On the use of MEIS cartography for the determination of $Si_{1-x}Ge_x$ thin-film strain

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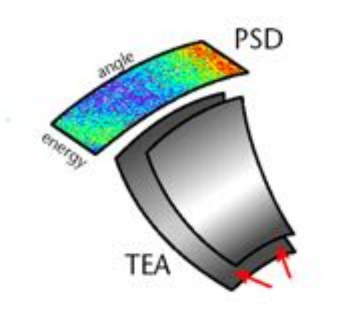
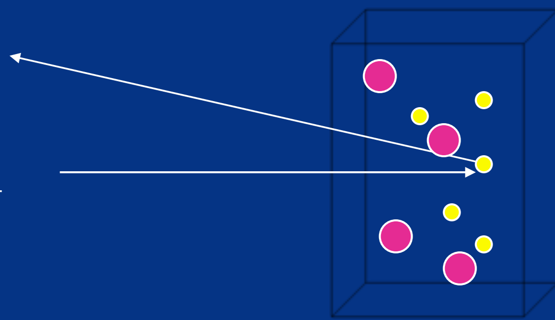
Outline

- Introduction (MEIS, strain)
- MEIS cartography technique
- New procedure to quantify strain through MEIS
- First results using $Si_{1-x}Ge_x/Si$ heterogeneous epitaxial structures
- Conclusions and perspectives

Medium Energy Ion Scattering MEIS

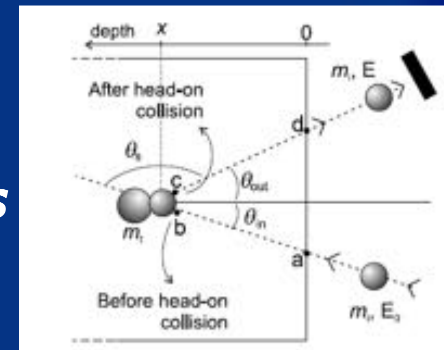


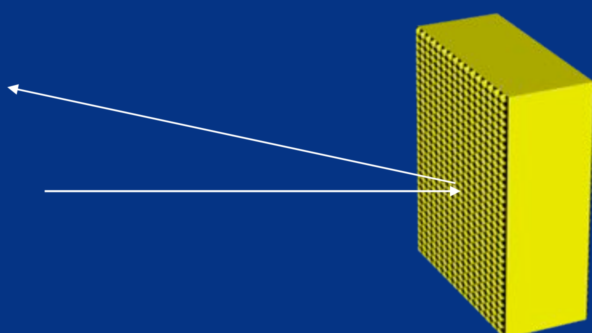
H$^+$



(amorphous)

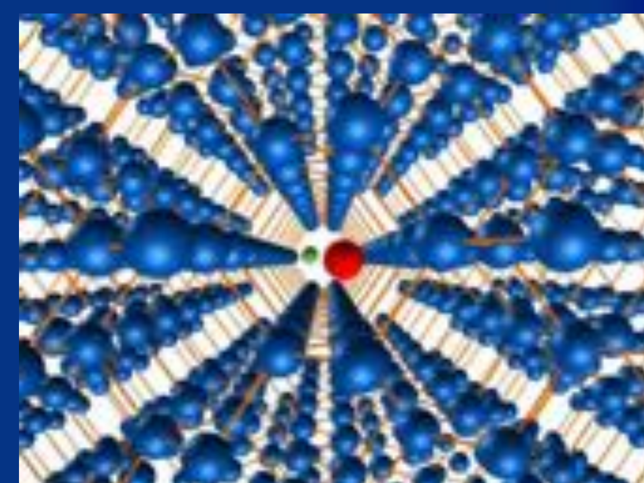
Improved depth and mass resolution

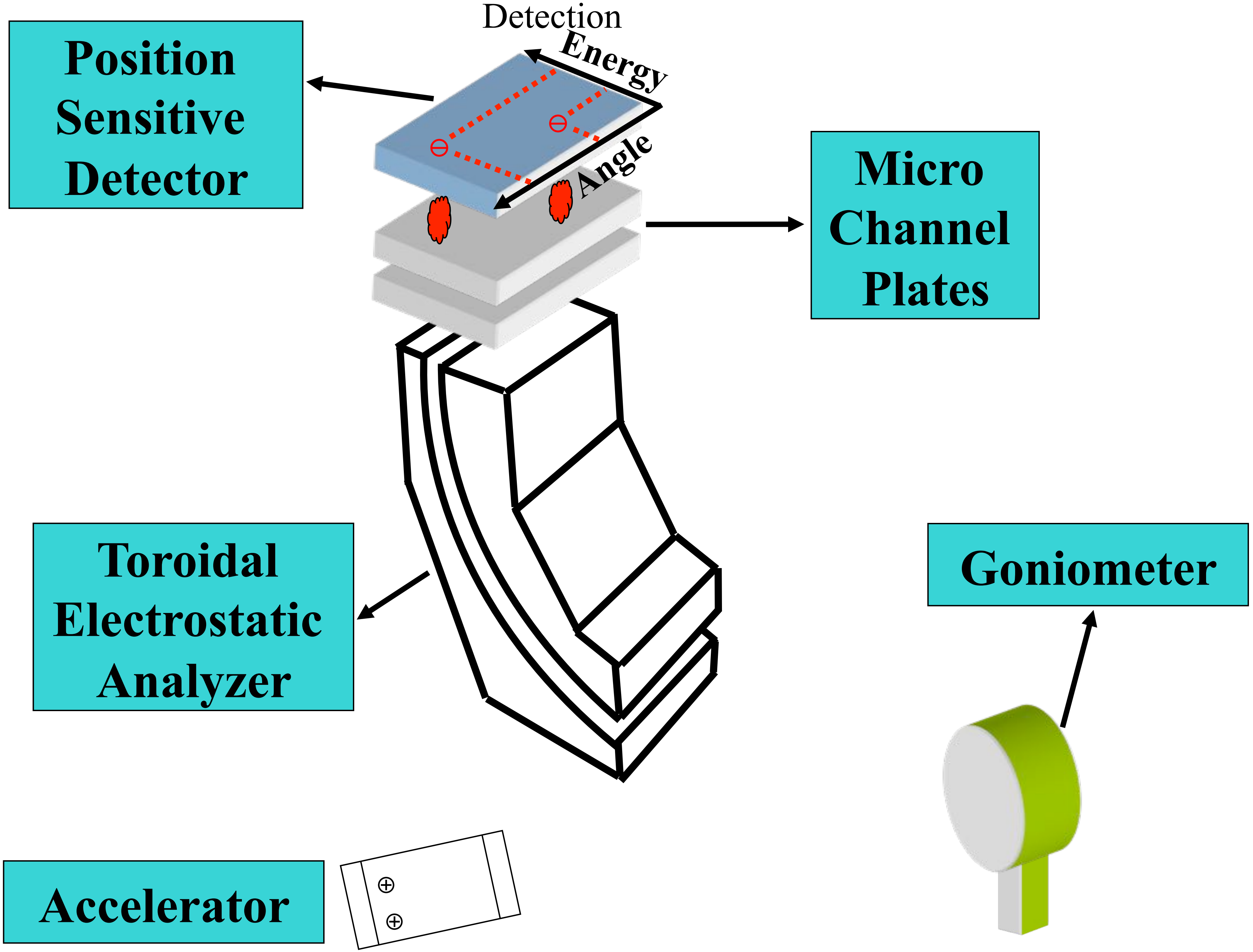




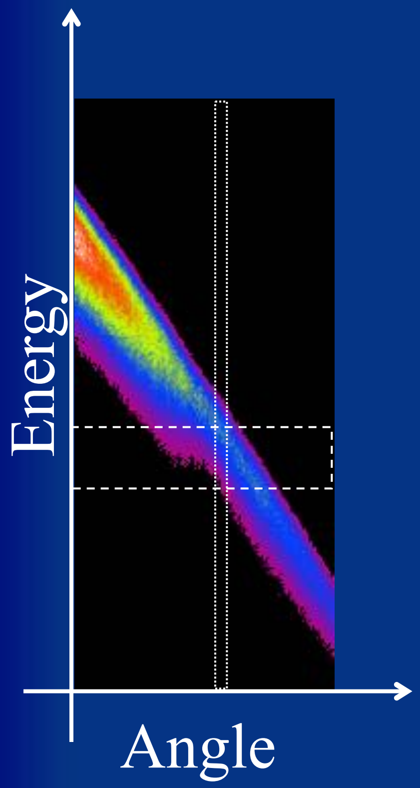
(crystal)

Surface sensitivity




Position Sensitive Detector
Detection
Energy
Angle
Micro Channel Plates
Toroidal Electrostatic Analyzer
Goniometer
Accelerator

MEIS 2D Spectrum



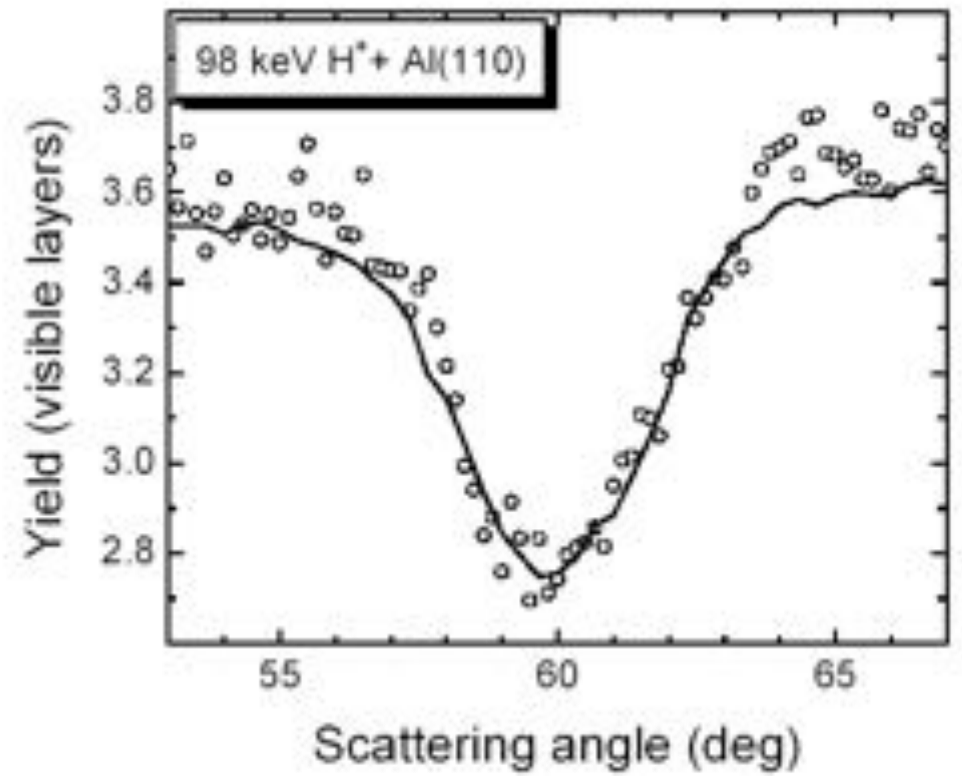


Figure 2 Angular distribution of protons scattered from Al(110) in the geometry of Fig. 1 (open symbols) and VEGAS simulation with optimized atomic positions and vibrational amplitudes (solid line).

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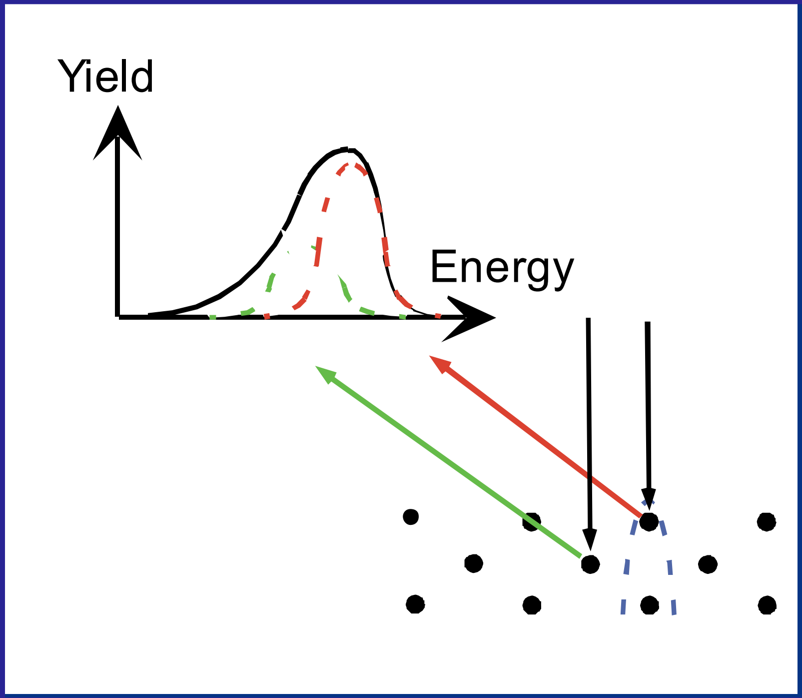
MEIS data collection

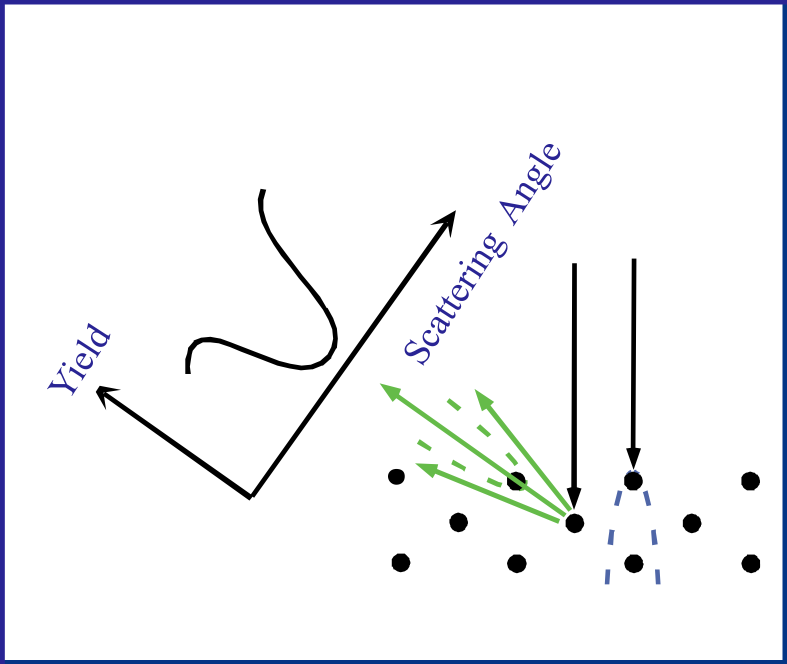
Schulte H. (Private communication)

Energy Spectrum



Deconvolution of ES gives depth profile (primarily for amorphous thin films).

