SIMULATION OF DISPLACEMENT FIELDS IN THE INP NANOWIRE. COMPARISON WITH X-RAY BRAGG PTYCHOGRAPHY RECONSTRUCTIONS.

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1.Introduction

The nanowires are perspective for the different directions of research. Due to the band structure of nanowires they are good semiconductors, and their microscopic size means that manufacturers could fit millions more transistors on a single microprocessor. As a result, computer speed would increase dramatically. Also the nanowires will improve the energy efficiency of solar cells. During the growth procedure formation of the defects and strain fields is possible inside the nanowire. So the quality of the crystals and their optical and electrical properties depends on the properties of their structure.

To investigate internal structure of such extended objects as nanowires we used coherent X-ray diffraction imaging (CXDI) technique [1]. CXDI is a relatively new imaging method that can produce an image of a sample without using optics between the sample and detector. The conventional CXDI experiment is performed with an isolated sample illuminated by a plane wave. The incident wave might be described by a complex field with uniform magnitude and phase. The radiation interacts with the sample, which affects both the amplitude and phase of this field. The scattered radiation from the sample propagates to a two-dimensional (2D) detector in the far field, and the diffracted intensities are measured. The detector can be positioned either in the forward direction, or in the case of a crystalline sample at the Bragg angle positions. The diffracted intensities cannot be directly inversed to real space because the phase information is lost. To retrieve the lost phases a special method ptychography was used [2]. Ptychography is similar to scanning microscopy, where the sample is scanned through the X-ray beam and number far-field diffraction patterns are collected from each point of the sample scanned. Importantly, the illuminated regions should overlap in the sample plane. The relationship between each scan point is used to reconstruct the exit surface wave.

To have a better understanding of results that we get from ptychographical reconstructions we performed simulations of the X-ray diffraction on InP nanowire.

2. Samples modeling

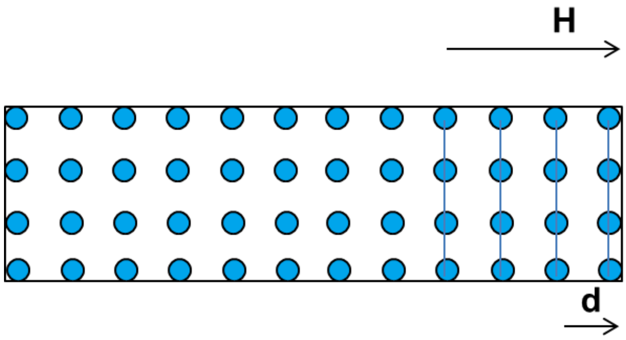


Figure 1. Sketch of the sample. **H** is the reciprocal lattice vector in 111 direction; d is interplanar spacing along **H** direction.

First, the atomic model of ideal crystal of the InP nanowire was obtained. The growth direction of the nanowire is collinear with the 111 crystalline direction for the zinc-blende structure of InP.

Modulus of the reciprocal lattice vector is related with the d as following:

