



# Stress State Determination in Nanoelectronic Silicon Devices Coupling COMSOL Multiphysics and a Recursive Dynamical CBED Pattern Simulation

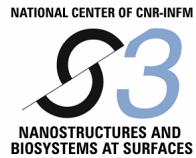
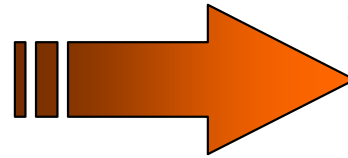
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# Affiliations



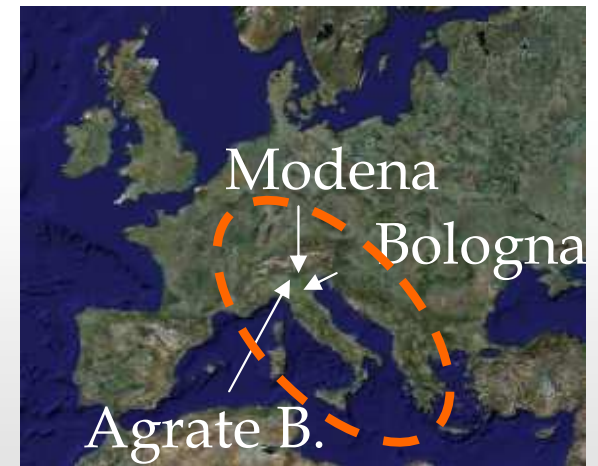
National Research Center S3, INFM-CNR



Department of Physics, University of Modena e Reggio Emilia, Modena (Italy)



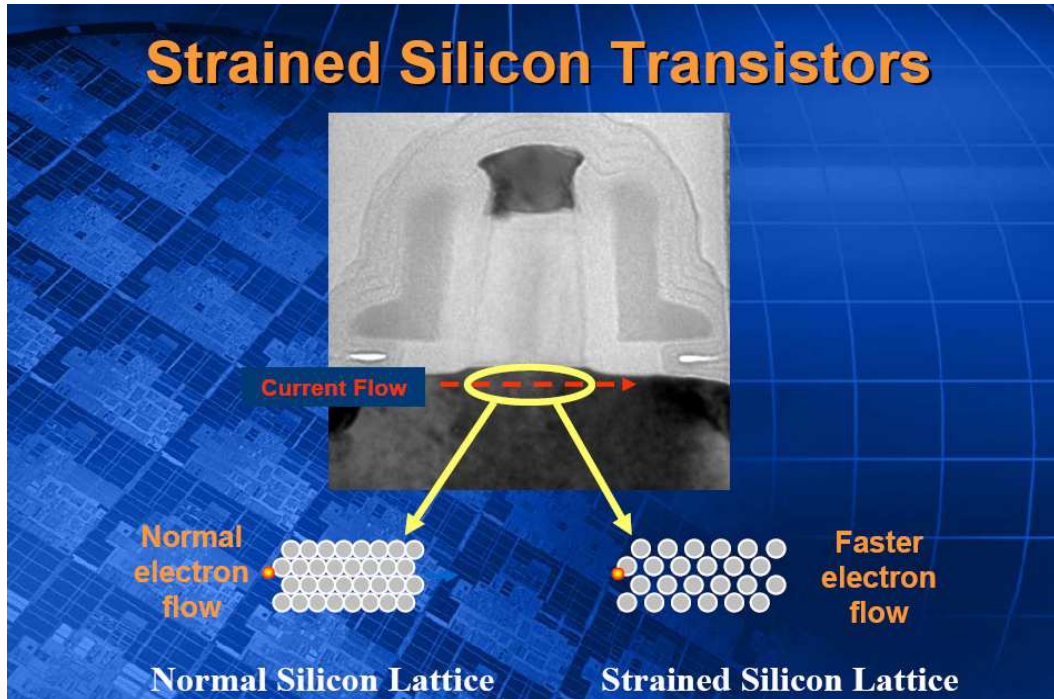
CNR-IMM Section of Bologna (Italy)



# Outlines

- Introduction on stress
- Experimental part
  - CBED/TEM: a powerful strain measurements tool
- Simulation:
  - Dynamical split HOLZ pattern simulation
  - our recursive method
- An example of application: COMSOL+CBED
- Check by a different technique: COMSOL+LACBED
- Conclusions

# Strain: a way to improve the performance of electronic devices



(\*) Examples of Strained-silicon technology applications:

- Extension of the performance of semiconductor transistors
- Power savings benefit
- Reduced device heat generation

**We need methods to map strain at a nanoscale resolution (in order to use it!)**

(\*) Intel site

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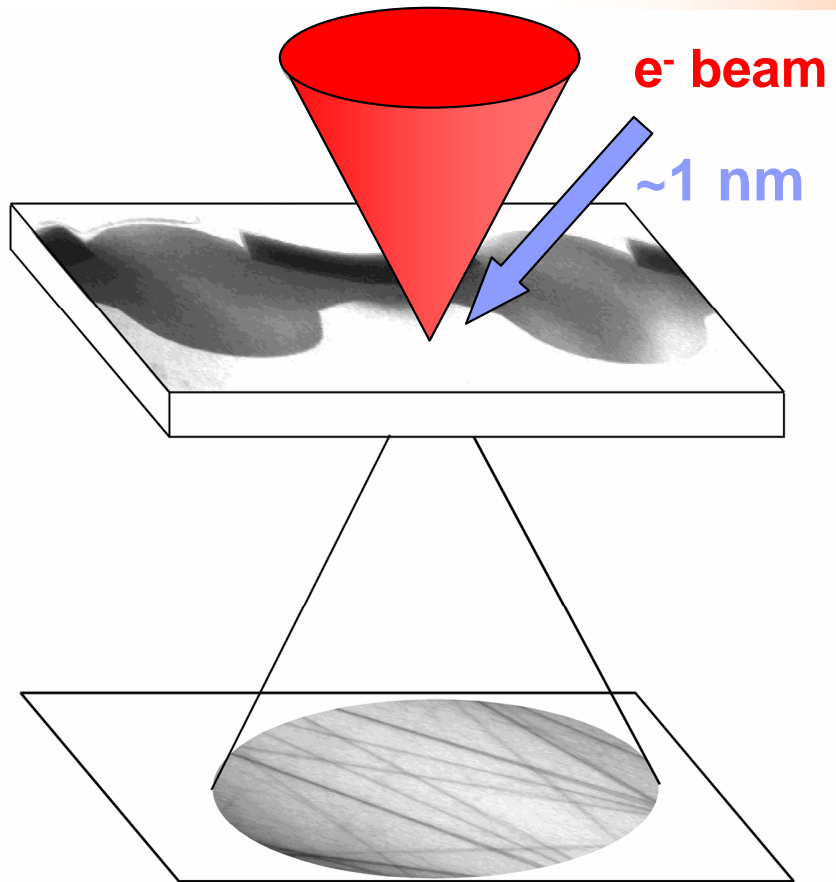
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# CBED/TEM technique