Angular Spectrum



MC ion scattering simulation of angular yield provides **surface structure.**

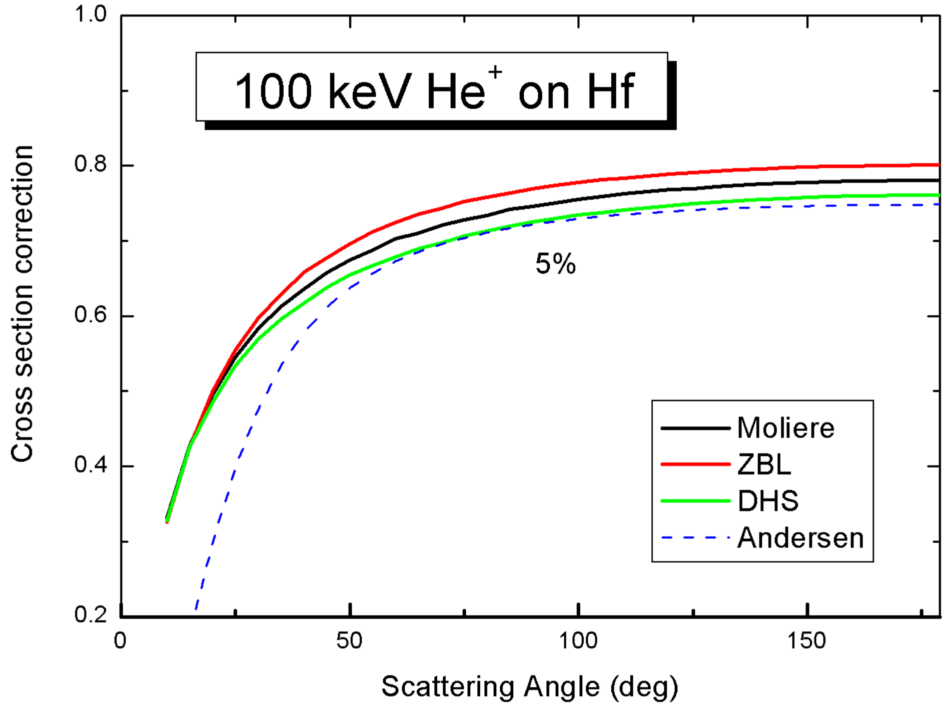
MEIS user community

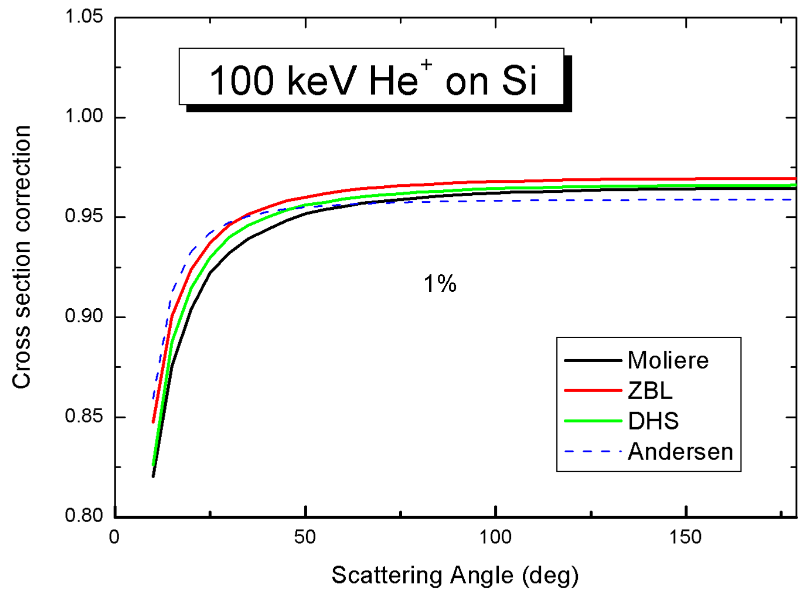
- Depth profiling (*amorphous*)
  - High-k materials
  - Thin films
  - …
- Structural determination (*crystal*)
  - Heterogeneous catalysis
  - Stress (Films, NWs)
  - …

MEIS – open problems

- Depth profiling (*amorphous*)
  - energy-loss (stopping, straggling and asymmetry)
  - neutralization
  - role of plural and multiple scattering
  - ~~cross section~~

- Structural determination (*crystal*)
  - line shape
  - trajectory dependent energy-loss
    - central collisions Q(0)
    - straggling
  - correlated thermal vibrations


100 keV He+ on Hf
Cross section correction
Scattering Angle (deg)
5%
Moliere
ZBL
DHS
Andersen
1.0
0.8
0.6
0.4
0.2
0
50
100
150


100 keV He+ on Si
Cross section correction
Scattering Angle (deg)
1%
Moliere
ZBL
DHS
Andersen
1.05
1.00
0.95
0.90
0.85
0.80
0
50
100
150

VEGAS Monte Carlo Simulation

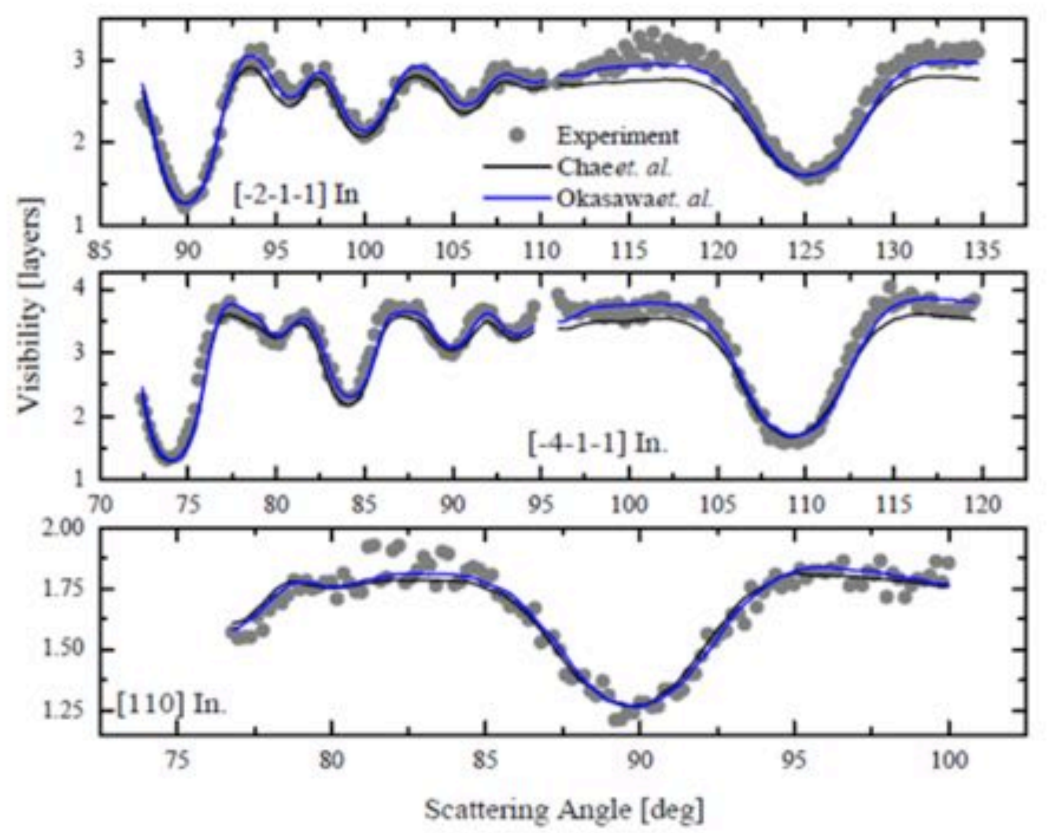
- well established in MEIS

  gives the **area** of the surface peak

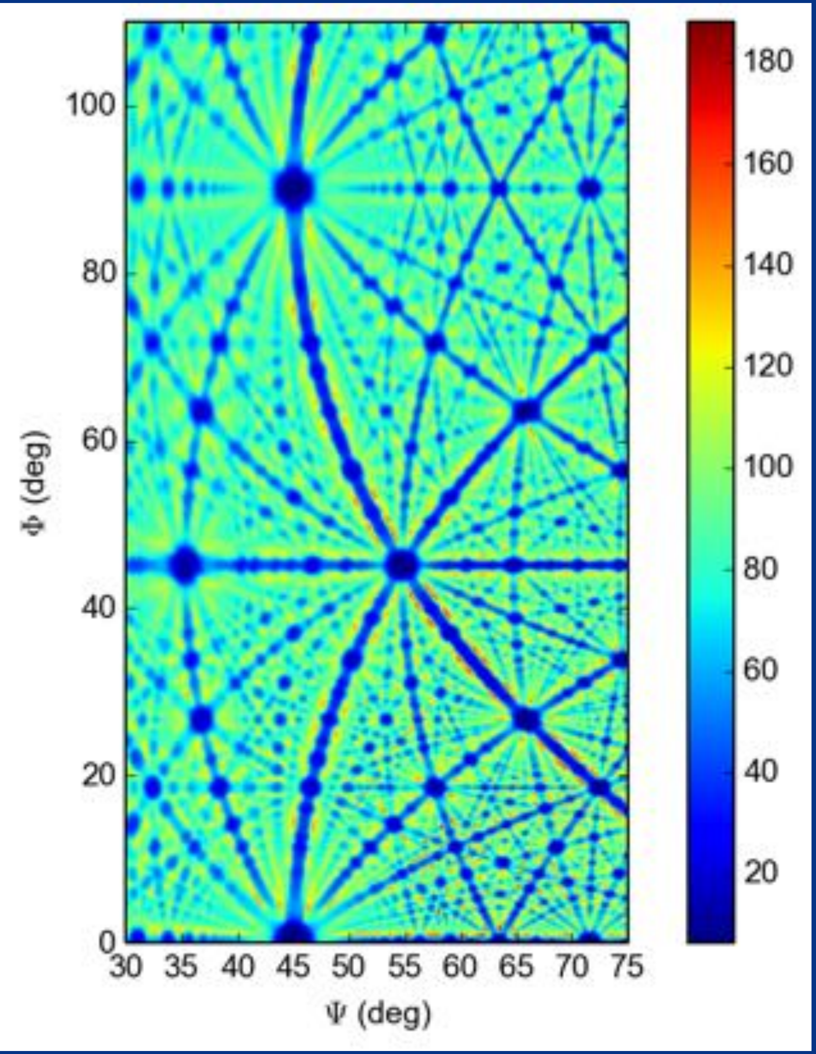
  P_{hit} and P_{det}

Blocking curves !

