An approach for Analyzing 3D Strain Distribution in Hybrid and Hetero Nanowires through NBED and FEM Iterative Model Fitting

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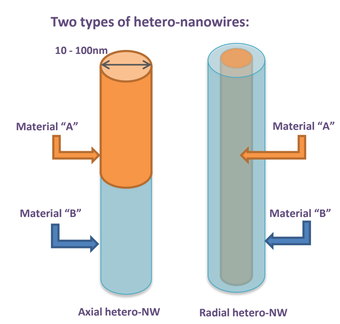
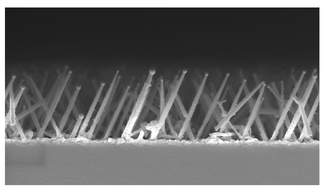
Highly Strained Semiconductor Nanowires



- Extremely high surface to volume ratio
- Ability to obtain defect-free structures even on highly mismatched substrates

Applications:
- Various sensing applications
- Nanoscale optoelectronics and photonics
- Micro- and Nano-Electro-Mechanical Systems
- Transistors …

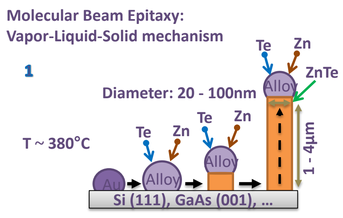
- strain changes electronic properties of the core and the shell
- **higher level of elastic strain without defects formation can be reached, comparing to 2D epilayers**
- **Thanks to surface energy**

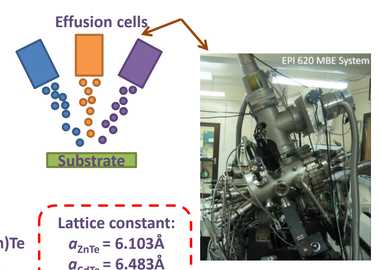


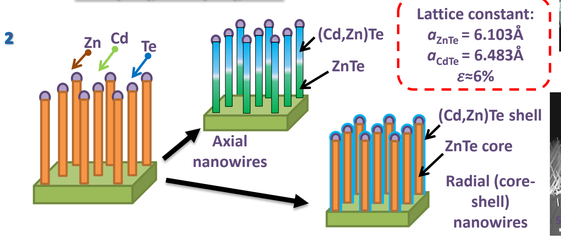
SEM image of ZnTe nanowires on Si substrate

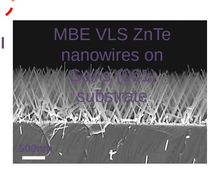
Fabrication of ZnTe/(Cd,Zn)Te hetero-nanowires

Molecular Beam Epitaxy:
Vapor-Liquid-Solid mechanism





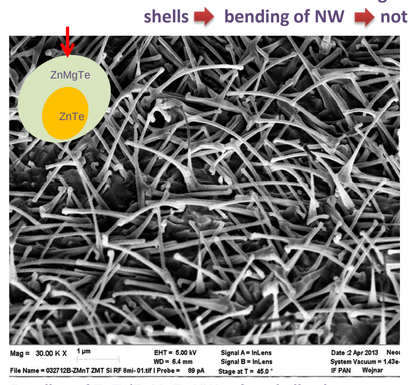




MBE Nanowires Piotr Wojnar at IP-PAS

Strain engineering

Directional flux of elements and shadowing effect in MBE ➡ asymmetric thickness of the shells ➡ bending of NW ➡ not symmetrical strain distribution



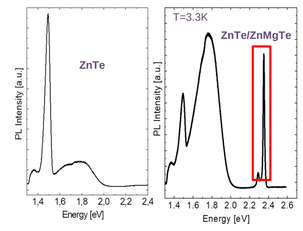
Bending of ZnTe/ZnMgTe NWs after shell epitaxy

P. Wojnar, et al., Nanotechnology 24, 365201 (2013).

STRAIN AND BANGAP ENGINEERING EXAMPLE

Activation of emission from ZnTe core at 2.35 eV (2.39 eV - free exciton in ZnTe)