TEM Convergent electron beam

sample

CBED pattern



Central disk  
(transmitted beam)

Zero Order Laue Zones (ZOLZ)



charge distribution

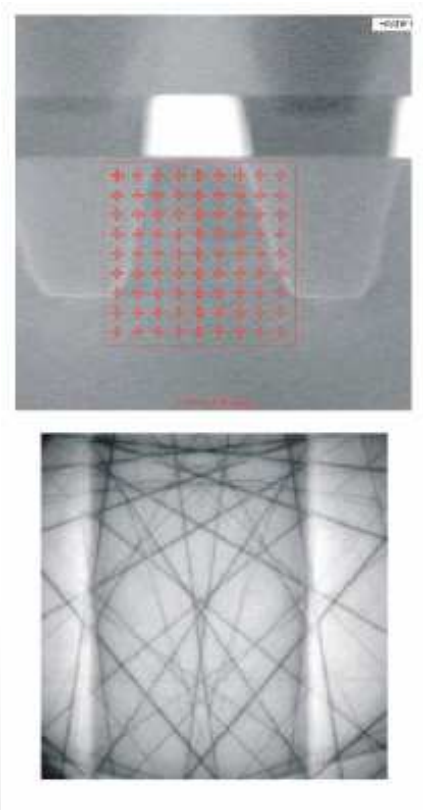
High Order Laue Zones (HOLZ)



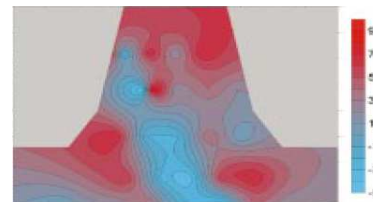
Static disorder & lattice displacement

# CBED: a powerful tool for strain analysis

## STATE OF THE ART: set of patterns analysis



2D strain maps



Determination of the strain tensor in the silicon active regions of deep sub-micron devices with:

- Automatic procedure (no deformation model required)
- very high spatial resolution
- good sensitivity

(\*) Armigliato A, Balboni R, Frabboni S, 2005 *Appl. Phys. Lett.* **86**, 63508

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# The problem of HOLZ line splitting

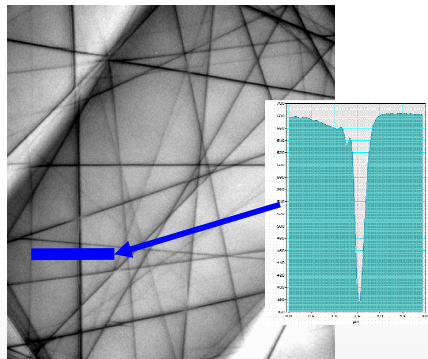
Large strain *gradients* in the electron direction



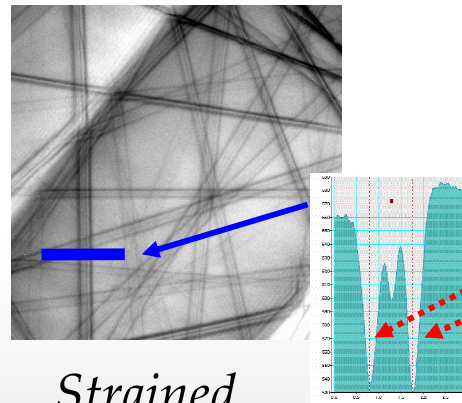
Local *bending* of the lattice planes



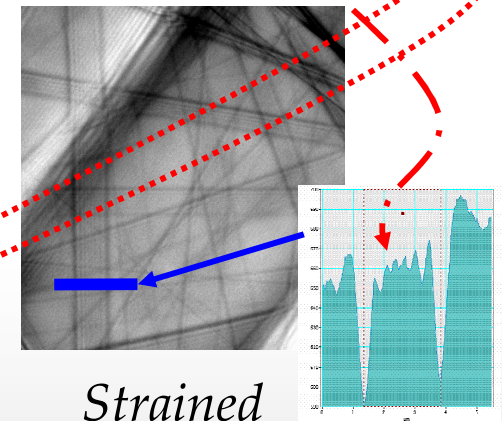
- 1) the HOLZ lines are *SPLIT* in two components
- 2) *INTERMEDIATE FRINGES* can be observed



Undeformed silicon  
HOLZ profile



Strained silicon  
HOLZ profile



Strained silicon  
HOLZ profile

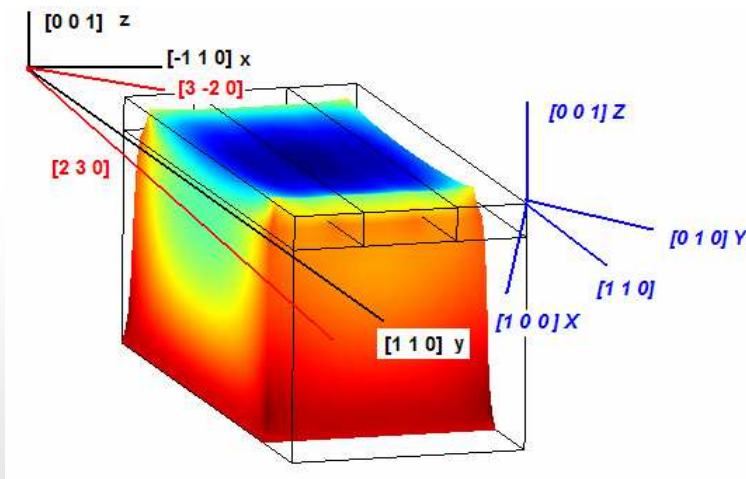


New methods are required

# Split HOLZ pattern recursive simulation (1)

- 1) Parametrized Displacement Field Modelization (from an Analytical Model or Finite Element Method)

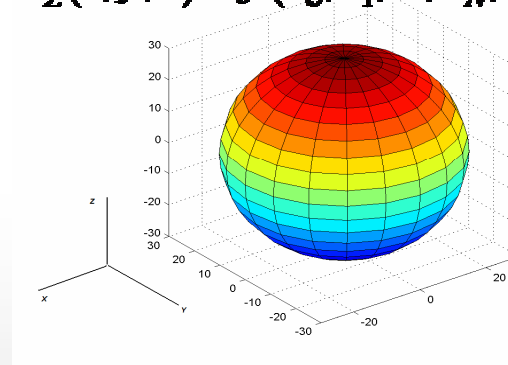
*FE model*



*e.g.: Pseudo-thermal relaxation*

*[example:  $(Si_xGe_{1-x} / Si)$ ]*

*Analytical model*  
 $R_Z(x,y,z) = f(n_0, n_1, \dots, n_N, x, y, z)$



*e.g.: Radial deformation*

*[example: spherical coherent precipitate]*

# Split HOLZ pattern recursive simulation (2)

2) Dynamical simulations (column approximation)