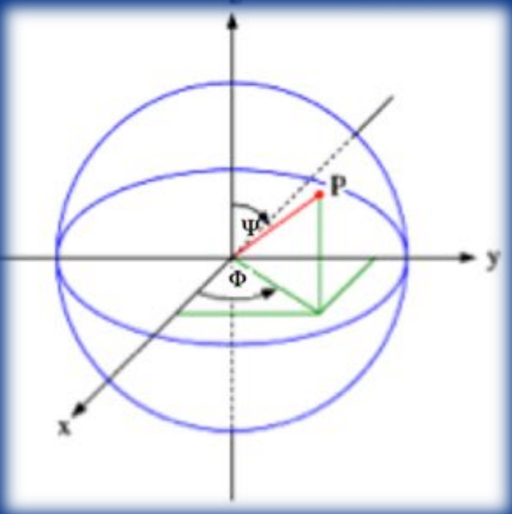
Blocking curves – Cu(111) surface



2D Blocking map – Si <100>



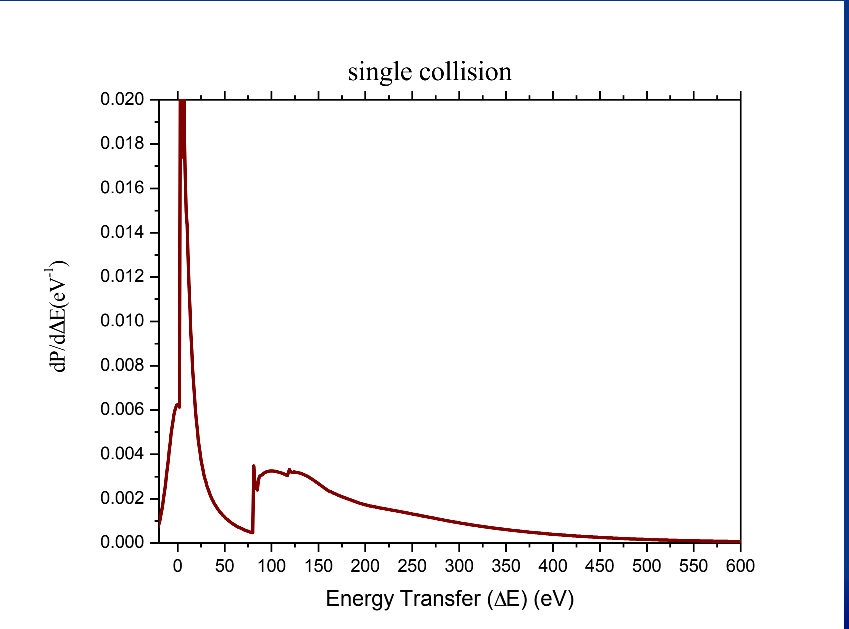
Sample normal



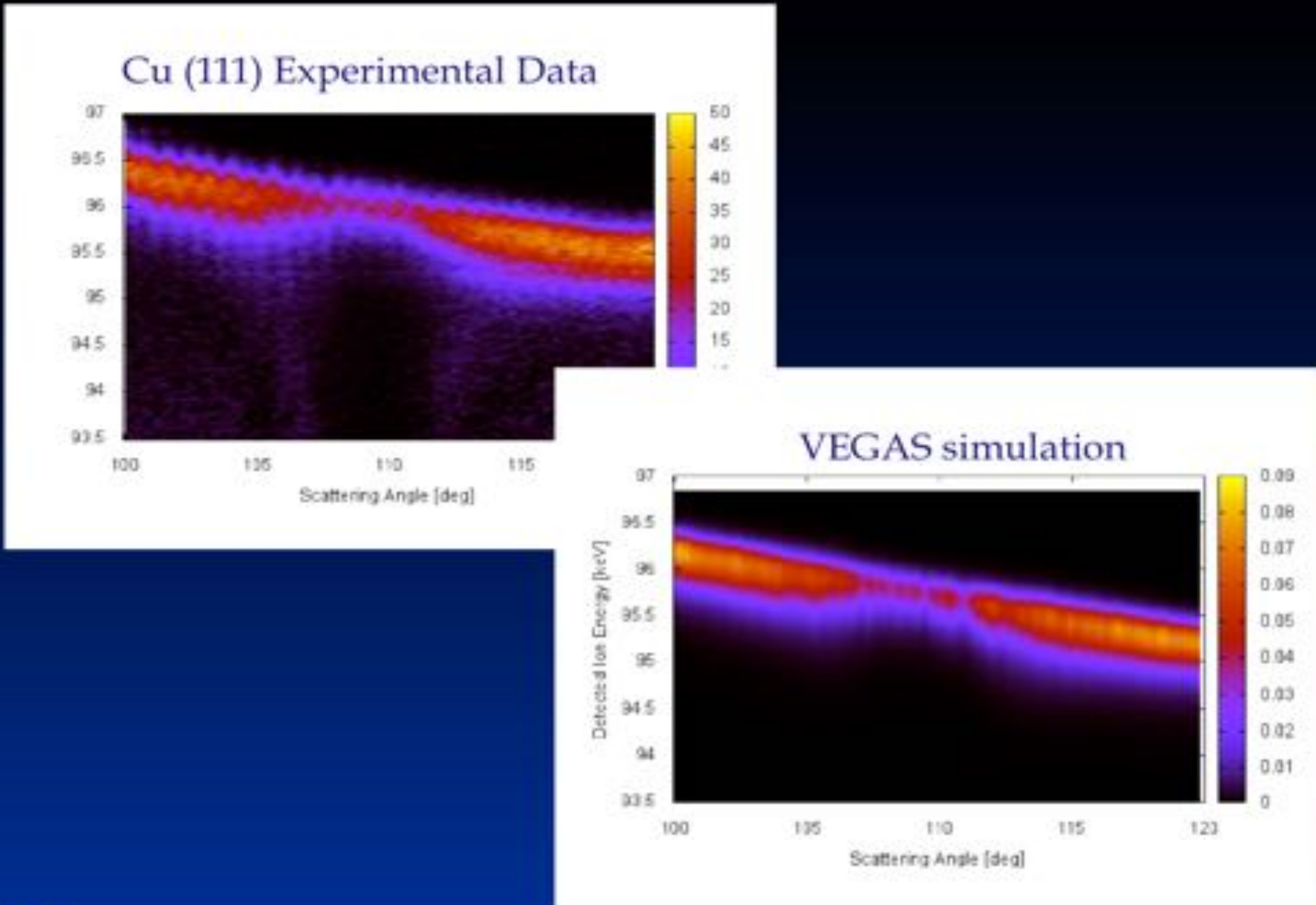
Modified VEGAS version

$$\Delta E = \Delta E_{in} + \Delta E_{out} + \Delta E_{backscattering}(b \approx 0)$$

$$\Delta E_{in} = \sum_i (\Delta E_{el}(b_i) + \Delta E_{nuclear}(b_i))$$



Full 2D MEIS spectrum



Ion beam facility @ Porto Alegre - Brazil

1)PIXE (Particle-Induced X-ray Emission)

2)RBS (Rutherford Backscattering Spectrometry)

3)NRA (Nuclear Reaction Analysis)

4)Microprobe

5)MEIS (Medium Energy Ion Scattering)

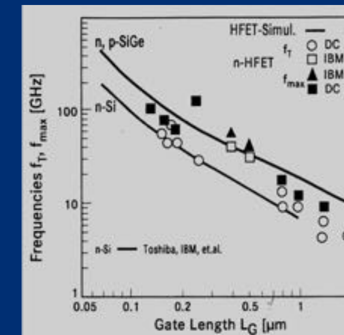
6) **Ion Implantation**

Current MEIS research @ Porto Alegre

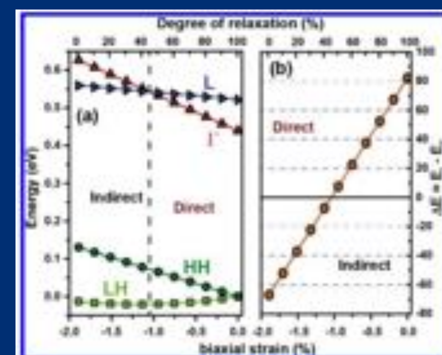
- 3D characterization of NPs (PowerMeis)
- Coulomb depth profile (using info from the Coulomb explosion)
- MEIS Cartography for crystalline materials

Importance of strain measurements

- Metal-oxide-semiconductor to boost CMOS performance

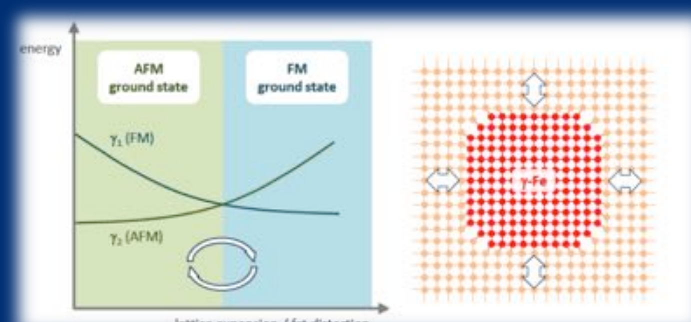


- Piezoelectric effect -> Electric field in QDs -> shift of luminescence
- Indirect to direct band-gap – lasing



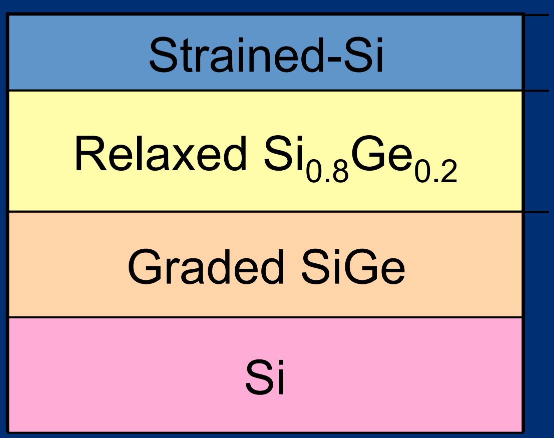
S. Wirths et al Nature photonics (2015)

- Strain-mediated magnetoelectric coupling



ISOLDE Newsletter 2016 - CERN

SiGe has been well investigated….



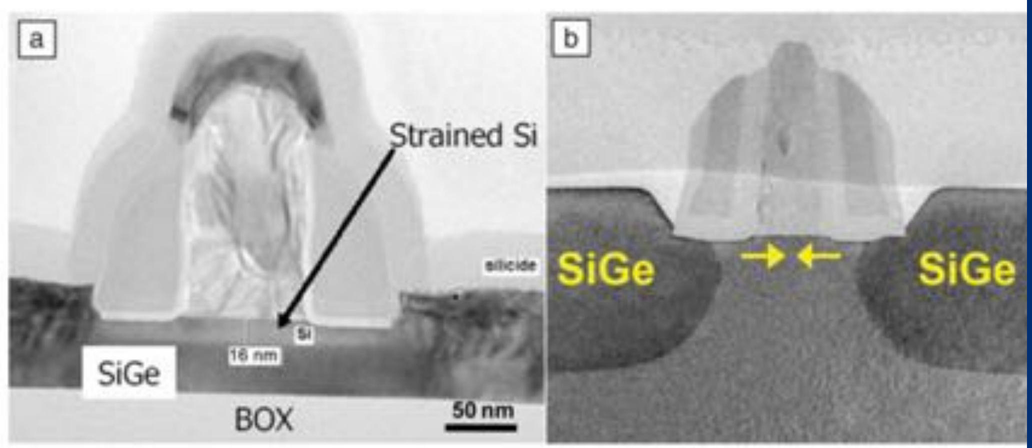


Figure 1. (a) Cross-sectional transmission electron microscopy (TEM) image of biaxial (tensile) strained Si *n*-type field-effect transistor (FET) fabricated using SiGe-on-insulator as a growth template. Reprinted with permission from Reference 8. © 2004 American Institute of Physics. (b) Cross-sectional TEM image of an uniaxial strained (compressive) *p*-type FET device using embedded SiGe in the source and drain regions. Reprinted with permission from Reference 10. © 2003 IEEE.

Typical Techniques

Lattice deformation and strain analysis

X-rays

XRD – X ray diffraction

…

Electrons

GAP – Geometrical Phase Analysis (from TEM images)

CBED – Convergent Beam Electron Diffraction

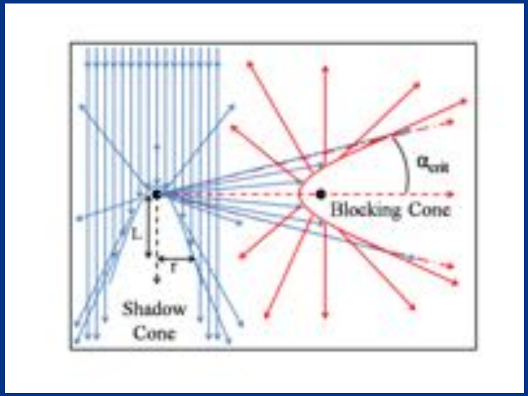
NBED – Nano Beam Electron Diffraction

…

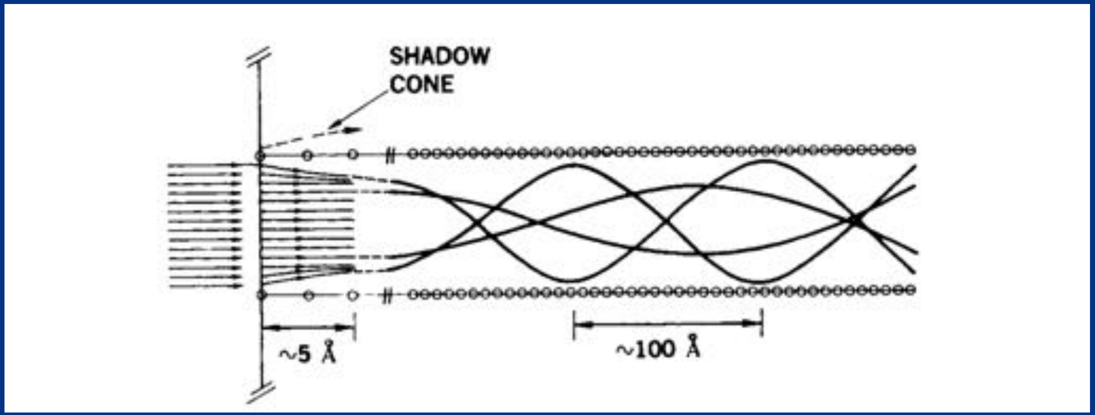
Ions

RBS, HRRBS, MEIS, Radioactive Ion Implantation,..

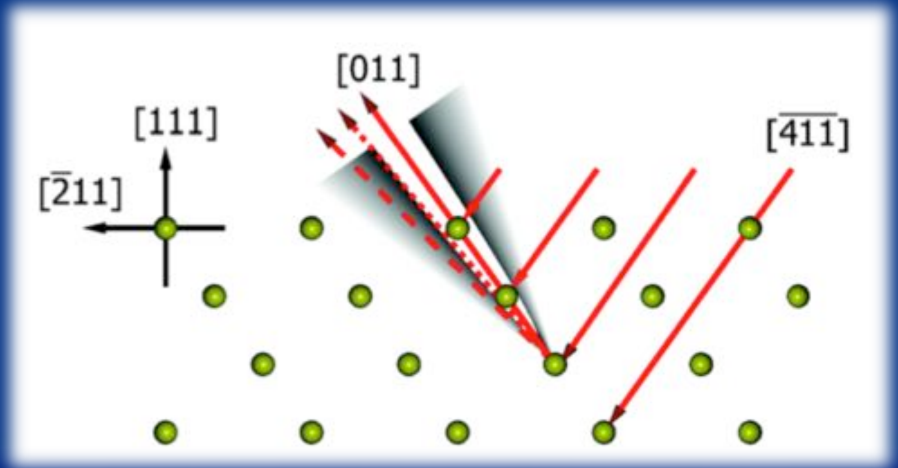
Blocking



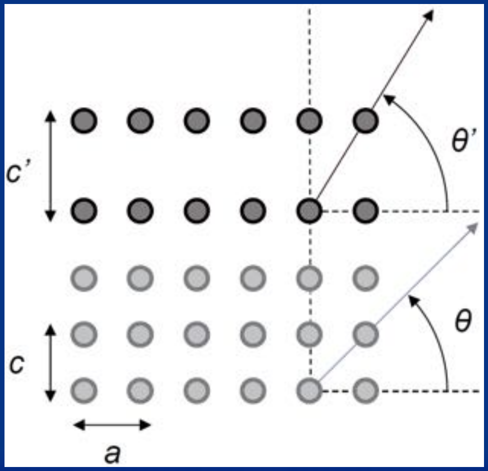
α_{crit}
Blocking Cone
L
r
Shadow Cone



SHADOW CONE
~5 Å
~100 Å



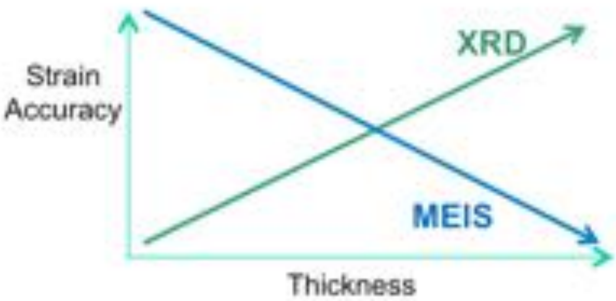
[011]
[111]
[$\bar{2}$11]
[$\bar{4}\bar{1}\bar{1}$]



c'
c
a
θ'
θ

Typical techniques - comparison

	MEIS	GPA	CBED	NBED	XRD
Depth Resolution	0.2 – 0.5 nm	0.1 nm	0.5 - 0.9 nm	2.5 - 3 nm	Not at the nanoscale
Lateral Resolution	Not at the nanoscale (monocrystal)	0.1 nm	0.5 - 0.9 nm	2.5 - 3 nm	200 nm
Strain Accuracy	$1\ 10^{-3}$	$\sim 1\ 10^{-2}$	$1\ 10^{-4}$	$6\ 10^{-4}$	$< 10^{-5}$ (bulk)
Surface	yes	no	no	no	Yes but diffraction limits



Jalabert IBA 2015

Limitation of XRD for nano objects

As in multiple slits….