$$|\boldsymbol{H}_{111}| = \frac{2\pi}{d}$$

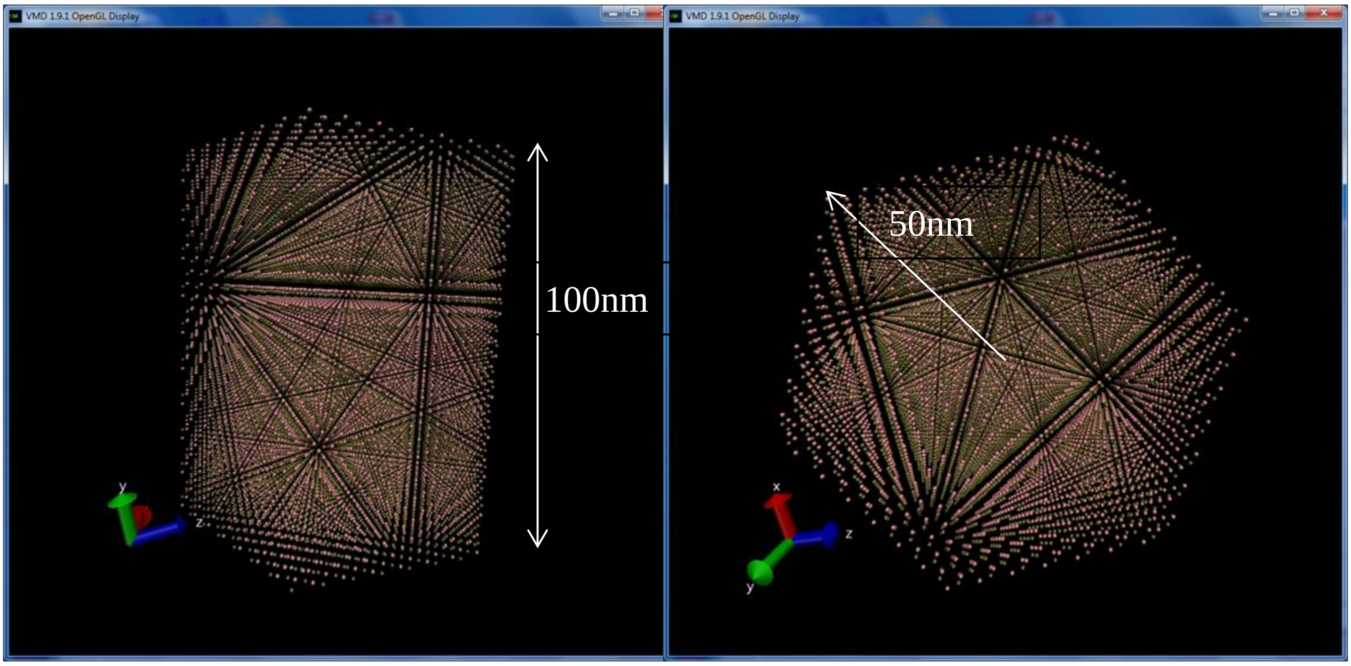


Figure 2. Two views of the generated crystal from side and from the top respectively (VMD software package).

direction.

Crystal of InP is face-centered cubic lattice, when **H** is parallel to the diagonal this cube.

Parameters of our sample: height 100 nm, radius 50 nm, interplanar spacing 3.38Å, unit cell constants (Å) : 5.8687 , 5.8687 , 5.8687.

The second model of the InP crystal includes a displacement field in some localized region.