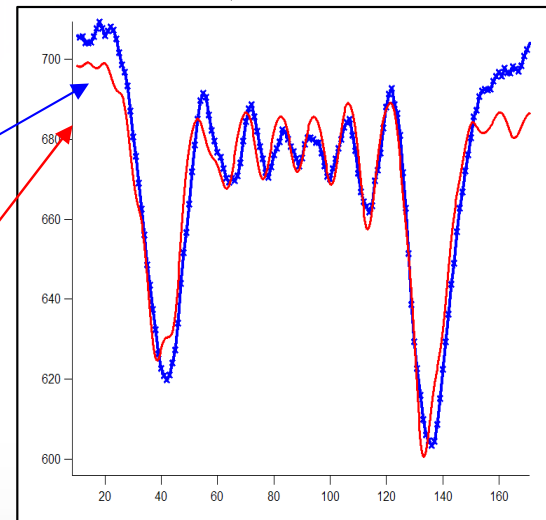
$$\Psi(z) = \prod_{k=1}^s [\mathbf{Q}_k \mathbf{P}_k(z_k) \mathbf{C}_k \gamma_k(t_k) \mathbf{C}_k^{-1} \mathbf{P}_k(-z_{k-1}) \mathbf{Q}_k^{-1}] \cdot \Psi(0) \quad (*)$$

$\uparrow$  Displacement  $\uparrow$

3) Comparison between experimental & simulation pattern (multiple line scan or 2D cross-correlation)

$$\chi^2 = \frac{1}{N-f-1} \cdot \sum_{i=1}^N \frac{(I_i^{(\text{exp})} - cI_i^{(\text{theo})} - I^{(\text{bg})})^2}{\sigma_i^2}$$

*Exp. (Blu) vs Sim. (Red)  
HOLZ Line Profile*



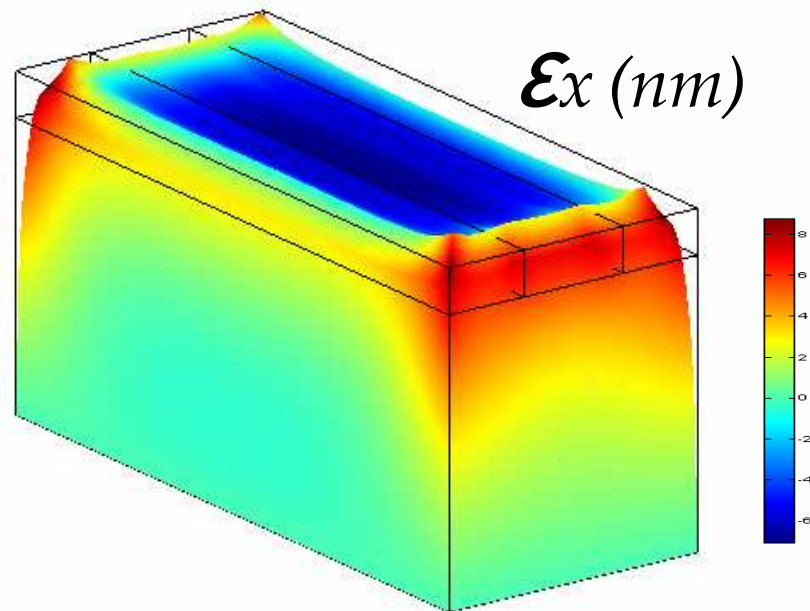
4) **Best Fit** (minimization of  $\chi^2$  with iterative simulation)

(\*) Peng & Whelan Many-Beams Matrix Formulation:  
L.M. Peng and M.J. Whelan, Proc.Roy.Soc. London A  
431, 111 (1990)

# Split HOLZ pattern recursive simulation (3)

DISPLACEMENT FIELD RECONSTRUCTION  
along  $z$  in the  $(x_i, y_i)$  surface point

SAMPLING THE DISPLACEMENT  
FIELD AT DIFFERENT  $(X_i, Y_i)$   
POSITIONS

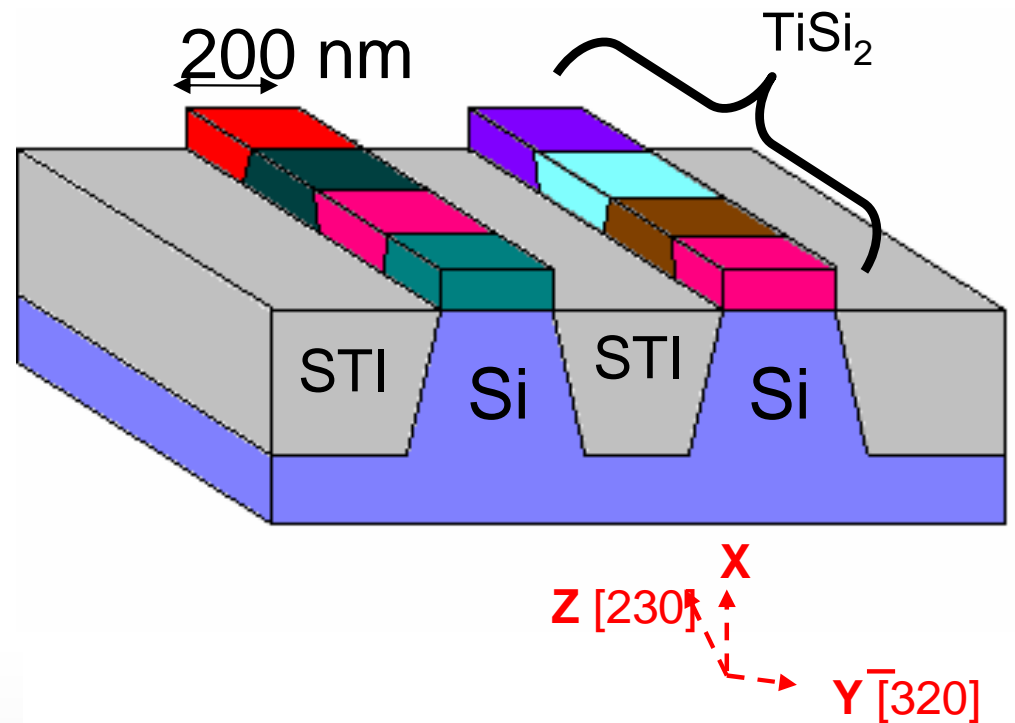
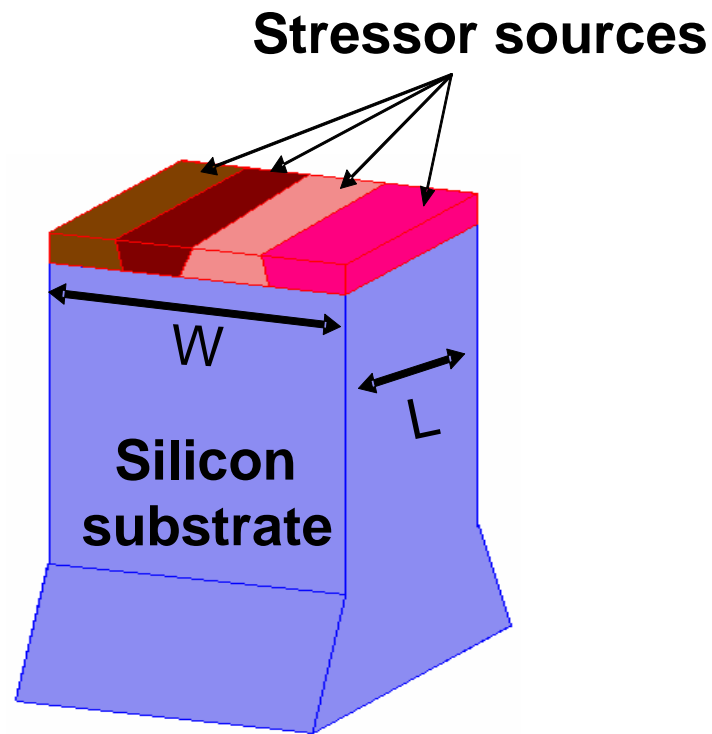


