X-ray Reciprocal Space Mapping of Dense Arrays of Heterostructured III-V Nanowires

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Arrays of vertically standing III-V nanowires (NWs) and related (radial/ vertical) heterostructures find potential applications in the photovoltaic[1,2] and photonic fields.[3] Analysis of such arrays by X-ray diffraction allows to probe million-to-billion of NWs altogether on the same sample. Observed diffraction patterns are expected to depend on the NW inner structure and the (NW-to-NW) size/compositional fluctuations associated with the growth process.

In this work we present a theoretical and experimental study of X-ray scattering from dense arrays of crystalline AlGaAs and GaAs-AlGaAs core-shell NWs grown by MOVPE. The scattering model is based on the kinematical diffraction theory. The model is suitable for the simulation of both high-resolution X-ray diffraction patterns (double-crystal diffraction scheme) and X-ray reciprocal space maps (RSMs).

For sake of simplicity, we considered the NWs having a cylindrical shape and use the appropriate and well-known form factor of the radial component expressed by the first-order Bessel function.[4,5] In general, diffraction simulation models for NWs consider only symmetrical diffraction schemes to analyze and evaluate the NWs average strain state along their axis, i.e., along the NW growth direction.[3] However, in order to precisely measure and evaluate the axial strain state, it is necessary to use asymmetric diffraction configurations too. We therefore generalize the scattering model in order to simulate diffraction patterns and RSMs in symmetric and the asymmetric diffraction schemes. The model was extended to calculate and simulate diffraction patterns of both core-shell and core-multishell NWs. Microstructural and morphological imperfections, such as NW length and diameter variations, NW inclination (tilt angle with respect to the substrate surface), and lattice strain gradients/fluctuations can be easily considered and implemented in the calculations.

$Al_xGa_{1-x}As$ NWs and GaAs/$Al_xGa_{1-x}As$ core-shell NWs were vertically grown on (111)B-GaAs substrates by Au-catalyst-assisted metalorganic vapour phase epitaxy (MOVPE),[6,] with typical length of 1000–5000 nm and diameters of 100–300 nm. Typical surface densities of as-grown NWs were in the 10^8–10^9 cm^{-2} range. X-ray scattering measurements were carried out using a laboratory high-resolution X-ray diffractometer equipped with a 4-bounce Bartels Ge monochromator and 3-bounce Ge analyzer crystals. The specific experimental conditions of a laboratory instrument imply reduced coherence length (about 1–2 μm) in the scattering plane. It follows that for our array densities only very few NW (less than 10) are illuminated coherently, and the NW array scattering intensity can be consequently calculated as the sum of the scattering

intensities of the single NWs.

Figure 1a shows the experimental RSM of a unintentional $Al_{0.50}Ga_{0.50}As$/ $Al_{0.30}Ga_{0.70}As$ core-shell NWs array,[7] with an NW average length of about 900 nm, a core diameter of ~50 nm and a shell thickness of ~100 nm. The NWs are in a relaxed state having a lattice mismatch along the [111] direction of about 1.2×10^{-3}. Fig. 1b refers to the best-fitted RSM, assuming a 10% fluctuation (Lorentz statistical distribution) for both the inner core diameter and shell thickness; Fig. 1c and 1d illustrate instead, the (ideal) case of no size fluctuations, and constant (x=y) Al-content in the NW core and shell (uniform $Al_xGa_{1-x}As$ NWs), respectively.