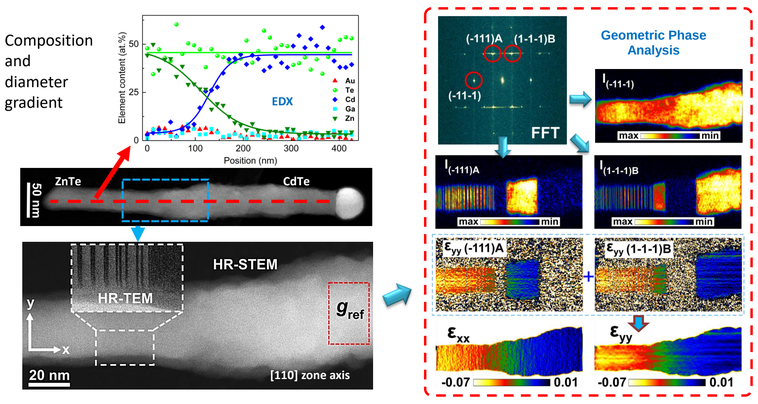
explanations: - **tensile strain – misfit MgTe/ZnTe ~5.4%!**



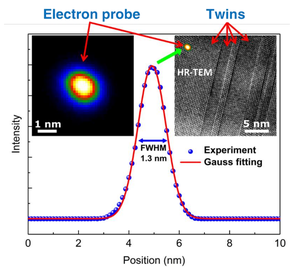
How we can experimentally determine the 3D strain state in individual bended core-shell NW?

Geometric Phase Analysis (GPA) nano-twinned axial hetero-nanowire

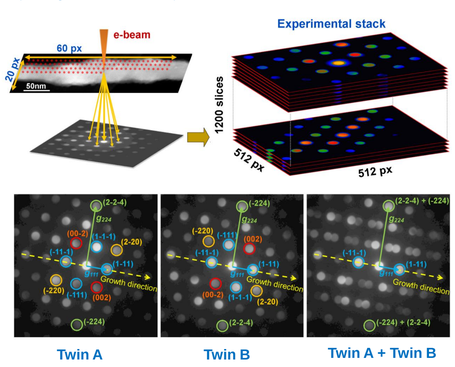
Composition and diameter gradient



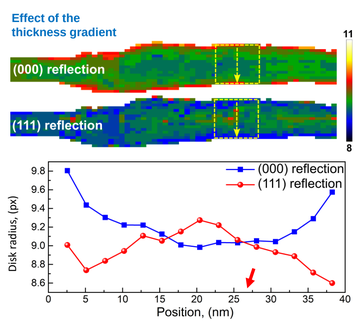
Nano Beam Electron Diffraction (no precession)



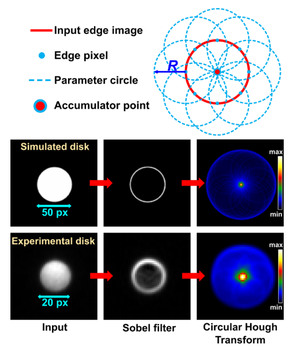
$$\varepsilon_{hkl}^{rel} = \frac{|g_{hkl}^{ref}| - |g_{hkl}^{exp}|}{|g_{hkl}^{exp}|}$$



Circular Hough transform for solving disk size variation issue

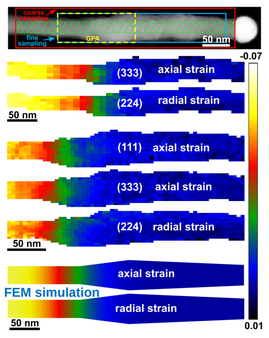


The thickness gradient in NW affect on diffracted intensities. This may lead variation of diffracted disk radius.
CCD scyntylator

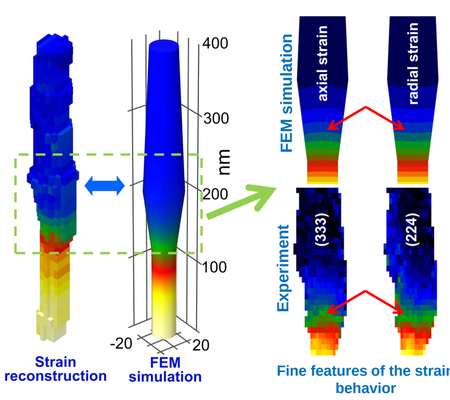


Circular Hough transform (CHT) with variable radius solves the problem of the variation of the disk radius