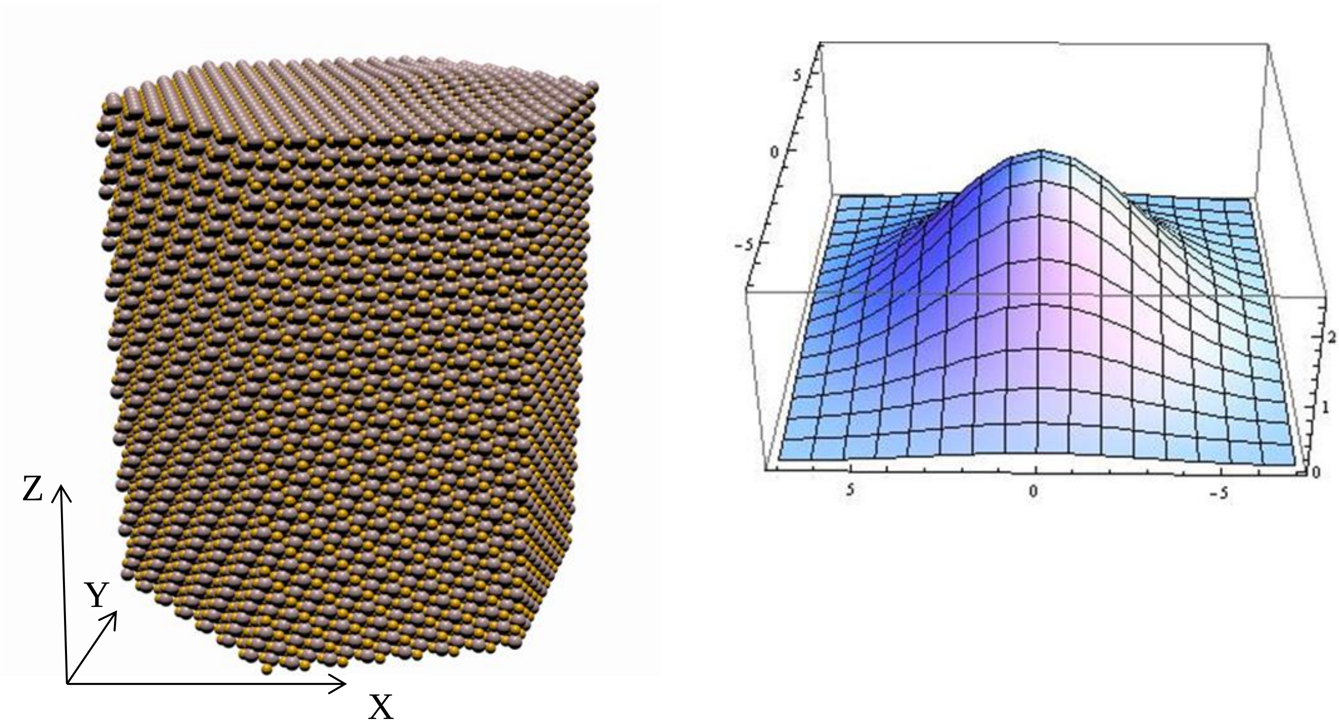


Figure 3. Model of sample with displacement

Distributions of dismplacement in the sample was set this equation with Gaussian distribution

$$d = d_0 + U_{\max} \cdot e^{\frac{(-x-\mu x)\hat{}2}{2\sigma x\hat{}2}} \cdot e^{\frac{(-y-\mu y)\hat{}2}{2\sigma y\hat{}2}}$$

U_{max}-maximum of displacement = 2.5Å.

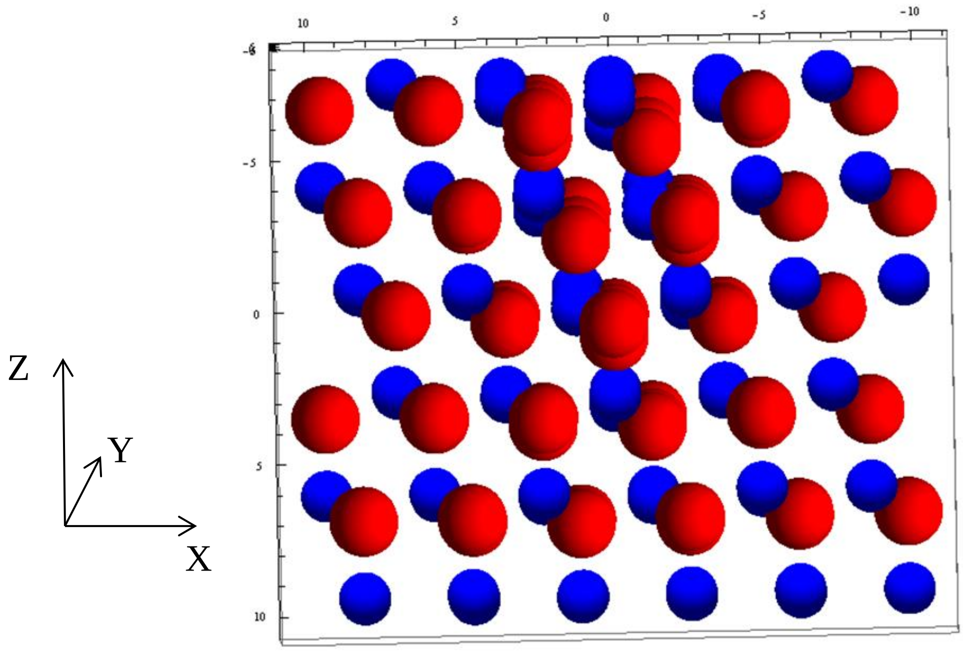


Figure 4. Model of sample with new displacement (Wolfram Matematica software)