STRAIN FIELD  
MAP

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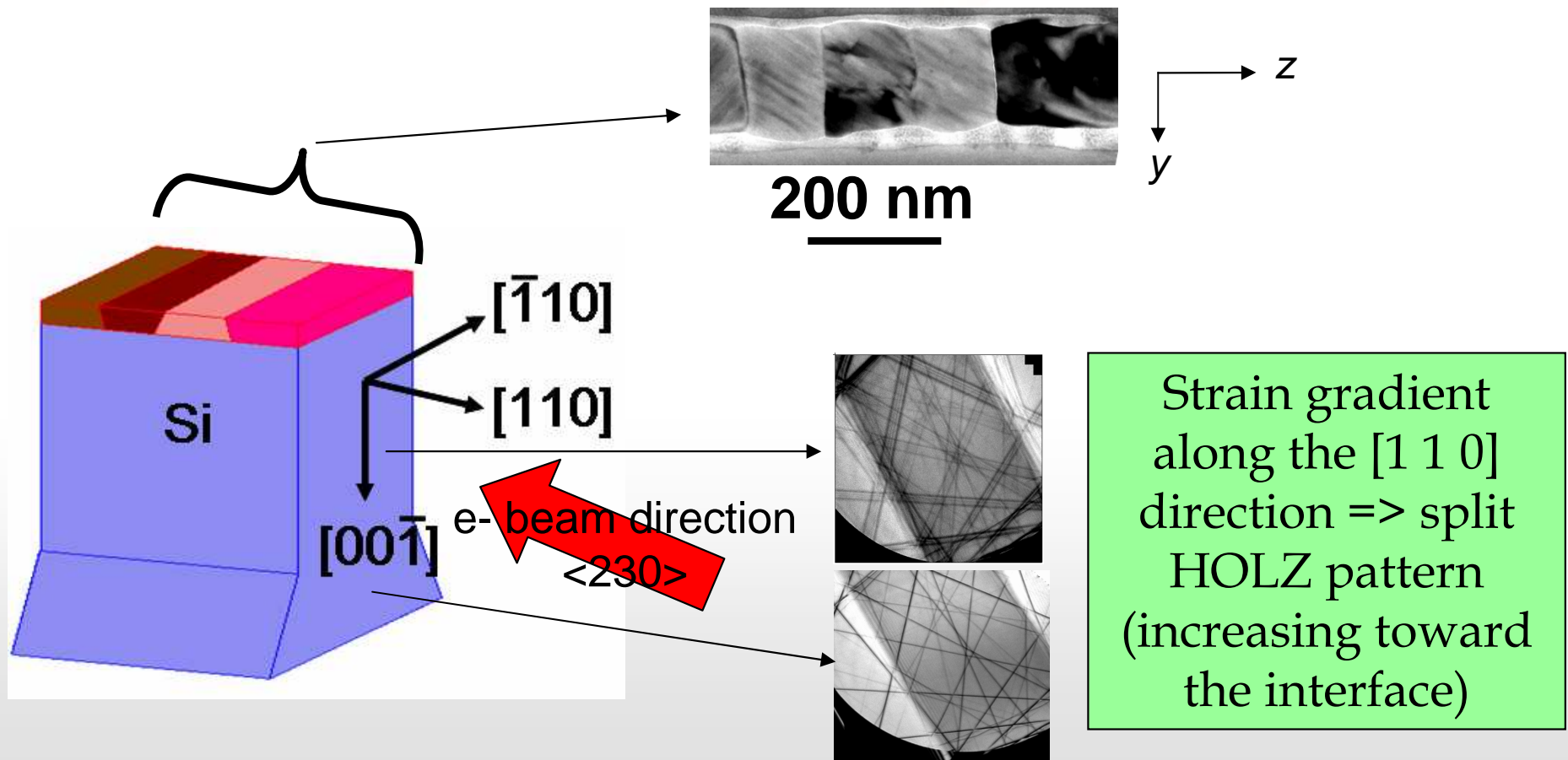
# CASE STUDY



TiSi<sub>2</sub> self-aligned silicides (“salicide”) overlayers onto the 200 nm wide active silicon areas of STI (Shallow Trench Isolation) structures

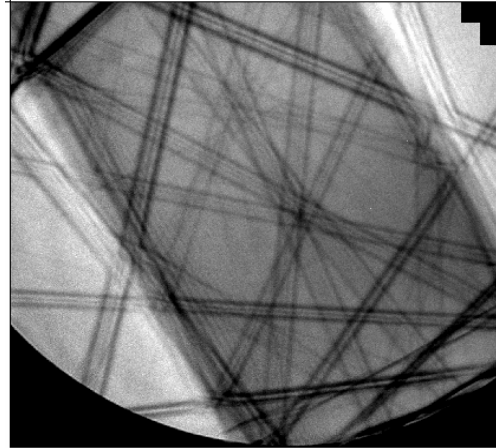
# Experimental Details

Bamboo-like distribution of grain boundaries (grain size:  $\sim 100$  nm)