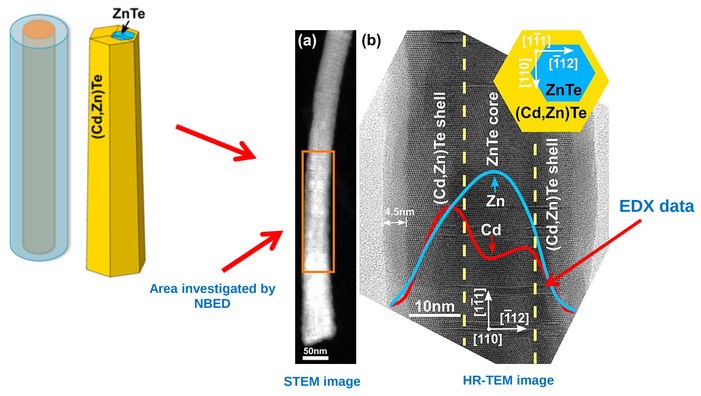
NBED-strain: assumption of radial symmetry



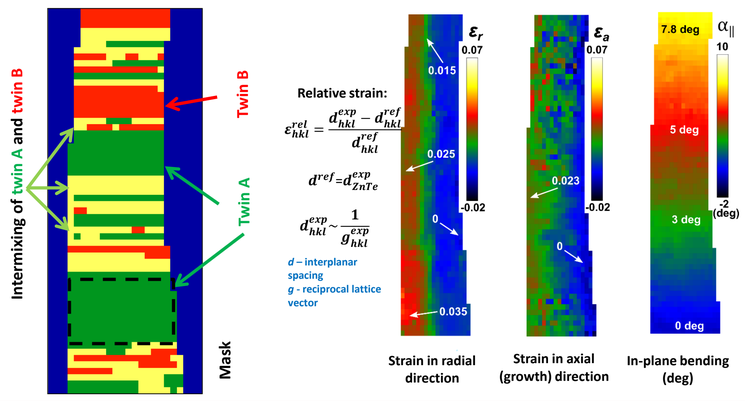
Experimental and projected maps of relative strain obtained by COMSOL simulation



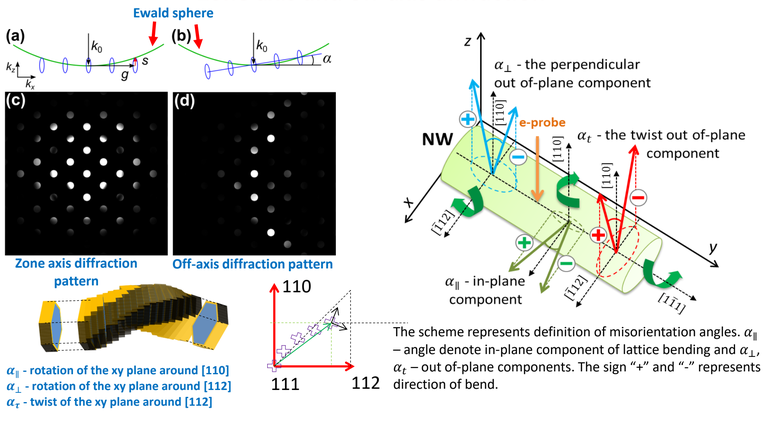
Radial hetero-nanowire: ZnTe core, CdZnTe shell