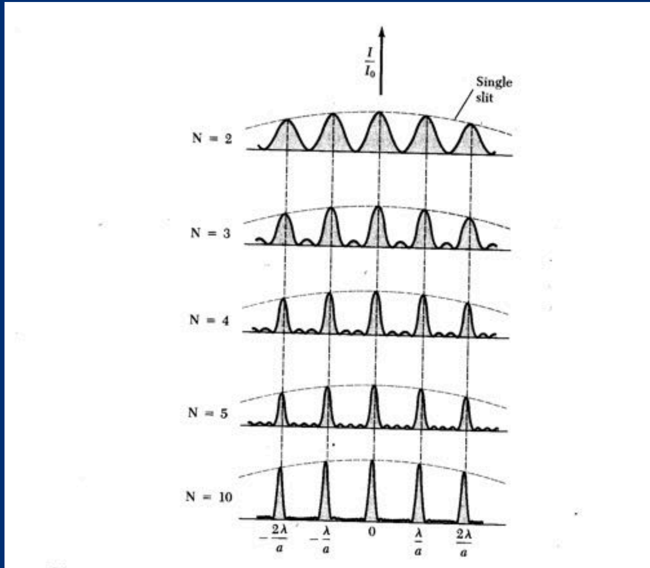
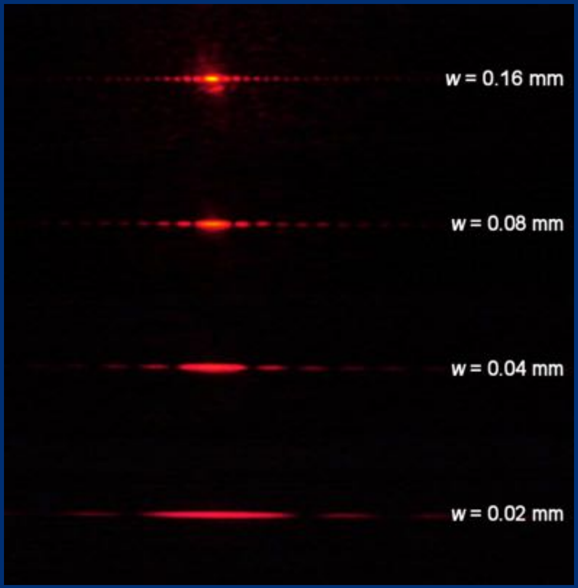


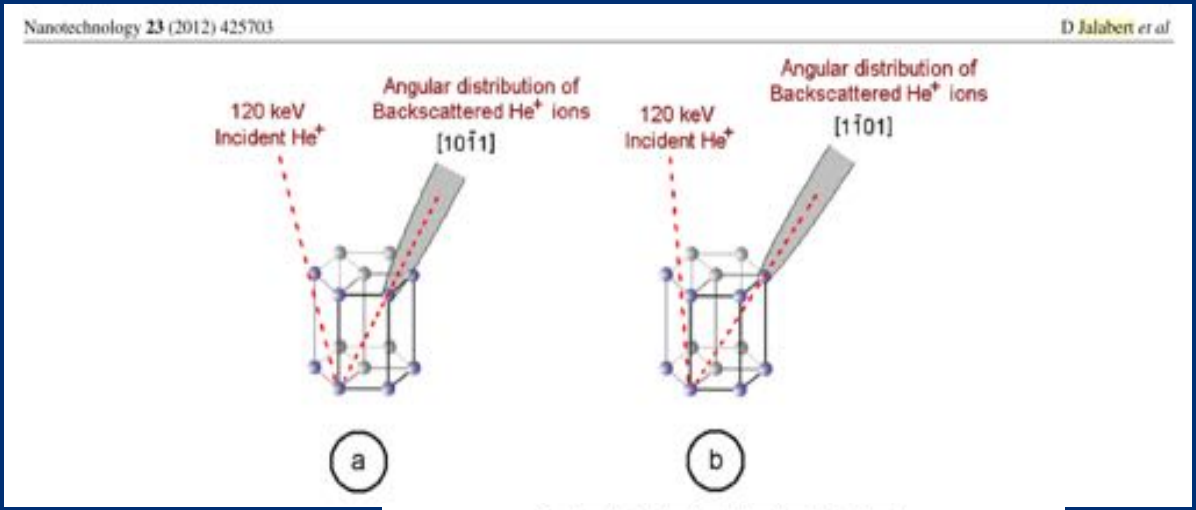
Figure 37.13 Multiple-slit interference patterns. Note that as the number of slits is increased, the primary maxima become narrower but remain fixed in position. Furthermore, the number of secondary maxima increases as the number of slits is increased. The decrease in intensity of the maxima, as indicated by the dashed lines, is due to the phenomenon of diffraction, which is discussed in Chapter 38.

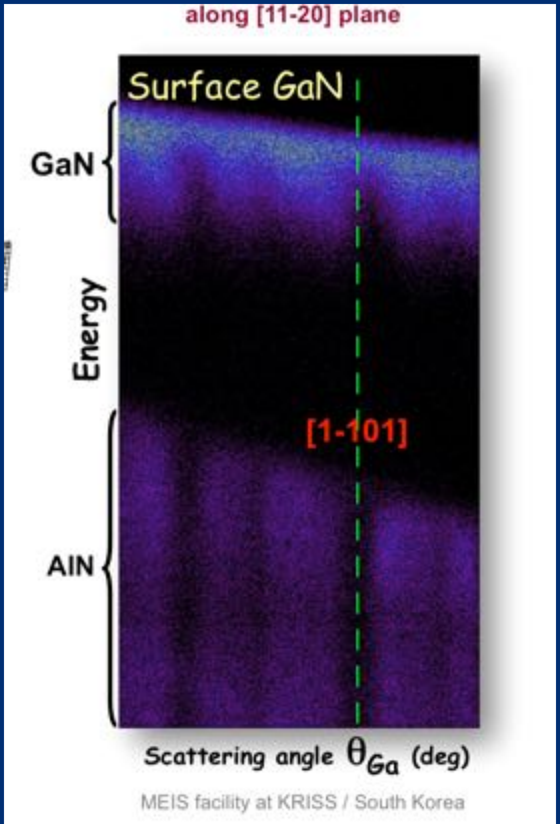


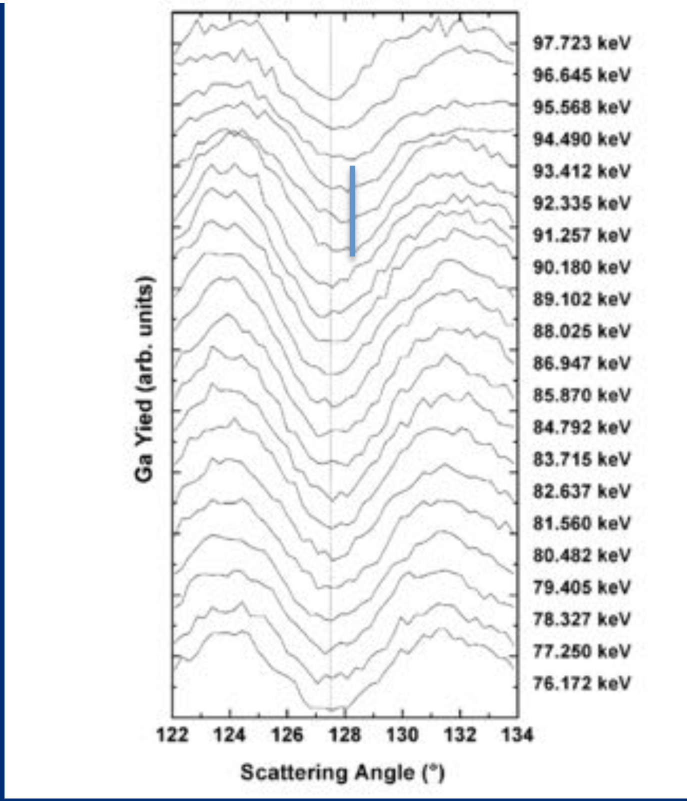
Crystal size decreases

- Peak size decreases
- Peak width increases
- Secondary peaks appear

MEIS examples

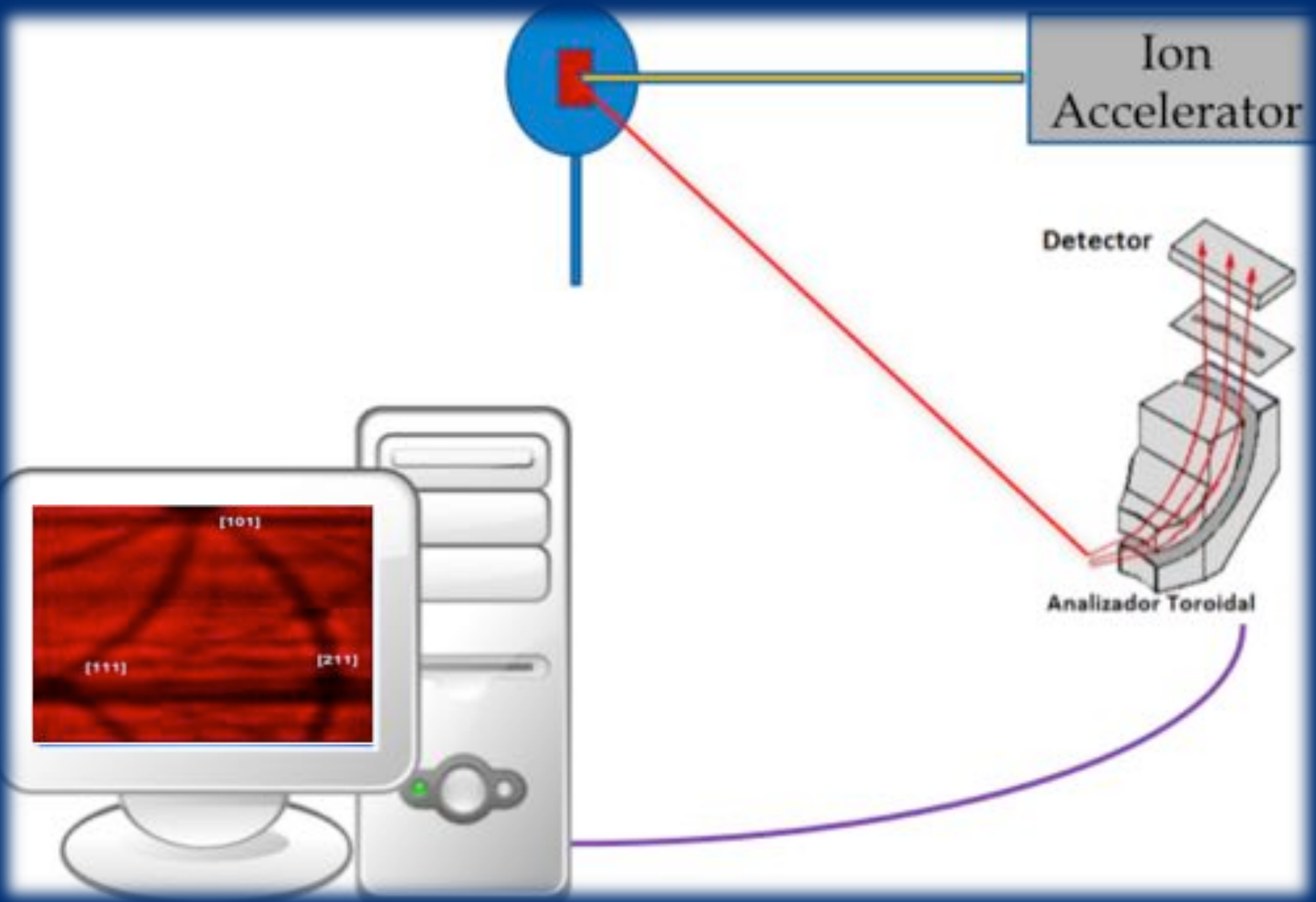


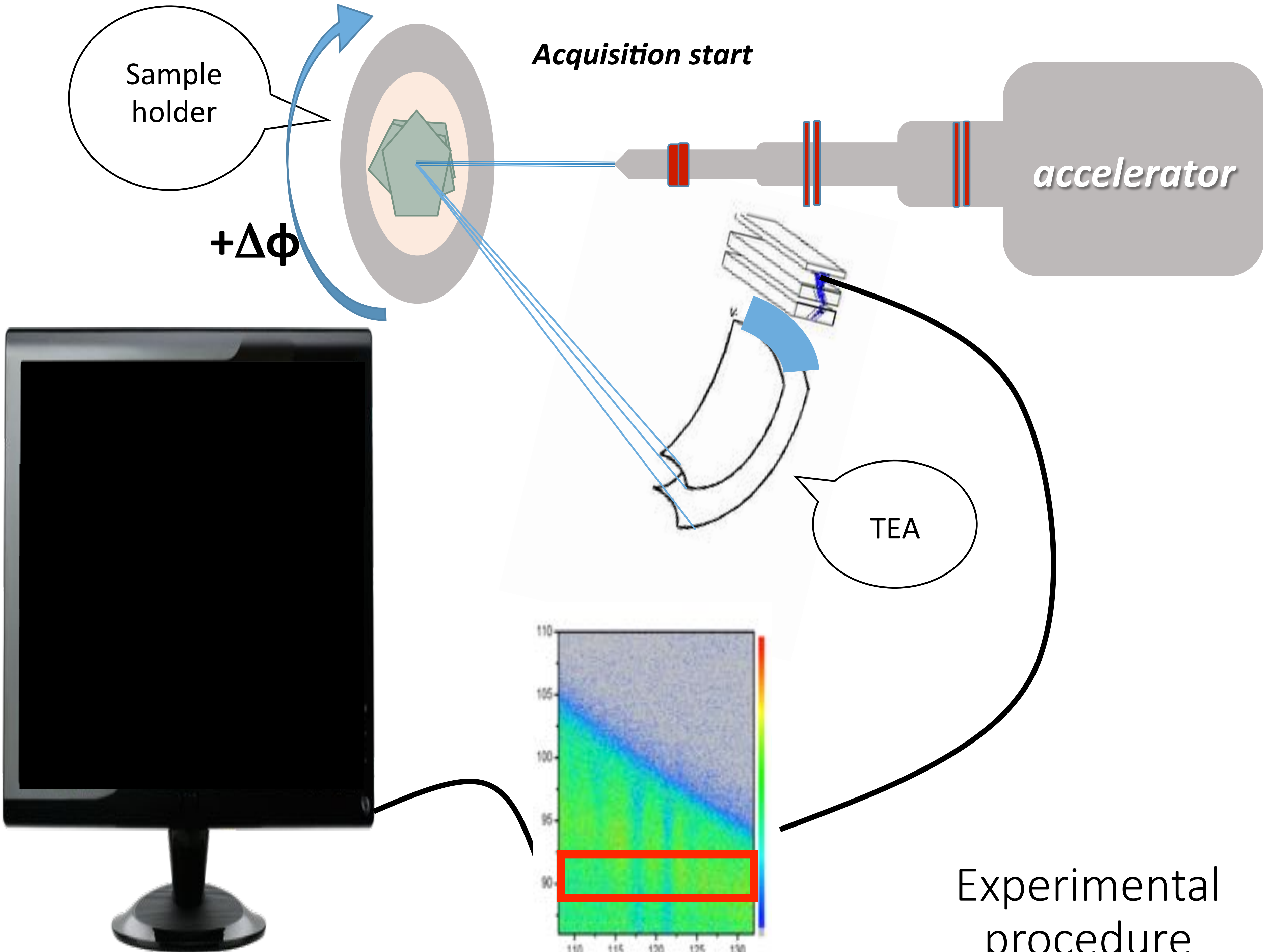




How to improve strain measurements with MEIS ?