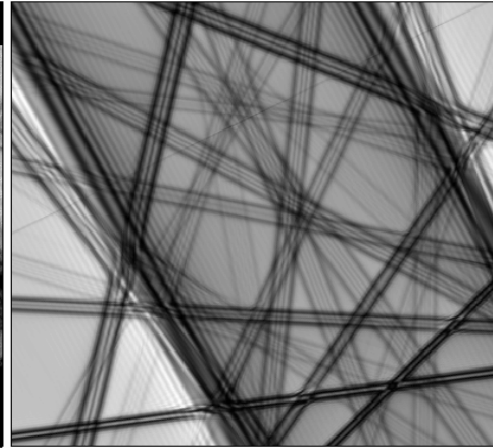


# Results: Example of strained pattern simulations

Z = 150 nm



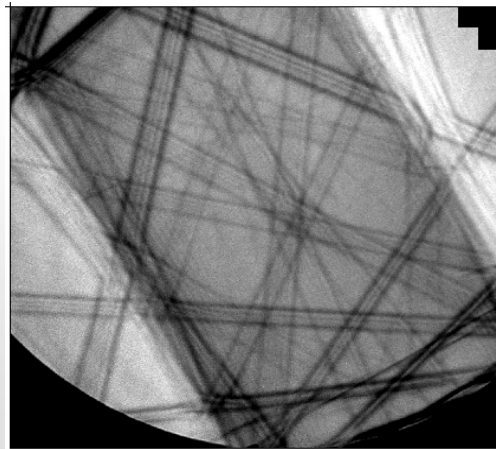
*Exp*



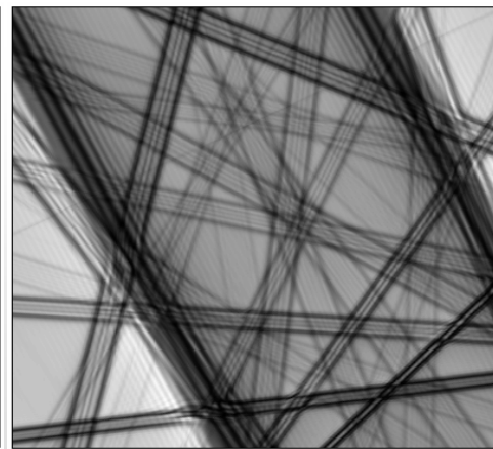
*Sim*

Matching

Z = 110 nm



*Exp*

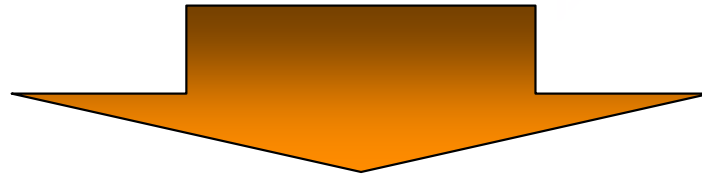


*Sim*

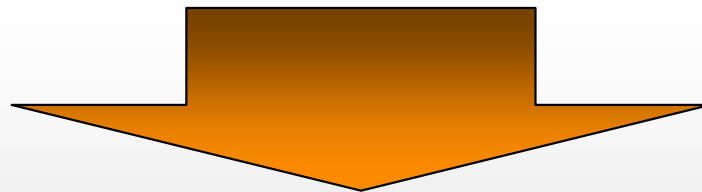


# Results: Discrimination between different deformation models (I)

Best fit deformation model in a CBED pattern



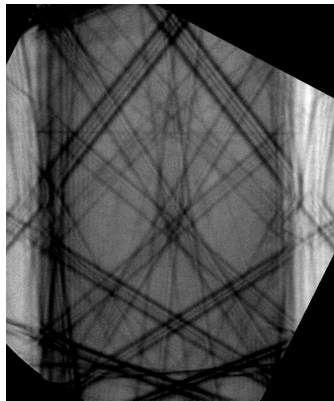
Test of the model in a sequence of CBED patterns



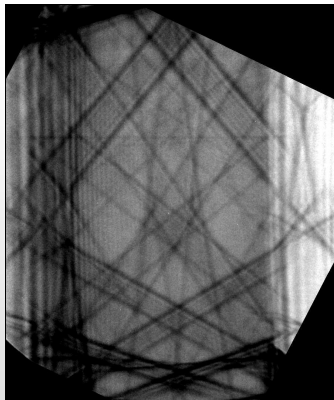
Discrimination between various models

# Results: Discrimination between different deformation models (II)

Exp.

