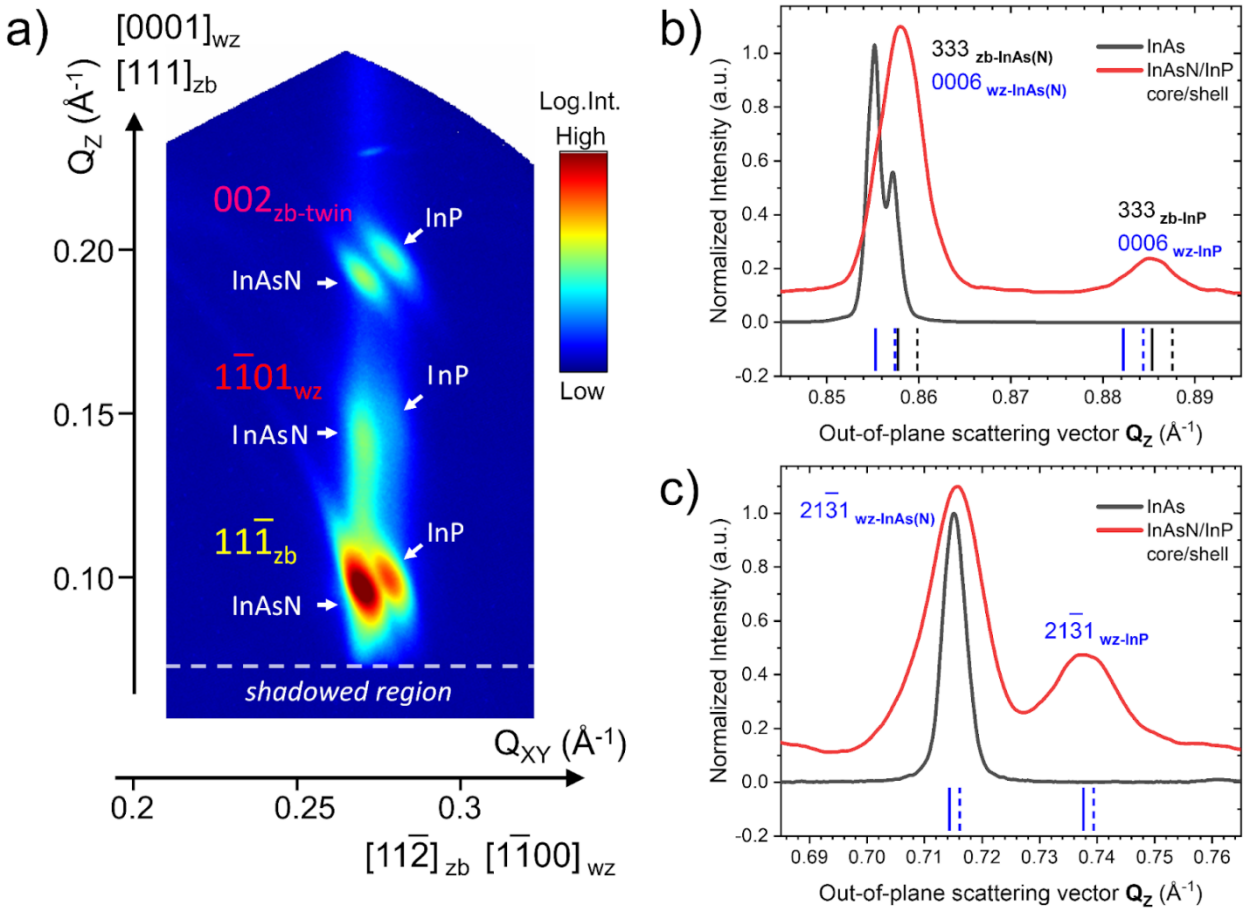

Figure S **XRD.** Normalized XRD intensity profiles in the out-of-plane (a) and in-plane (b) directions for symmetric (a) and asymmetric (b) Bragg reflections of the InAs (dark gray line) and InAsN / InP core / shell NW samples. c) 2D cross section of XRD-RSM taken in the vicinity of the <-1-100> Bragg reflection of the WZ-phase of InAs(N). White arrows indicate the Bragg reflections corresponding to the InAs(N) and InP materials. Bright 002 and 11-1 Bragg reflections of the cubic ZB phase and its rotational twin are visible. XRD-RSM is presented in logarithmic intensity scale.