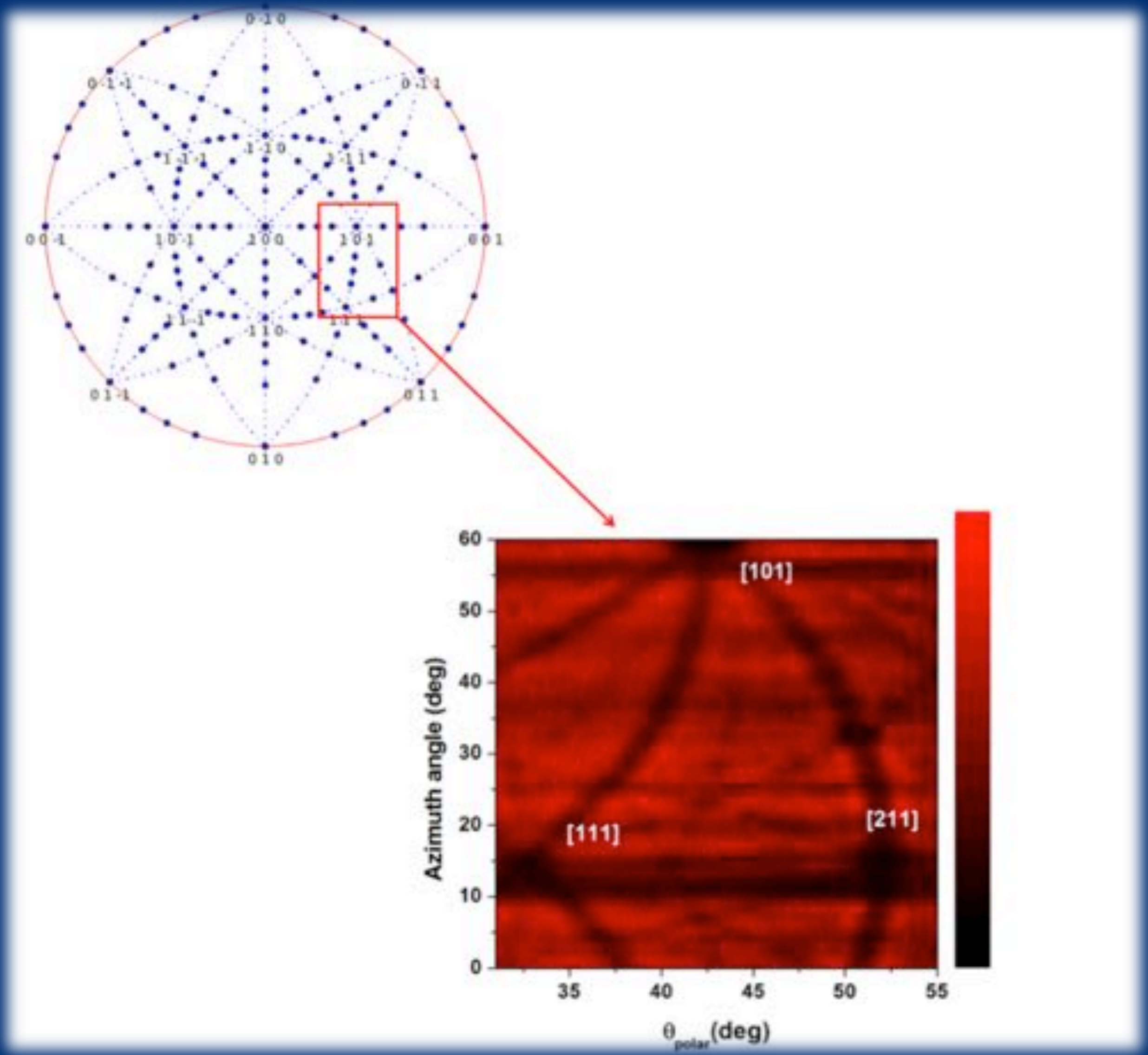
MEIS Cartography





Experimental procedure

Stereographic projection



Denis Jalabert (HRDP6)

Nuclear Instruments and Methods in Physics Research B 270 (2012) 19–22

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journal homepage: www.elsevier.com/locate/nimb

Real space structural analysis using 3D MEIS spectra from a toroidal electrostatic analyzer with 2D detector

D. Jalabert*

CEA-INAC/UJF-Grenoble 1 UMR-E, SP2M, LEMMA, Minatec Grenoble F-38054, France

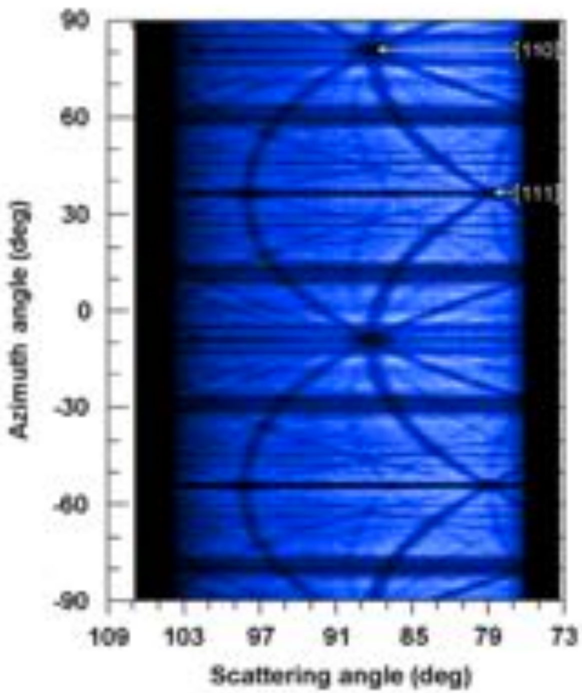


Fig. 3. Cartography of He$^+$ ions scattered by the germanium atoms in a SiGe layer to a depth of 18 nm below surface.

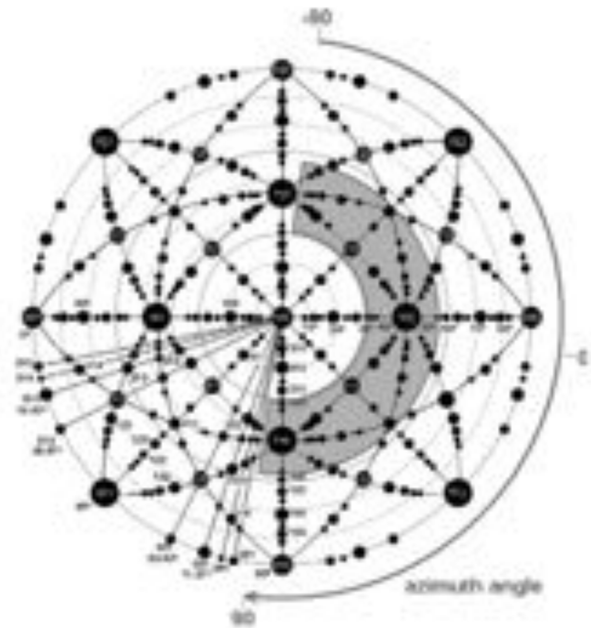
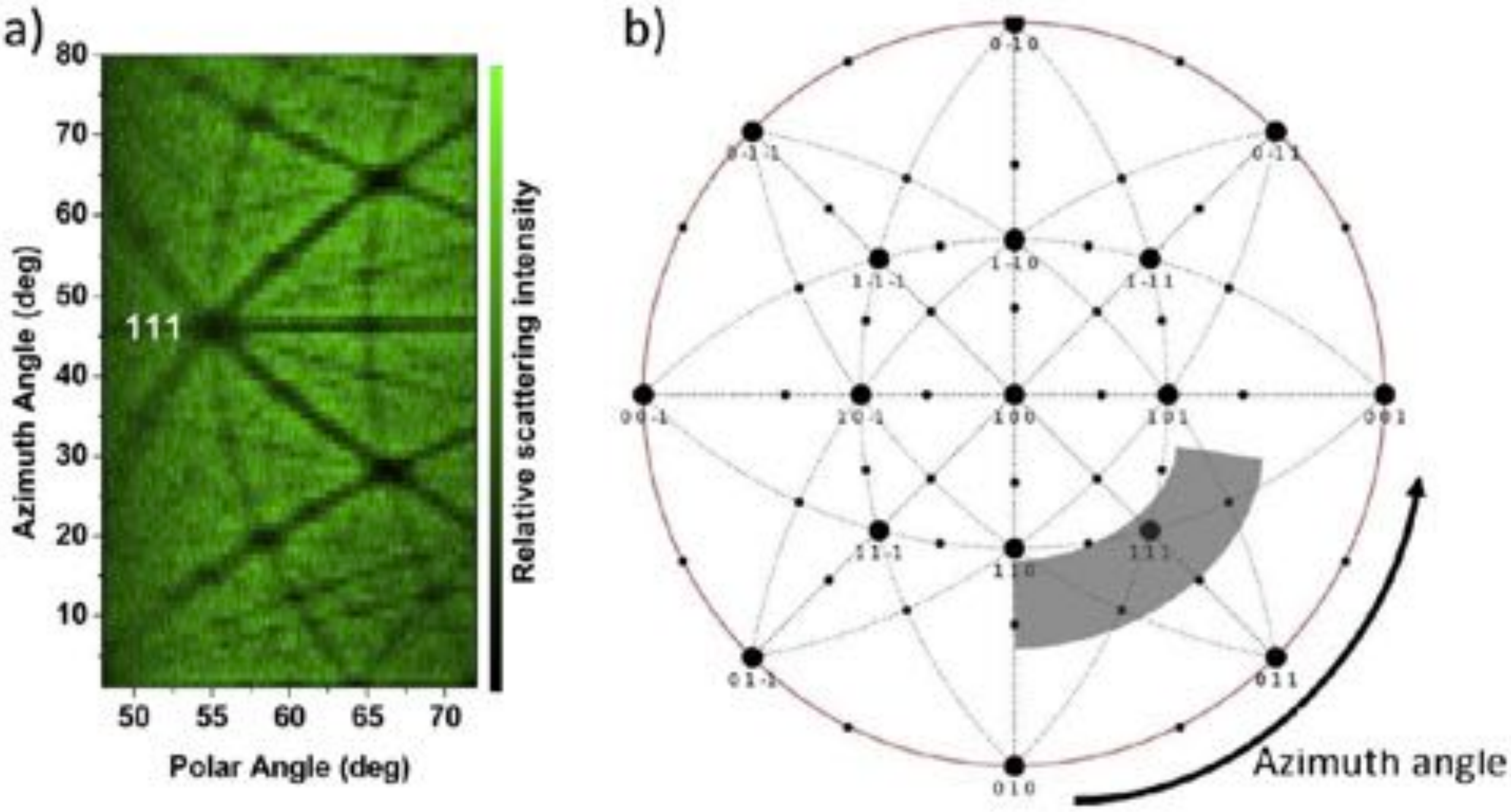


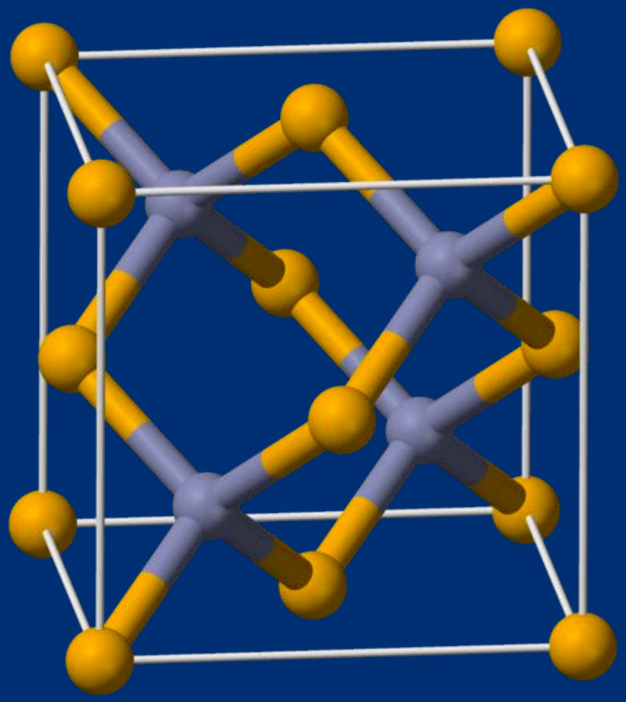
Fig. 4. Stereographic projection of a face-centered cubic crystal on the [100] direction [17]. The gray area corresponds to the experimental cartography shown in Fig. 3. The relation between the scattering angle θ_{sc} and the polar angle θ_{pol} of the figure is $\theta_{sc} = 180 - \theta_{inc} - \theta_{pol}$.