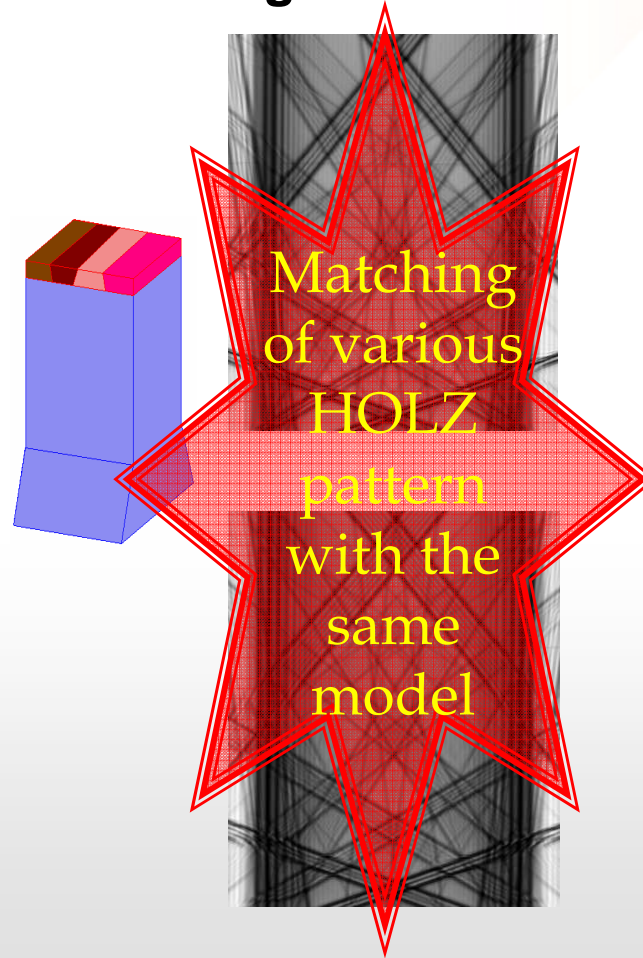


x = 110 nm

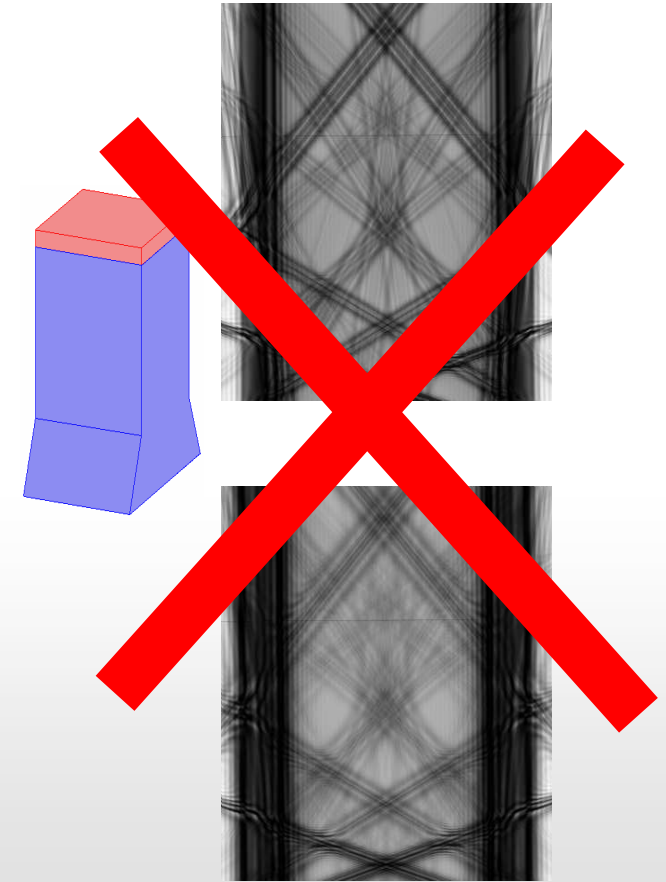


x = 70 nm

Inhomogeneous Model



Homogeneous Model



# FEA Theory:

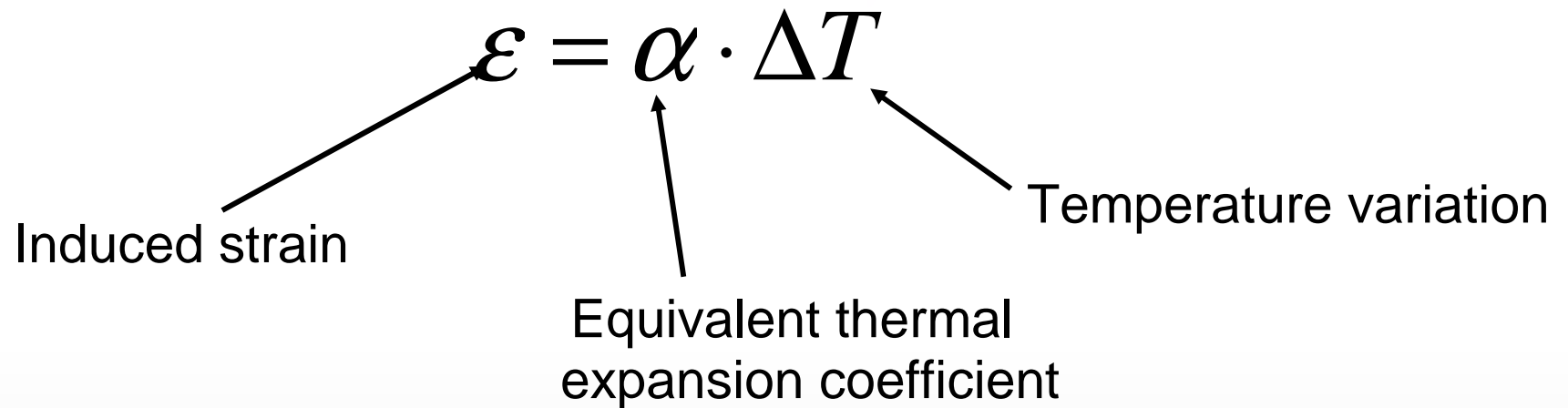
- Deformation calculated with a pseudo thermal relaxation
  - Assumption of lattice mismatch between lattice and stressor sources

$$\epsilon = \alpha \cdot \Delta T$$

Induced strain

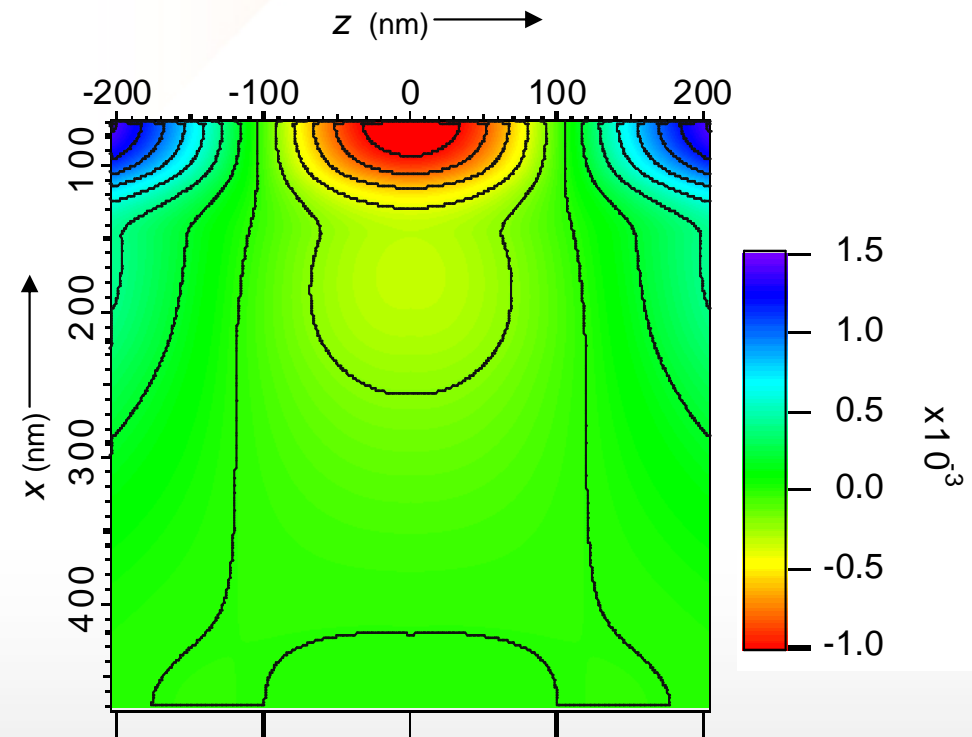
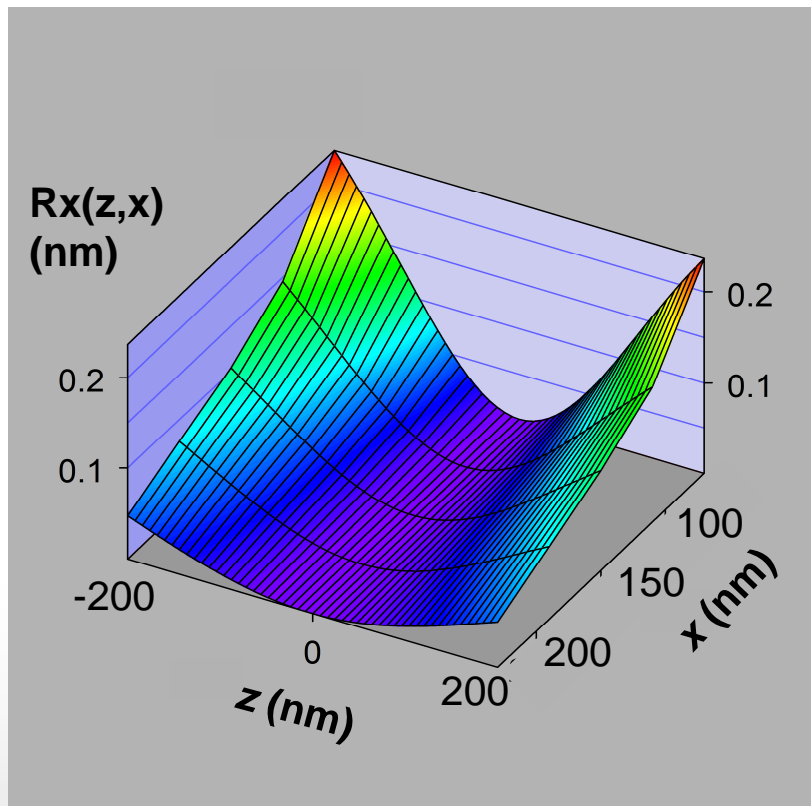
Equivalent thermal expansion coefficient

Temperature variation

The diagram shows the equation  $\epsilon = \alpha \cdot \Delta T$  centered on the page. Three arrows point from text labels below to the variables in the equation: one from 'Induced strain' to  $\epsilon$ , one from 'Equivalent thermal expansion coefficient' to  $\alpha$ , and one from 'Temperature variation' to  $\Delta T$ .