STEP I Projected Strain mapping



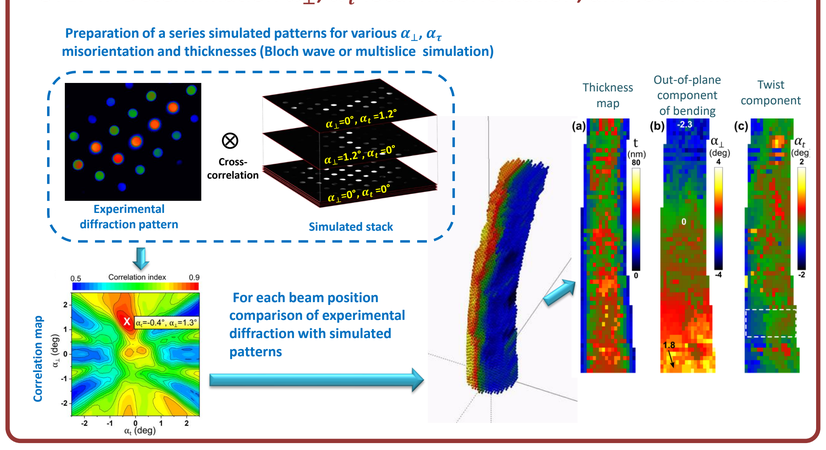
Zone axis and off-axis diffraction



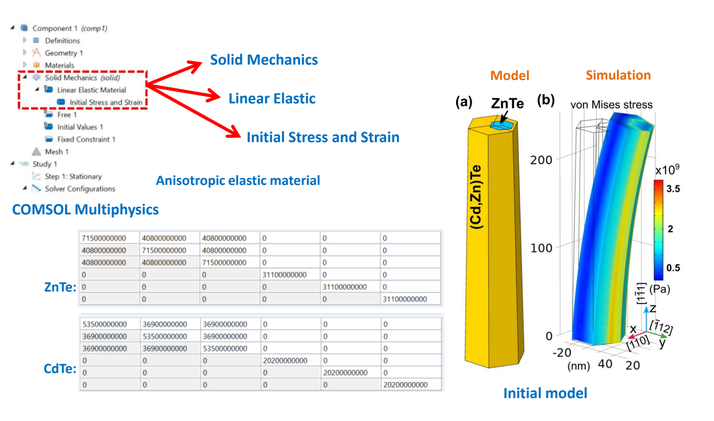
$\alpha_{||}$ - rotation of the xy plane around [110]
$\alpha_\perp$ - rotation of the xy plane around [112]
α_τ - twist of the xy plane around [112]

STEP II Determination $\alpha_\perp$, α_τ local misorientation, and local thickness

Preparation of a series simulated patterns for various $\alpha_\perp$, α_τ misorientation and thicknesses (Bloch wave or multislice simulation)



FEM modeling of core-shell hetero-nanowires



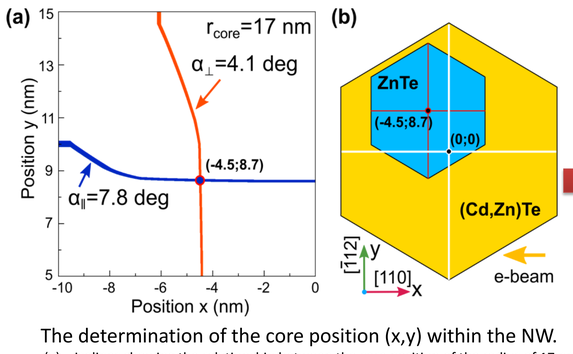
STEP III: Iterative Fitting of FEM and experimental maps

We have:
- Asymmetrical core-shell configuration
- Core -> ZnTe
- Shell -> $Cd_xZn_{1-x}Te$
- Radius of whole c-s the NW

We still need:
- Cd content in the shell?
- Core radius?
- Core position in the NW (x,y)?
- And we make same additional assumption that the taper of the core is the same as the nanowire