Si <100>

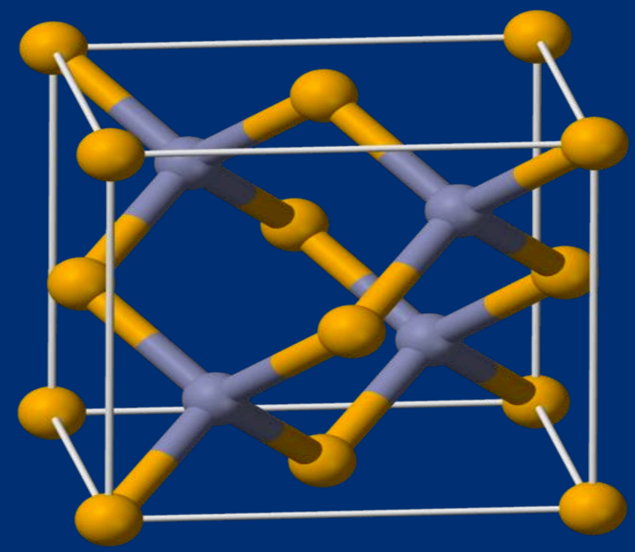
T.S. Avila et al. / Thin Solid Films 611 (2016) 101–106



Strain Analysis



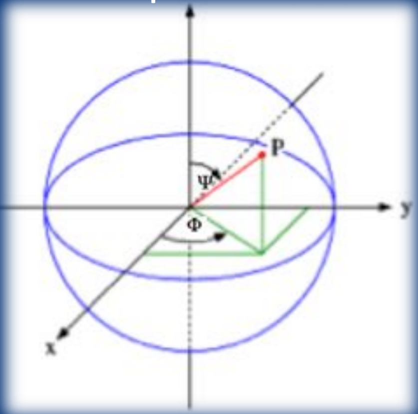
cubic cell

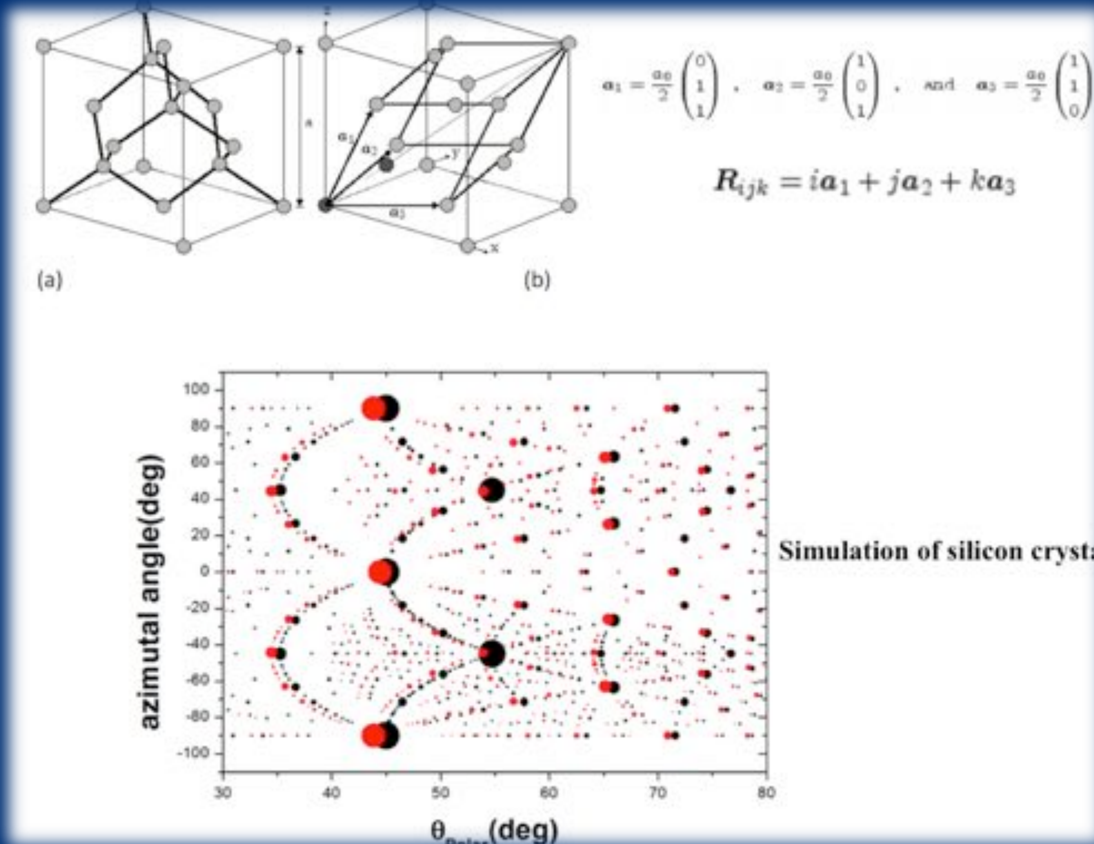


uniaxial strain

Getting crystal directions…..

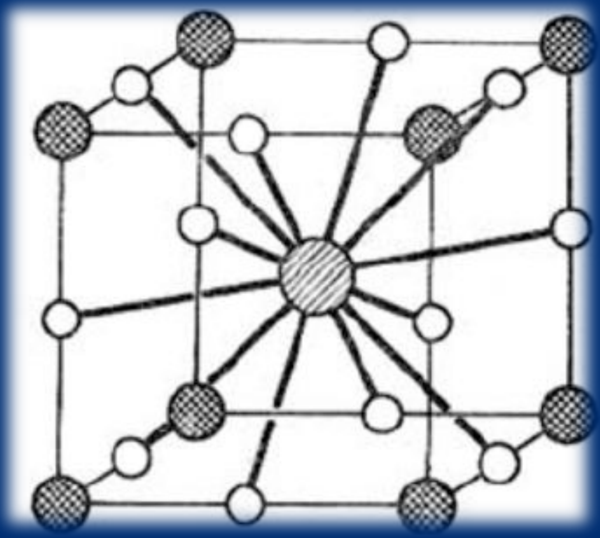
Sample normal

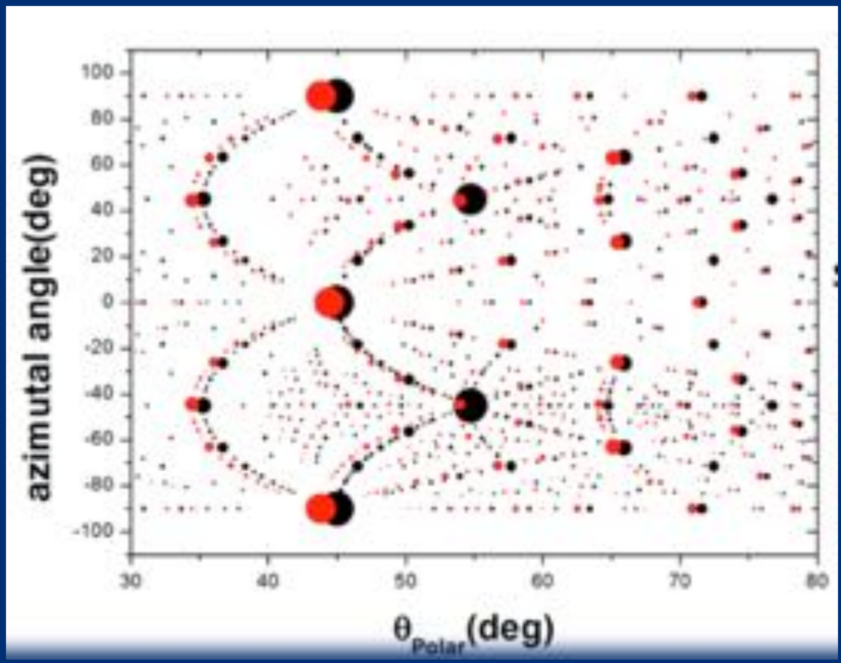




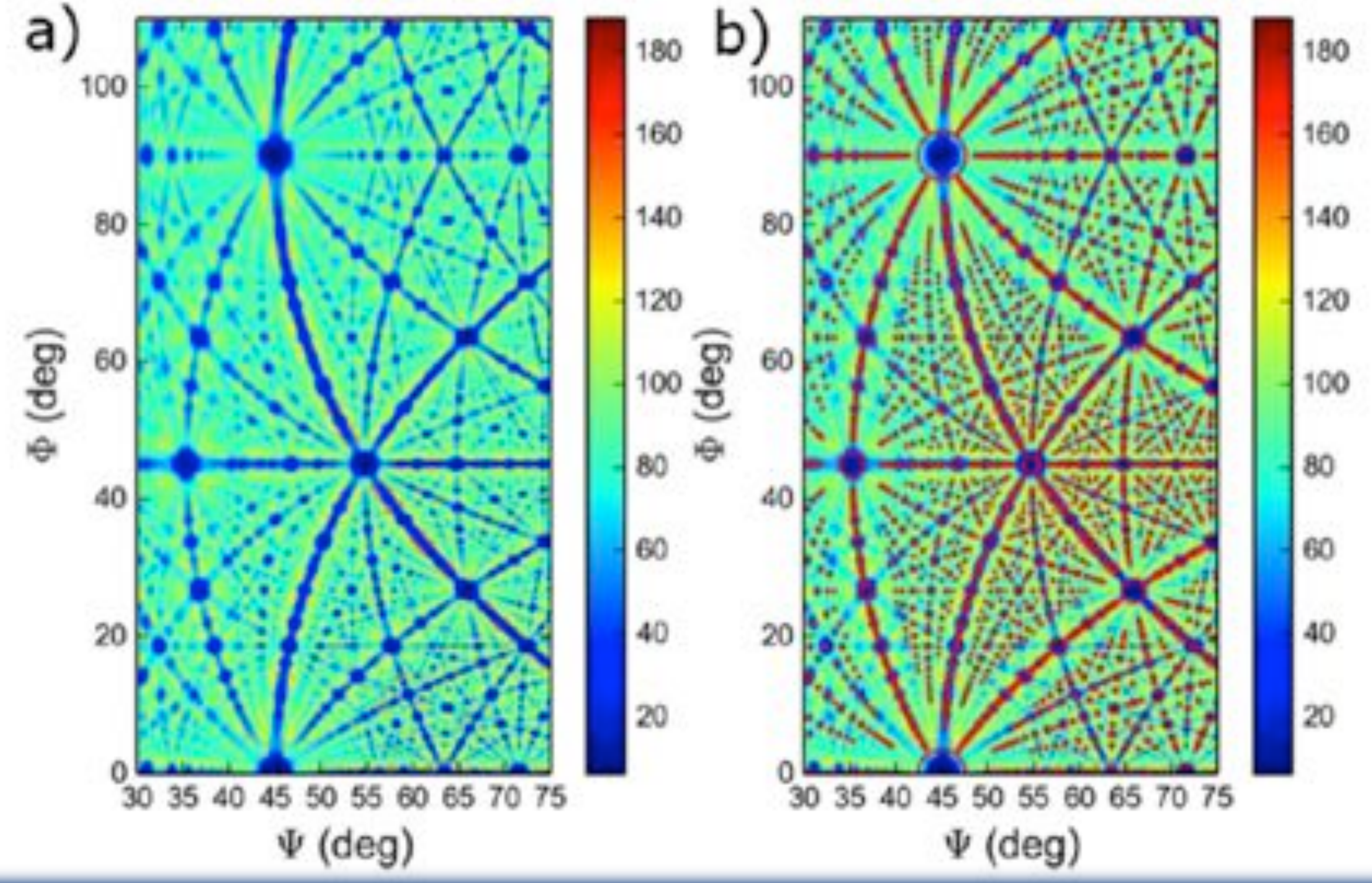
Blocking *strength* of each direction

$$w(\Psi;\Phi) = \sum_{i=1}^{N_i(\Psi;\Phi)} \frac{1}{d_i^2},$$





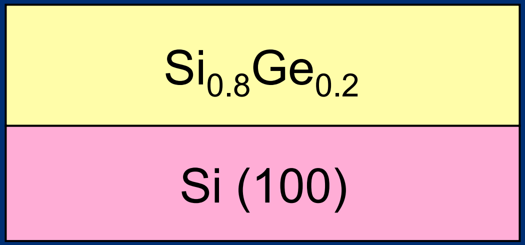
VEGAS simulation



SiGe Benchmark Samples

Table 1
Description of samples used in MEIS analysis.

Sample	SiGe thickness	Nominal strain
$Si_{0.7}Ge_{0.3}$	87 nm	2.06%
$Si_{0.8}Ge_{0.2}$	127 nm	1.33%



MBE

MEIS – 150 keV He^+ ions on SiGe

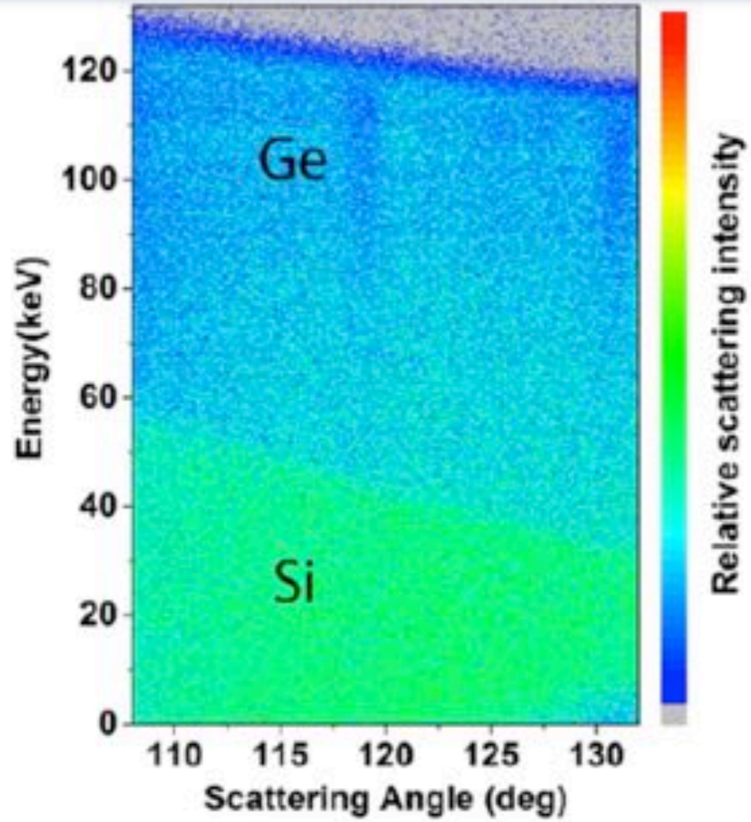
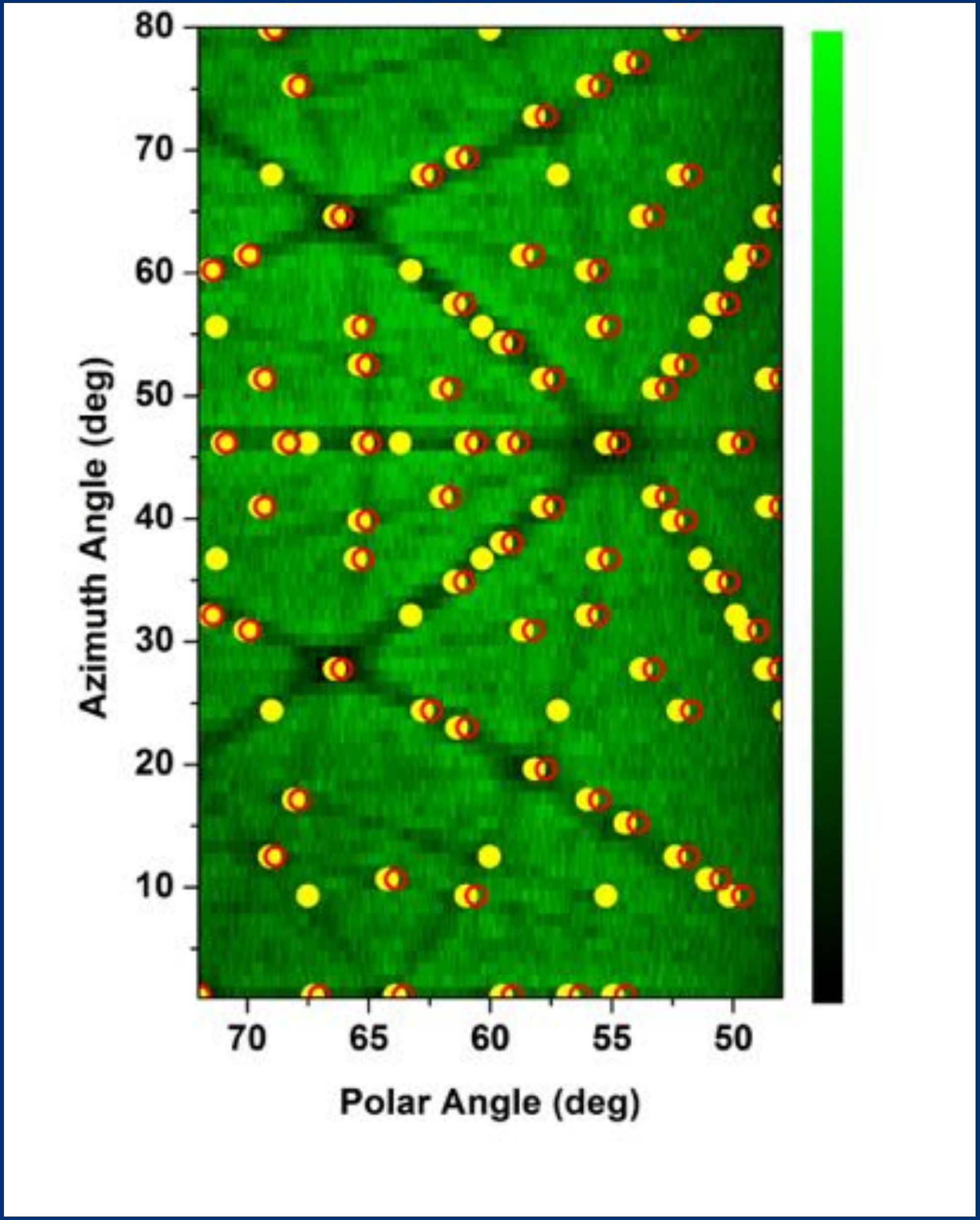