- Large displacement taken into account
- Extrusion of the 2D deformation into 3D model

# Results: Displacement and Strain Field in the analyzed TEM sample

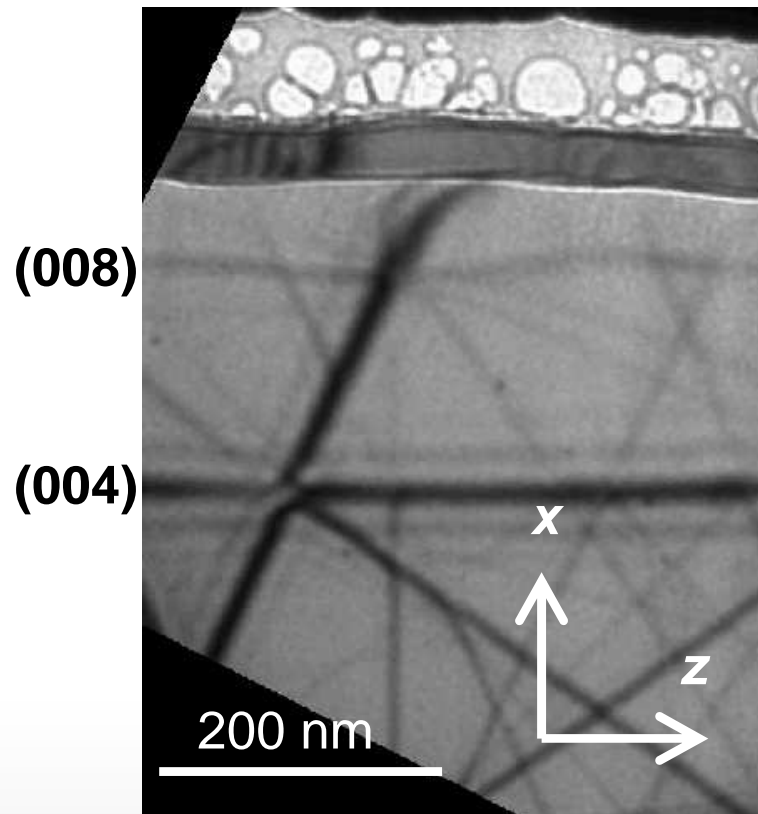


By numerical interpolation, the strain field can be evaluated in points where the experimental CBED patterns cannot be acquired

# Outlines

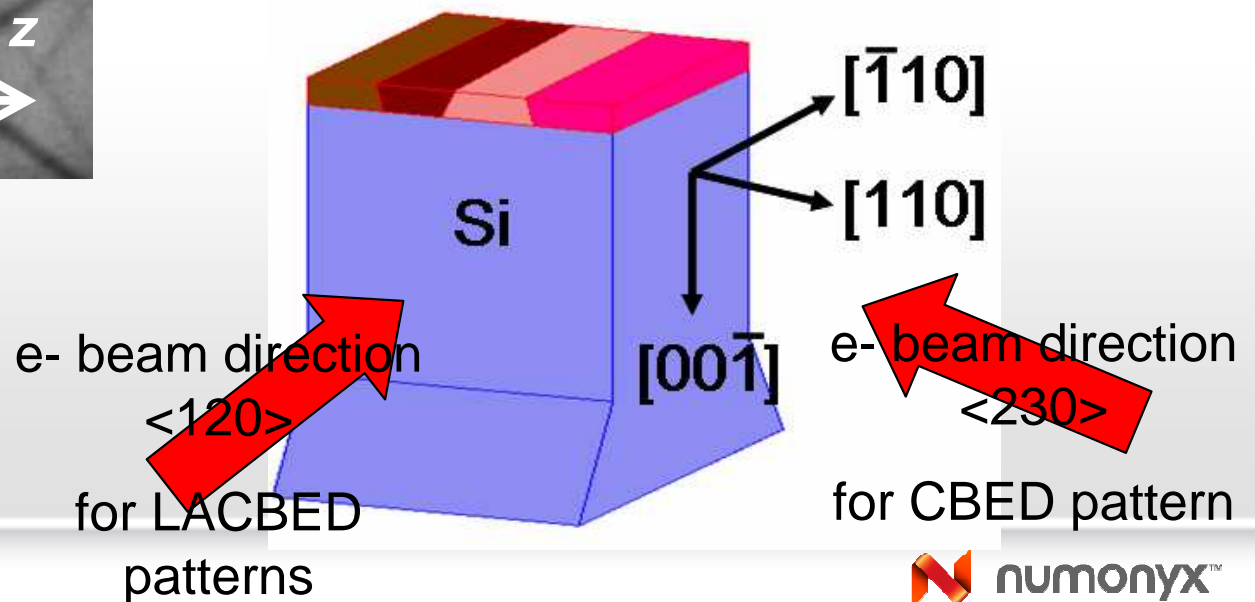
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# LACBED patterns



-The diffraction pattern is superimposed to the image

-Every point is connected with the strain state of a different area of the sample