Distributions of displacement in the sample was set this equation

$$d = d_0 + Umax \cdot e^{\frac{(-x-\mu x)^2}{2\sigma x^2}} \cdot e^{\frac{(-y-\mu y)^2}{2\sigma y^2}} \cdot e^{\frac{(-z-\mu z)^2}{2\sigma z^2}}$$

We want to get displacement with changing vector ***d.***

Was made simulation of last sample with given displacement

$$d = d_0 + Umax \cdot e^{\frac{(-z-\mu z)^2}{2\sigma z^2}}$$

3. Diffraction patterns simulation.

We used scheme of experiment in Bragg geometry. Beam illuminated the sample. Beam was reflected at the Bragg angle and diffraction patterns were recorded at the detector.

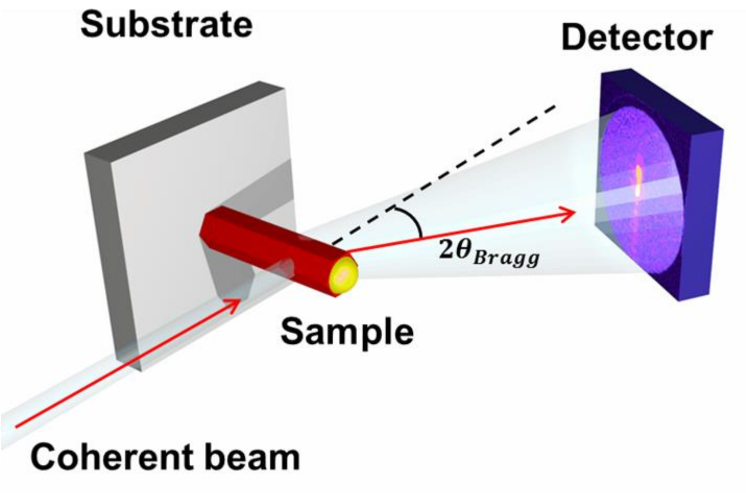


Figure 5. Scheme of experiment

Parameters of Gaussian beam: full width at half maximum 100*100nm, energy 15.25 keV, Bragg angle 6.89 degree.

Parameters of detector: the number of pixels 896x896, distance to detector 2.3 m, the rotation of detector 13.78 degree.

As result we obtained diffraction pattern of single Bragg reflection [Fig.6.].