Fig. 1. 2D MEIS spectrum measured with 150 keV He^+ projectiles under normal incidence on the SiGe heterostructure grown over crystal Si. The following signals are observed from top to bottom: Ge and Si from the $Si_{0.7}Ge_{0.3}$, Si from the substrate. Blocking lines in Ge are also visible.

Cartographic map $Si_{0.7}Ge_{0.3}$

○ unstrained

● out-of-plane strained



Cartographic map : $Si_{0.7}Ge_{0.3}$

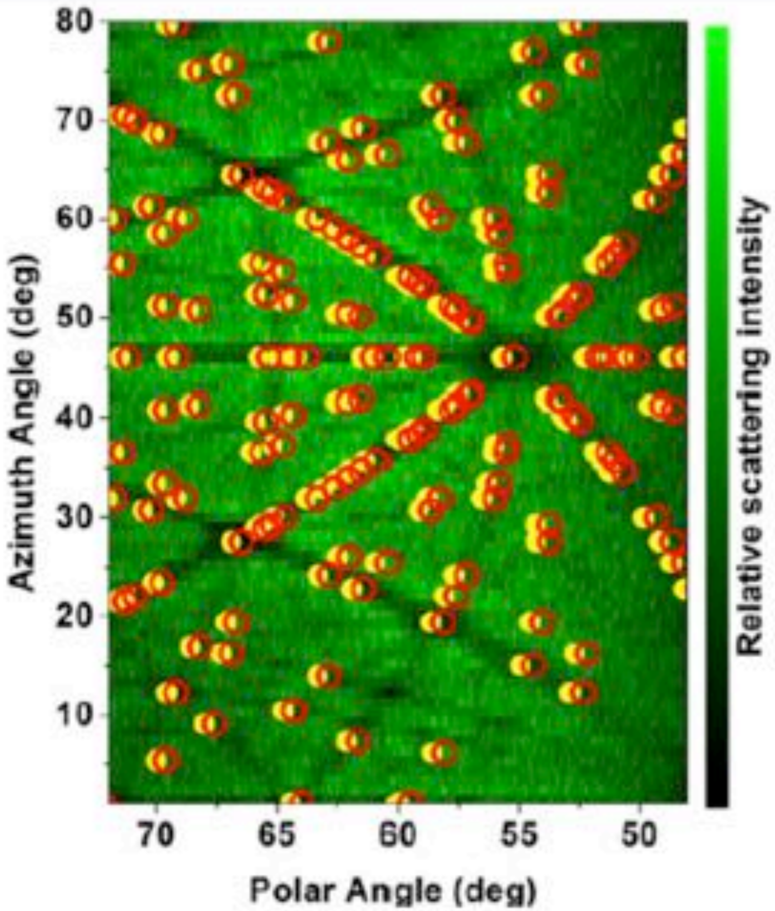


Fig. 4. Cartographic map of a strained-layer $Si_{0.7}Ge_{0.3}/Si$ using 150 keV He^{+}. Each superimposed circle corresponds to a direction in a relaxed layer (full circles) and 2% uniaxial strain (open circles).

However…..

Strain ~ $\Delta\Psi$

↓

Reference / angular calibration

Pure Si $Si_{0.8}Ge_{0.2}$

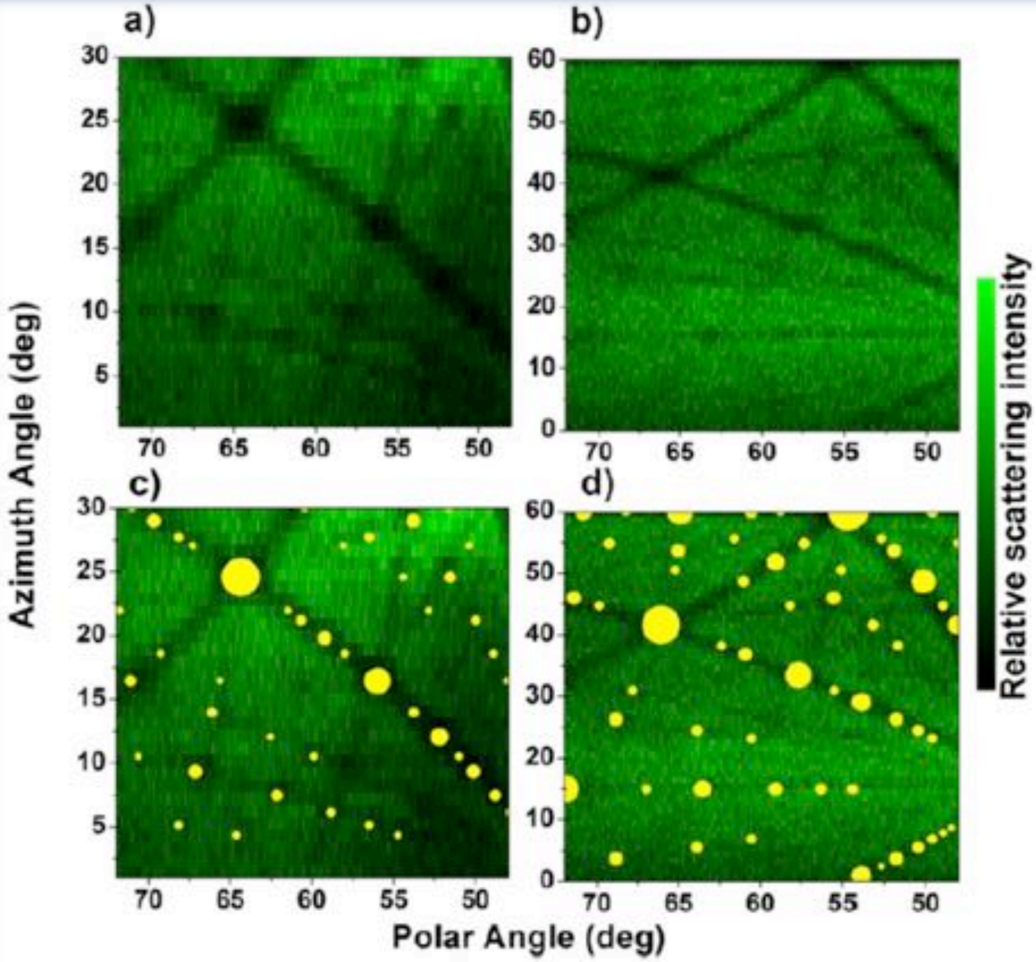
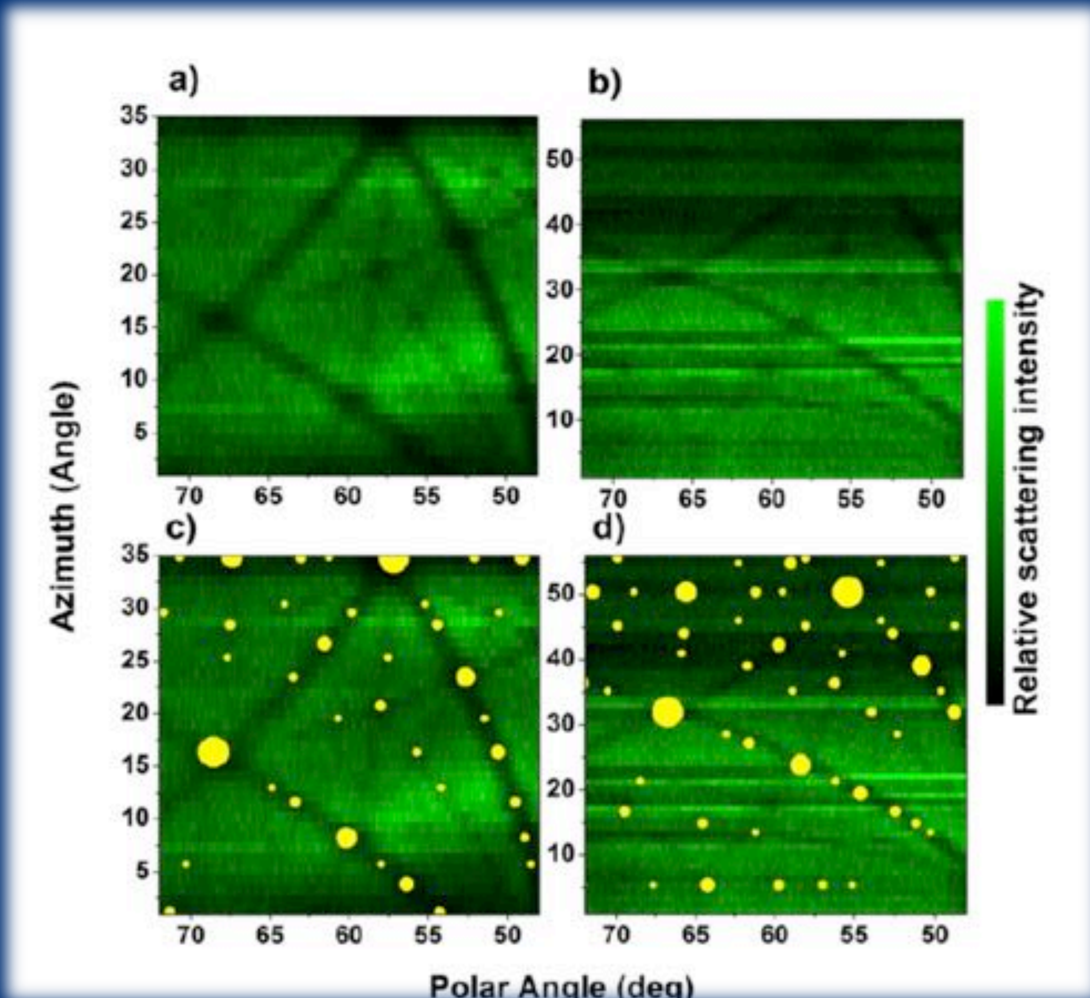


Fig. 6. (a) MEIS cartography of a reference Si (100) sample used for angular calibration. (b) MEIS cartography for $Si_{0.8}Ge_{0.2}$. (c) and (d) are the same as in (a) and (b) including the main directions represented by circles.