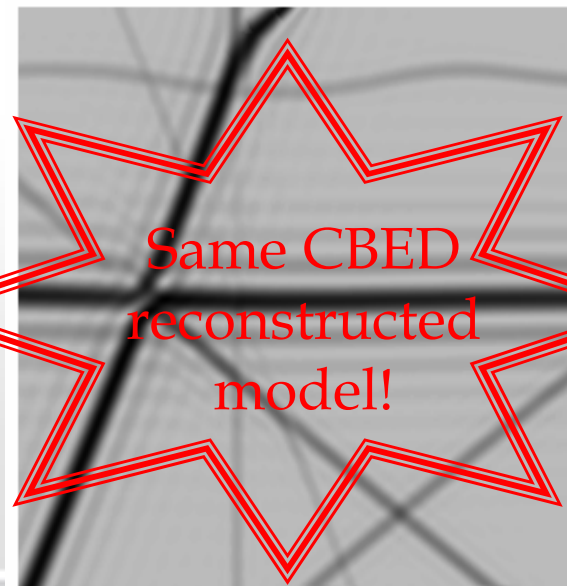
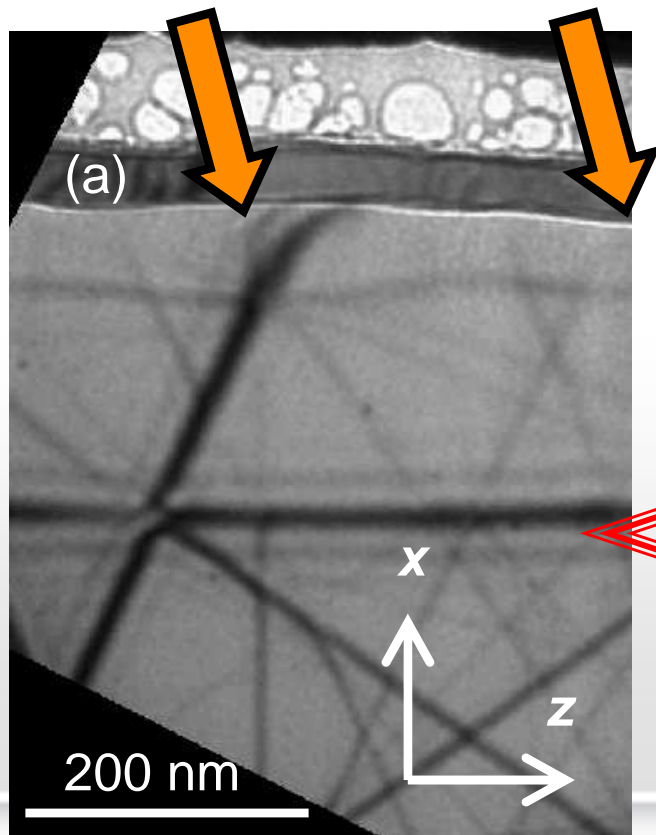
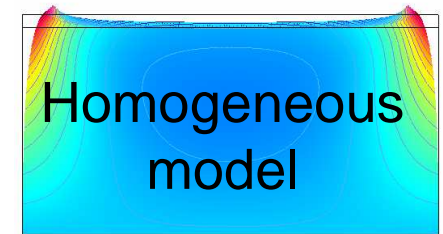
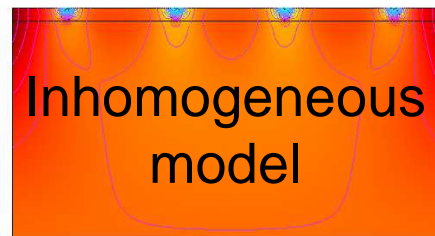


# Check of the CBED results by LACBED

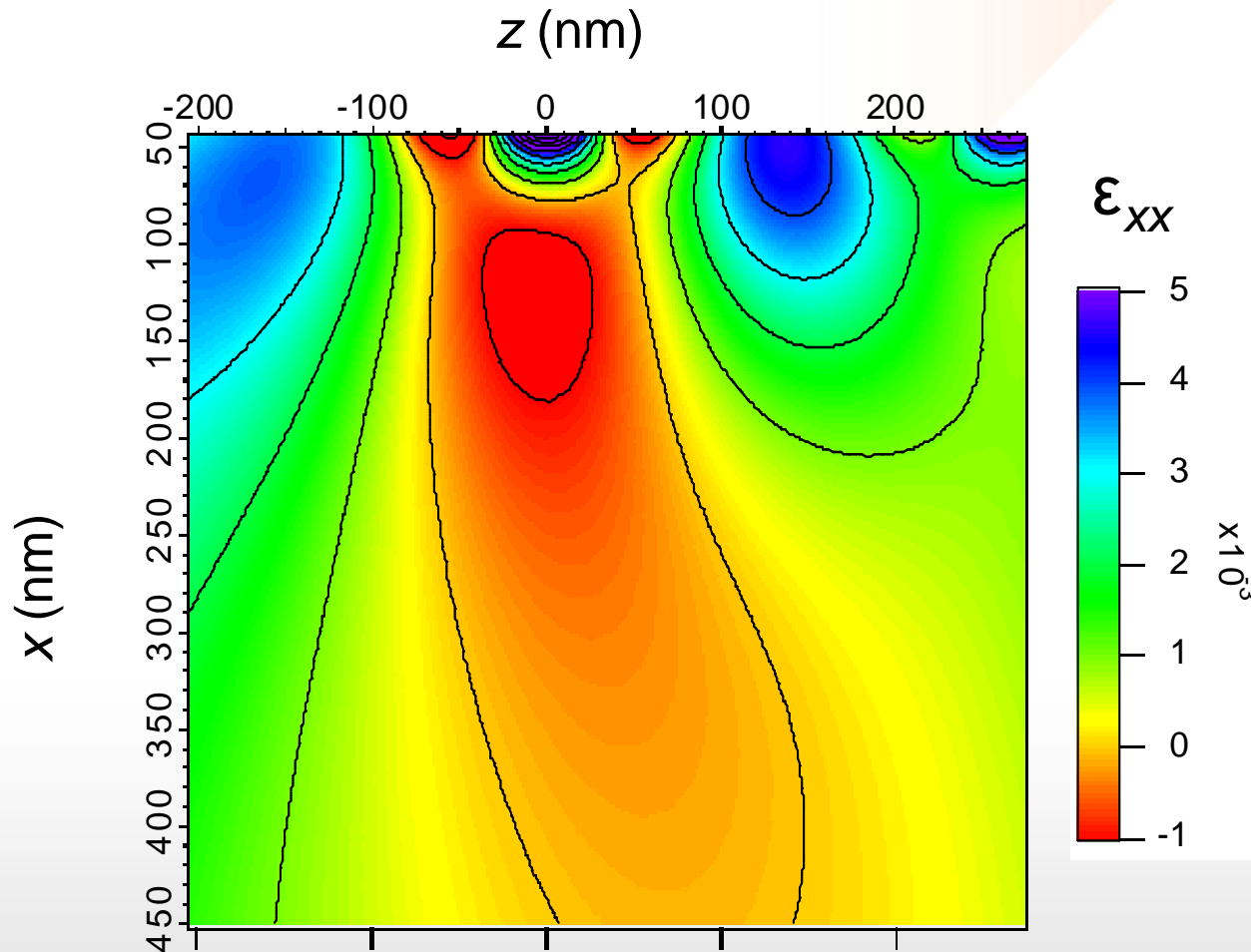
Exp.

Sim. 1

Sim. 2



## Check of the strain field obtained by CBED in $\langle 230 \rangle$



Strain field obtained in the  $\langle 120 \rangle$  by LACBED is in agreement with the CBED results



# Conclusions

- 1) By *CBED* simulation, the displacement field is reconstructed in the TEM sample by the analysis of an experimental database of patterns. Coupling the experimental data with the COMSOL simulation, the strain gradient can be evaluated
- 2) The strain field can be checked in the LACBED simulation even in the inhomogeneous case, and used to reconstruct the unthinned situation with the help of FEA simulation