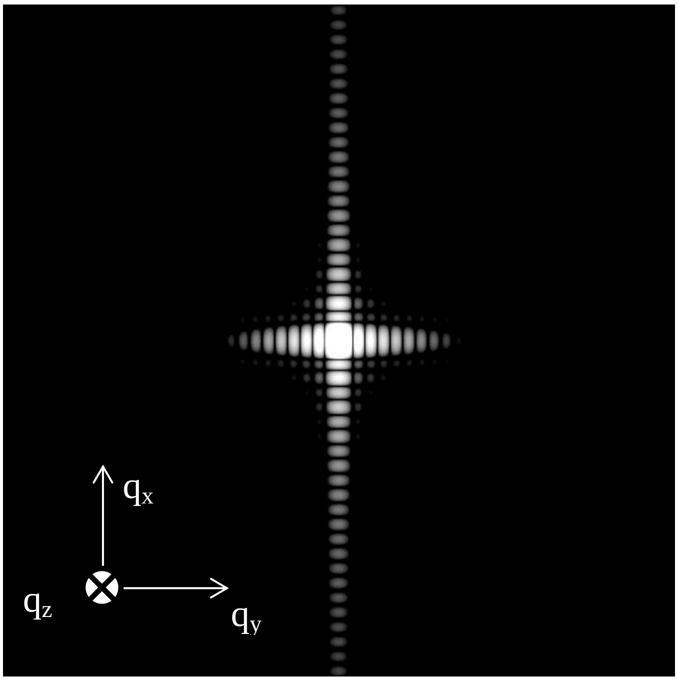


Figure 6. Diffraction from ideal crystal q_x and q_y are vector in reciprocal space.

Vectors in reciprocal space collinear vectors in the real space. The horizontal line corresponds to long part of sample and the vertical line corresponds to short part of sample. [3]

To understand how diffraction image changes, we have made difference between ideal and strained crystal.

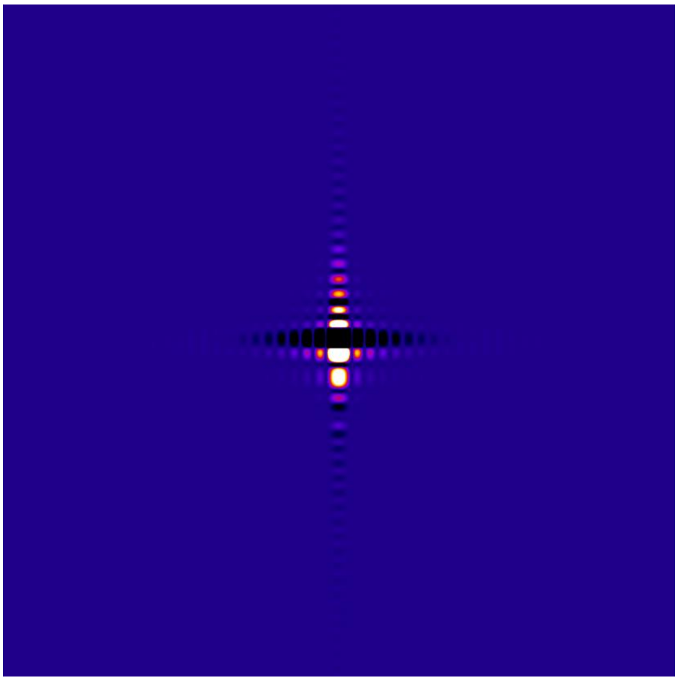


Figure 7. Difference between diffraction patterns from ideal and strained crystal

The phase ramp in the vertical direction in the real space leads to the shift of the intensities on the diffraction image in the same direction.

4.Ptychography simulations

By means of ptychography we can reconstruct the phases of the samples of various sizes.

For the reconstruction of phase we need to set the **U** vector is the vector of displacement, because

$$\varphi = \boldsymbol{H}_{111} \cdot \boldsymbol{U}$$

$$\boldsymbol{U} = \boldsymbol{d} - \boldsymbol{d}_0$$

$\boldsymbol{d}_0$-is the initial distance between atoms, $\boldsymbol{d}$ –is the final distance between atoms .

The next step was ptychography.

We have made 4x4 scanning.