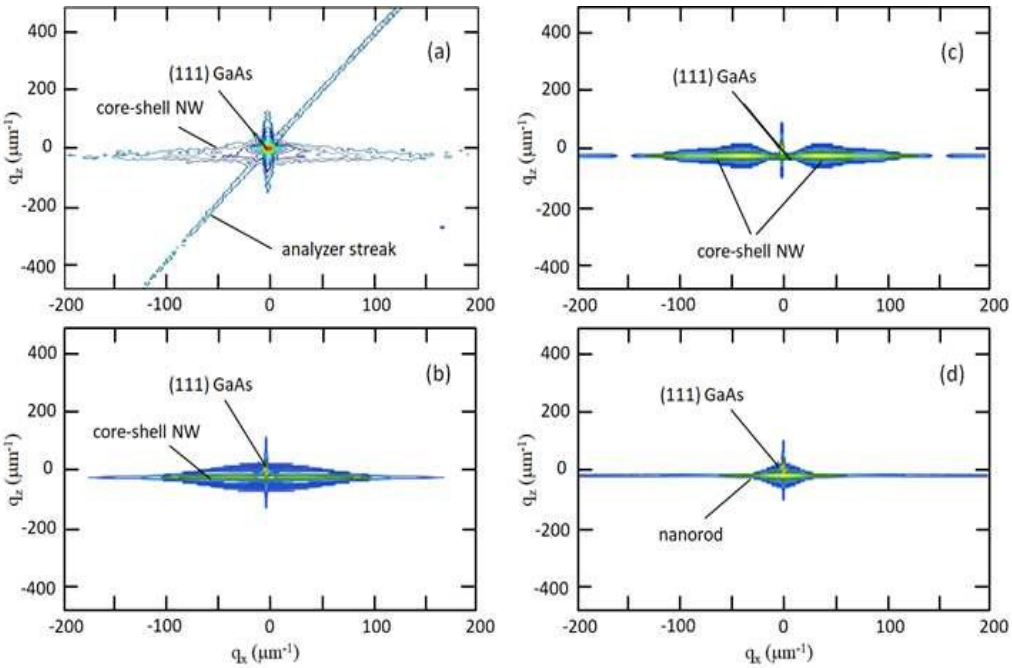

Figure 1: (a) Experimental and (b) calculated RSMs close to the (111)GaAs rlp of an array of core-shell $Al_{0.50}Ga_{0.50}As/Al_{0.30}Ga_{0.70}As$ NWs vertically standing on the (111)GaAs substrate. The RSM in (b) was obtained assuming a core diameter and shell thickness fluctuation of 10%. For comparison, the RSMs calculated for arrays of $Al_xGa_{1-x}As/Al_yGa_{1-y}As$ core-shell NWs having (c) constant diameter, and (d) constant Al-content (x=y) are also shown.

***References**:*

[1] P. Prete, N. Lovergine, *Progr. Cryst. Growth Character. Mater.* **2020**, 66, 100510. https://doi.org/10.1016/j.pcrysgrow.2020.100510

[2] A. Cretì, P. Prete, N. Lovergine, M. Lomascolo, *ACS Appl. Nano Mater.* **2022**, 5, 18149-18158. https://doi.org/10.1021/acsanm.2c04044

[3] P. Prete, D. Wolf, F. Marzo, N. Lovergine, *Nanophotonics* **2019**, 8, 1567–1577. https://doi.org/10.1515/nanoph-2019-0156

[4] V.M. Kaganer, M. Wölzr, O. Brandt, L. Geelhaar, H. Riechert, *Phys. Rev. B*, **2011**, 83, 245321.

[5] V.P. Kladko, A.V. Kuchuk, H.V. Stanchu, N.V. Safriuk, A.E. Belyaev, A. Wierzbicka, M. Sobanska, K. Klosek, et al., *J. Cryst. Growth*, **2014**, 401, 347-250. http://dx.doi.org/10.1016/j.jcrysgro.2014.01.042

[6] P. Paiano, P. Prete, E. Speiser, N. Lovergine, W. Richter, L. Tapfer, A.M. Mancini, J. Cryst. Growth **2007**, 298C, 620-624. https://doi.org/10.1016/j.jcrysgro.2006.10.107

[7] B. Buick, E. Speiser, P. Prete, P. Paiano, N. Lovergine, W. Richter, *Phys. Status Sol. (b)* **2010**, 247, 2027–2032. https://doi.org/10.1002/pssb.200983948

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