Pure Si $Si_{0.7}Ge_{0.3}$

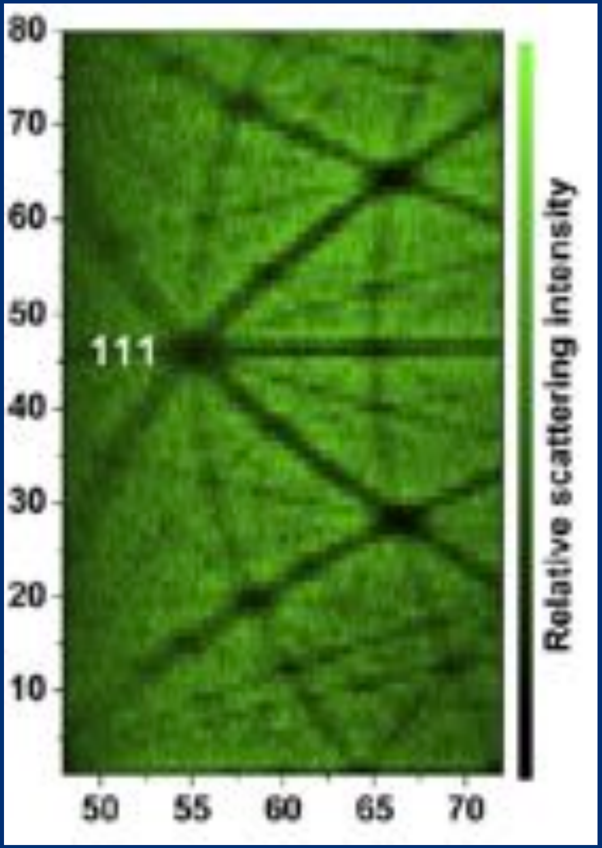


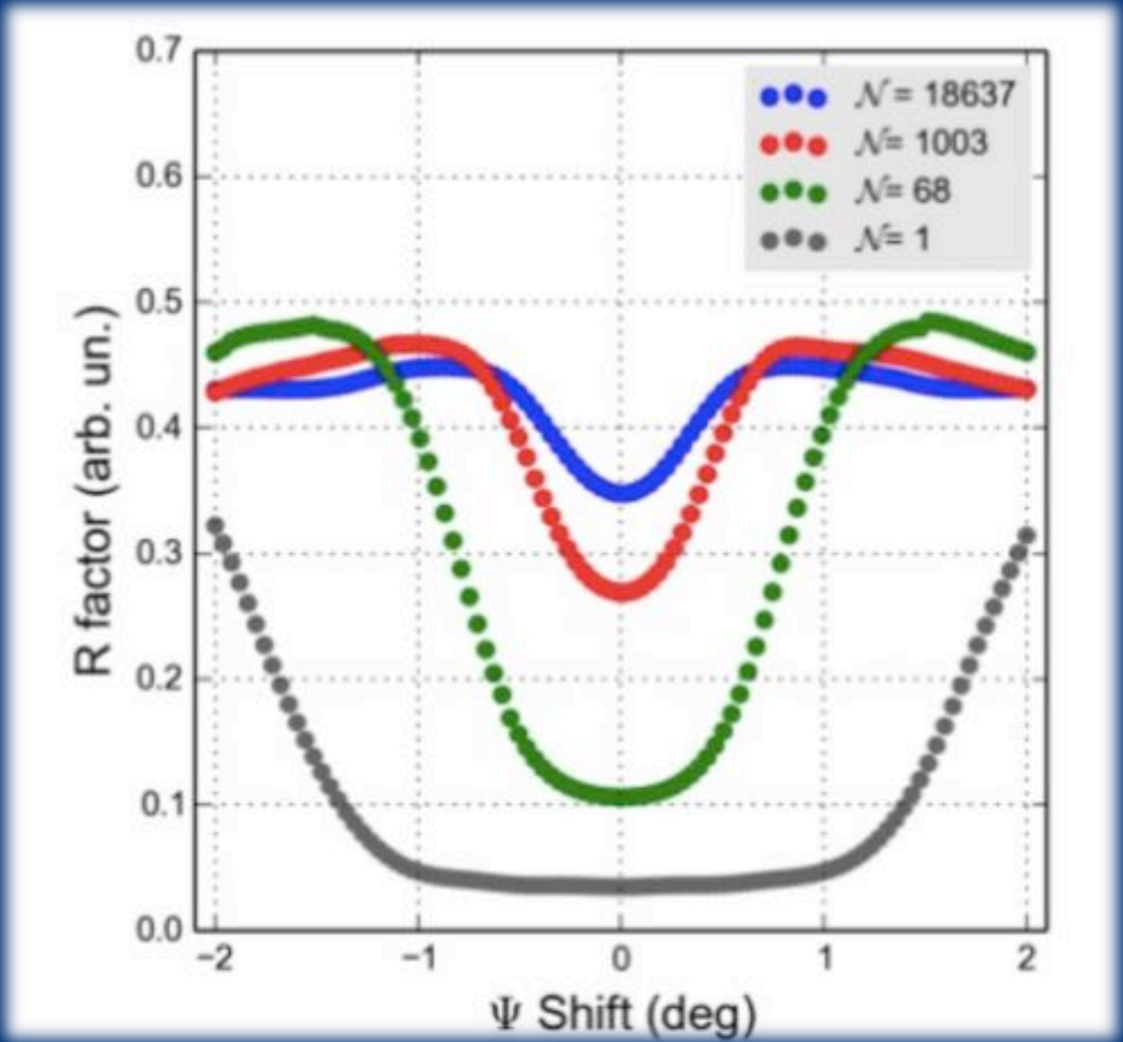
Reliability Function

$$R = \frac{1}{\mathcal{N}} \sum_{i} Y(\Psi_i, \Phi_i)$$

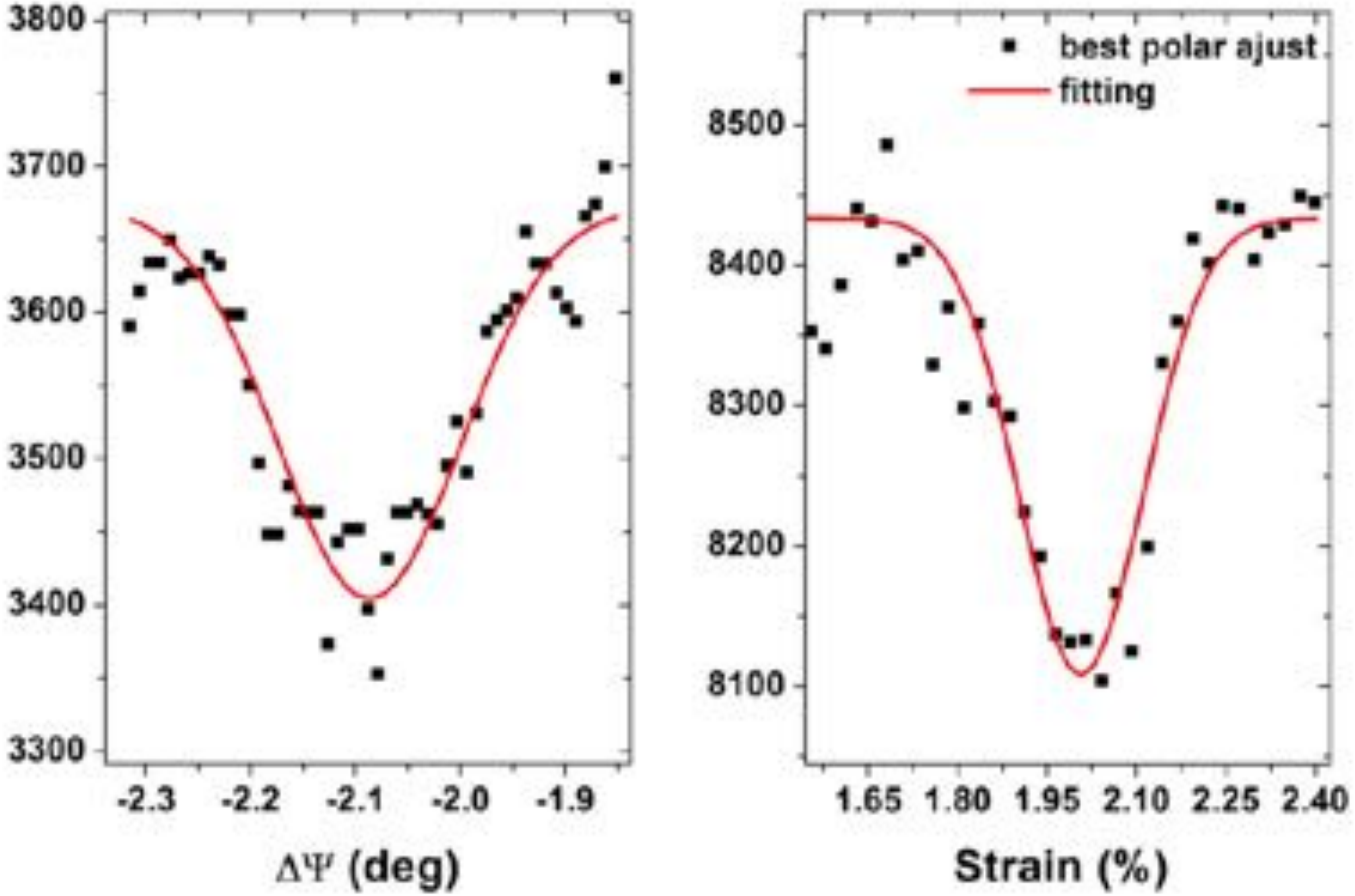
Experimental Cartography MEIS Yield

Best number of directions





Best strain

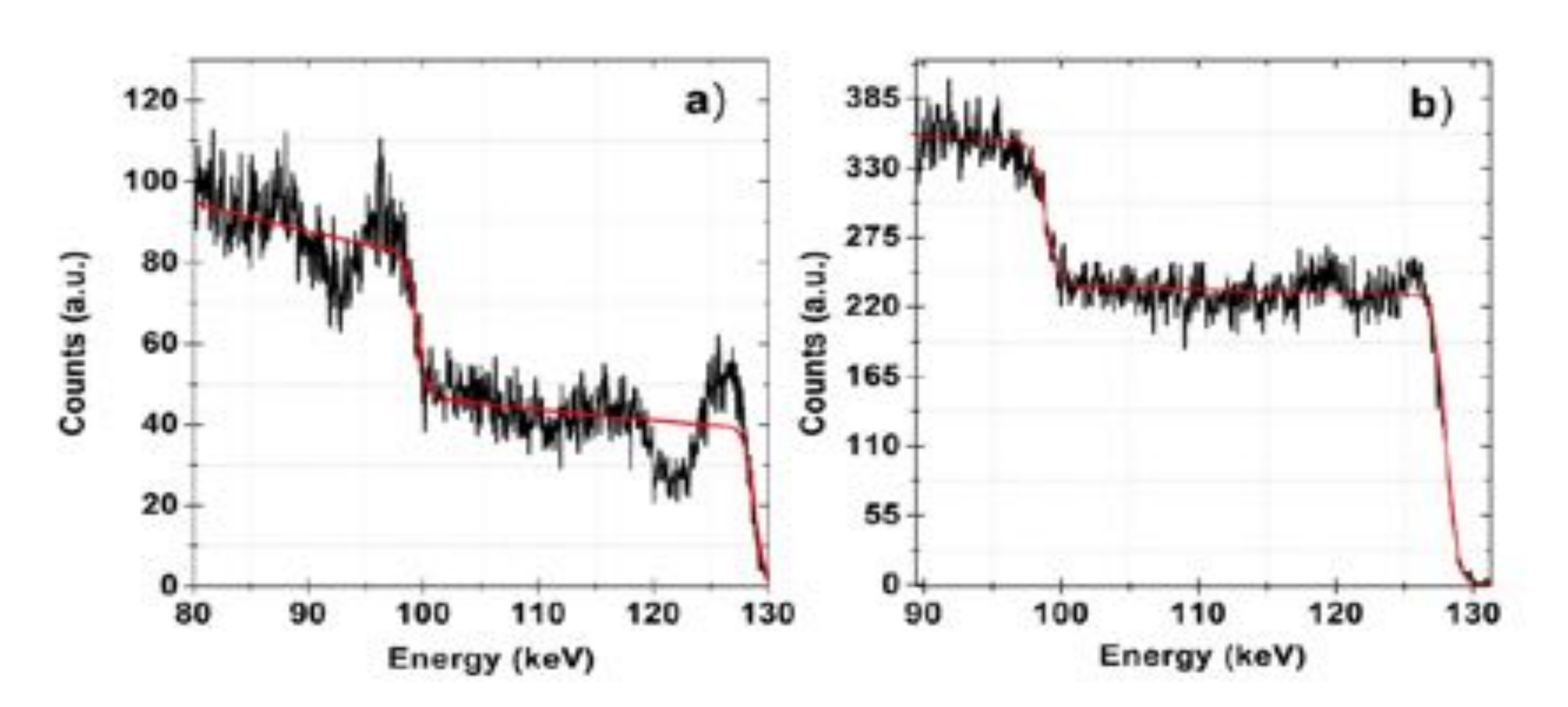

3800
3700
3600
3500
3400
3300
-2.3
-2.2
-2.1
-2.0
-1.9
ΔΨ (deg)
best polar ajust
fitting
8500
8400
8300
8200
8100
1.65
1.80
1.95
2.10
2.25
2.40
Strain (%)

MEIS Results

Table 2
MEIS results for the strain and Ge concentration.

Sample	Ge/Si concentration	Nominal strain	Measured strain	ΔΨ (deg)
$Si_{0.7}Ge_{0.3}$	0.31/0.69	2.05%	2.00% ± 0.07	0.48
$Si_{0.8}Ge_{0.2}$	0.21/0.79	1.33%	1.37% ± 0.07	0.34

Stoichiometry : Replica Method



$$F(E) \sim \alpha F_{Ge}(E-\Delta E) + F_{Ge}(E)$$

$$\alpha = \frac{\sigma_{Si}}{\sigma_{Ge}} \boxed{\frac{N_{Si}}{N_{Ge}}} \frac{[S]_{Ge}}{[S]_{Si}}$$

Summary

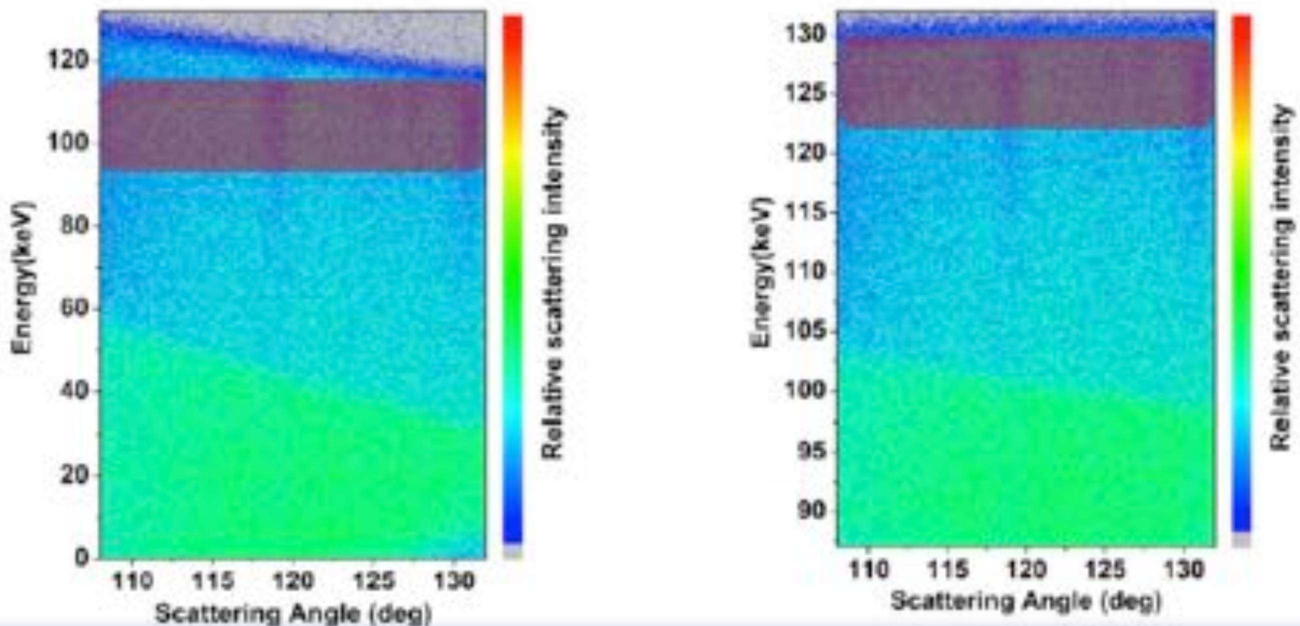
- Cartography method to measure the lattice deformation in a model-case material consisting of strained $Si_{1-x}Ge_x/Si$ heterogeneous epitaxial structures.

- The higher index directions are more sensitive to strain and lead to a clear quantification of the strain.

- We have proposed a method to analyze the map of ion scattering intensities as a function of polar and azimuthal angles and cross checked it using full VEGAS calculations.

Perspectives

- It can be extend to analyze depth-dependent strain in thin films or any other nano-structured material..



Thank you for your attention !