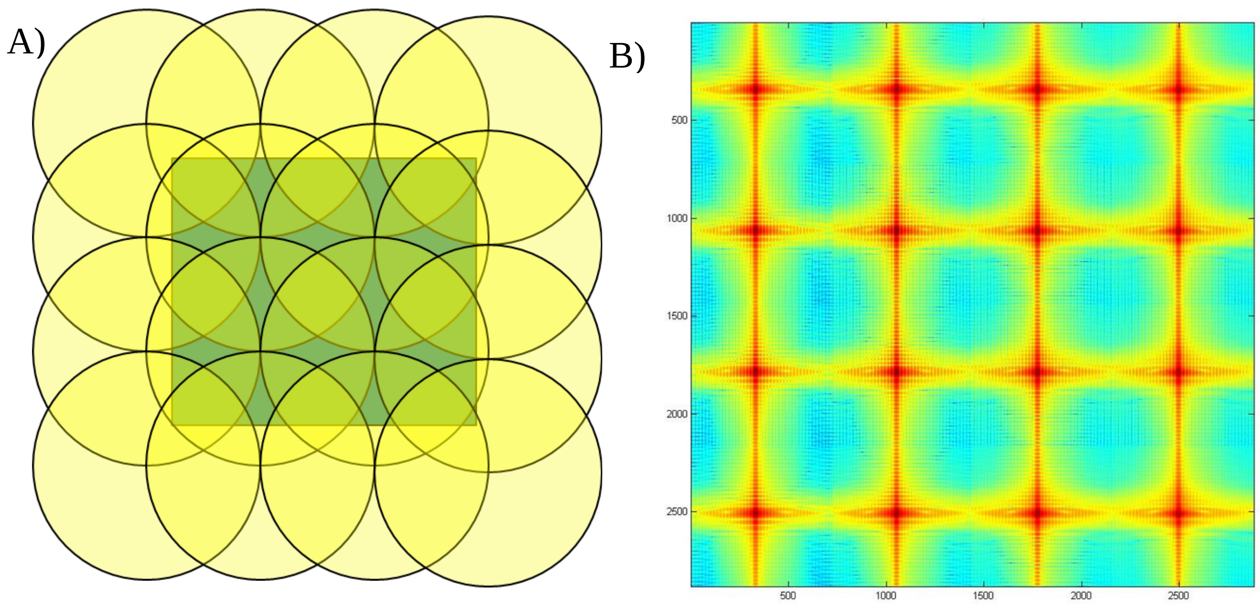


Figure 8. A) positions of probe during scan procedure B) Diffraction map of scan

FWHM 80nm; overlap 40nm; first position of scan (-60nm,60nm)