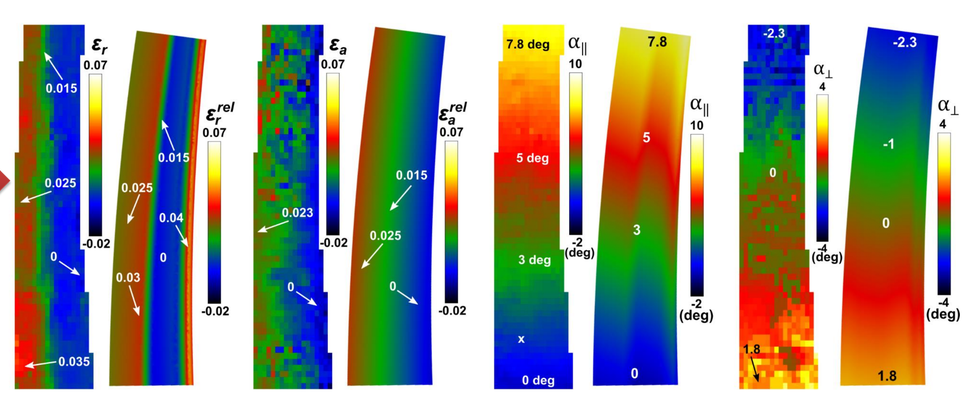
1. Finding Cd content in the shell:
Fitting only *min* and *max* strain values on experimental and simulated ε_r maps.
Min and *max* values on ε_r map depend mainly on chemical composition but not on the radius and position of the core.
2. Finding the core positions within the NW (*x,y*):
- **Performing FEM simulation for different core position (*x,y*) for each core radius r.**
- **Finding which (*x,y*) positions correspond experimental in-plane $\alpha_{||} = 7.8$ deg and out-of-plane bending $\alpha_\perp = 4.1$ deg of the NW. > For each core radius r we obtained (*x,y*) positions that that correspond experimental bending angles: r(*x,y*)**

3. Finding the core radius r:
Comparing of the FEM simulated ε_r maps for defined above core parameters r(*x,y*) to the experimental map.
This is possible due to the sharp transition region on the ε_r map.

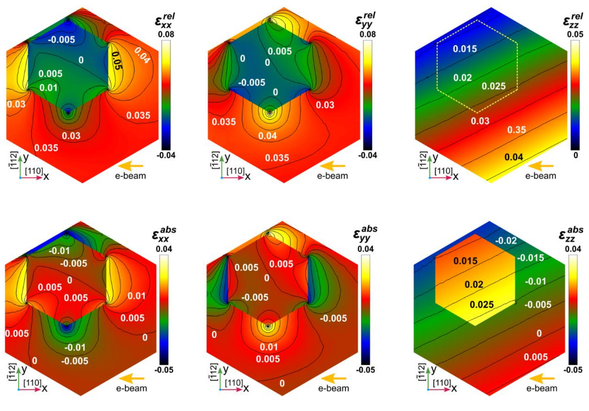


The determination of the core position (x,y) within the NW.
(a) – isolines showing the relationship between the core position of the radius of 17 nm in the NW and bent angles $\alpha_{||}$ (blue line) and $\alpha_\perp$ (red line).
Those lines' intersection corresponds to the bent NW's core position.
(b) – the scheme of the asymmetric core-shell NW.

Comparison best fit FEM simulation and experimental results



Cross-section of best fit simulated core-shell NW ➡ quasi/pseudo-Tomography from one projection ➡ limited radiation damage, the same object structure



$$\varepsilon_{ZnTe}^{rel} = \frac{d_{ZnTe}^{core} - d_{ZnTe}^{teor}}{d_{ZnTe}^{teor}}$$

$$\varepsilon_{CdZnTe}^{rel} = \frac{d_{CdZnTe}^{shell} - d_{ZnTe}^{teor}}{d_{ZnTe}^{teor}}$$

Absolute strain calculated in terms of relaxed ZnTe core and $Cd_{0.57}Zn_{0.43}Te$ shell values

Summary

- Improved algorithm for the detection of the centres of diffraction disks based on the Sobel filtering and Hough transform suitable to CCD cameras and high thickness gradient (GMS script Sobel+Hough + nano-twin filter)
- We demonstrate the method for the 3D strain reconstruction in the core-shell NW with sub-nanometer spatial resolution based on single zone axis diffraction.
- Object conservation due to limited dose, for radiation sensitive materials
- Full dynamic simulations are needed

REFERENCES
S. Kryvyi, S. Kret and P. Wojnar, Precise strain mapping of nano-twinned axial ZnTe/CdTe hetero-nanowires by scanning nanobeam electron diffraction. *Nanotechnology*, **33**(19), 195704, (2022)
S. Kryvyi, S. Kret, J. Domagała and P. Wojnar, Reconstruction of three-dimensional strain field in an asymmetrical curved core-shell hetero-nanowire. *Nanotechnology* 34 (44), 445705, (2023)

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