After that we could to do ptychography reconstruction

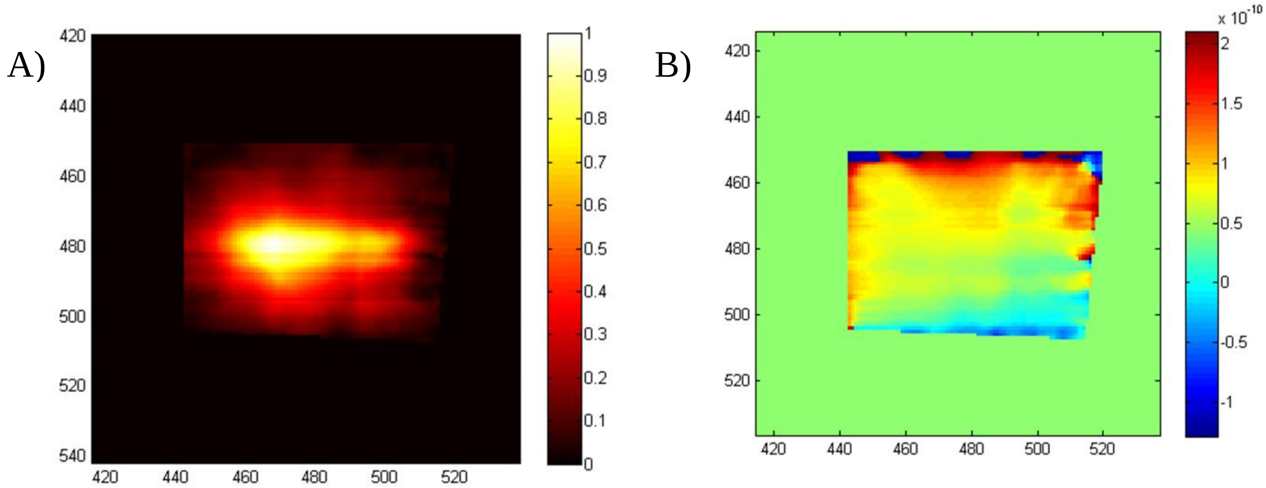


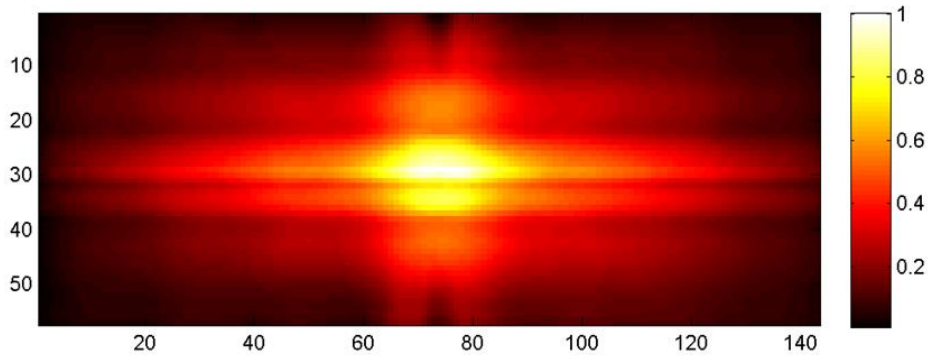
Figure 9. Result of ptychographical reconstruction

A) Distribution of amplitudes ; B) Distributions of displacement

In these pictures we can see the gradient of the displacement and that maximum of amplitudes corresponds to given maximum.

Scanning grid of 6x6 was measured.

A)



B)

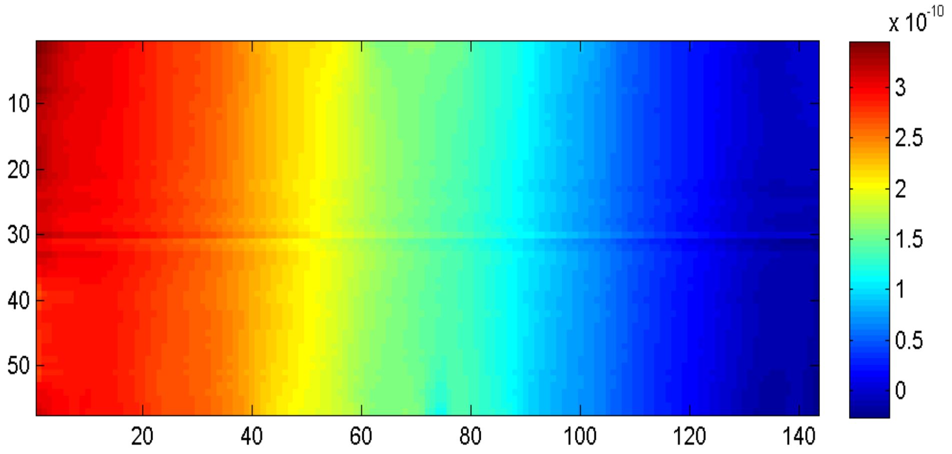


Figure.10 Result of ptychographical reconstruction.

A) Distribution of amplitudes ; B) Distributions of displacement

These are reconstruction have shown that changing of displacement was changed the phase. And the maximum in distribution of displacement corresponds to the maximum of displacement in my model.

5.Conlusions

As result in this work it was done the three simulations of nanowires and two modulations of diffraction and in the end ptychography reconstructions.

References

[1] Vartanyants IA, Pitney JA, Libbert JL, Robinson IK (1997) Reconstruction of surface morphology from coherent X-ray reflectivity, Phys Rev B, 55, 13193–13202.

[2] Yefanov OM, Zozulya AV, Vartanyants IA, et al. (2009) Coherent diffraction tomography of nanoislands from grazing-incidence small angle X-ray scattering, Appl Phys Lett, 94, 123104.

[3] Jens Als-Nielsen , Des McMorrow Elements of Modern X-ray Physics,(2010)