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Determination of Bi positions in $GaAs_{(1-x)}Bi_x$ heterostructures with atomic column resolution

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The University of Nottingham

M.F. Chisholm

Oak Ridge National Laboratory

UCA
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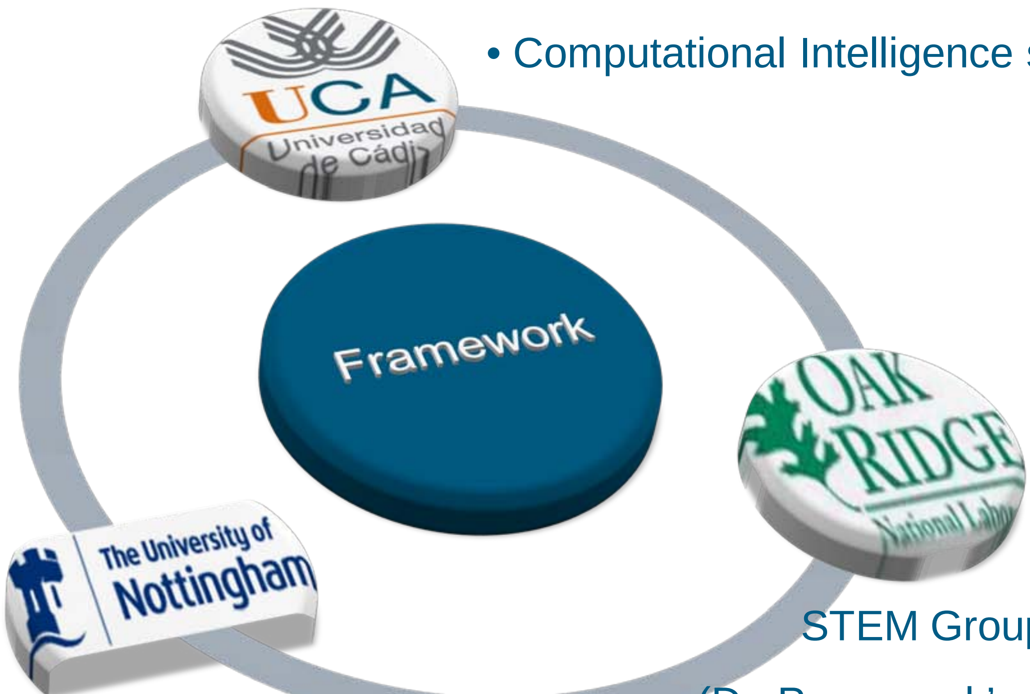
Framework

- Materials Science & Engineering Group
- Computational Intelligence systems



STEM Group

(Dr. Pennycook's group)

Dr. Henini's Group

Transmission electron microscopes

JEOL 2010 FEG

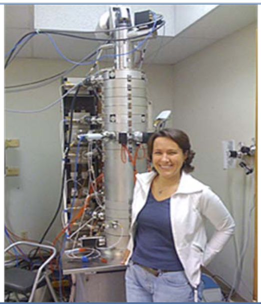
JEOL 2011 LaB_6

JEOL 1200 EX

Aberration-corrected

VG-HB603

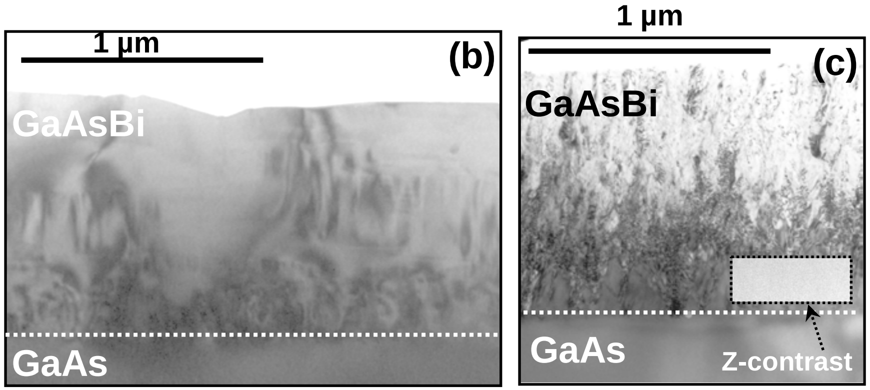
VG-HB501



NION UltraSTEM

Previous TEM work in GaAsBi

- **Molecular beam epitaxy of GaAsBi on (311)B GaAs substrates**



(001) **(311)B**

M. Henini et al. Appl. Phys. Lett. **91, 251909 2007**

Previous TEM work in GaAsBi

J. F. Rodrigo et al. Applied Surface Science 256 (2010) 5688–5690

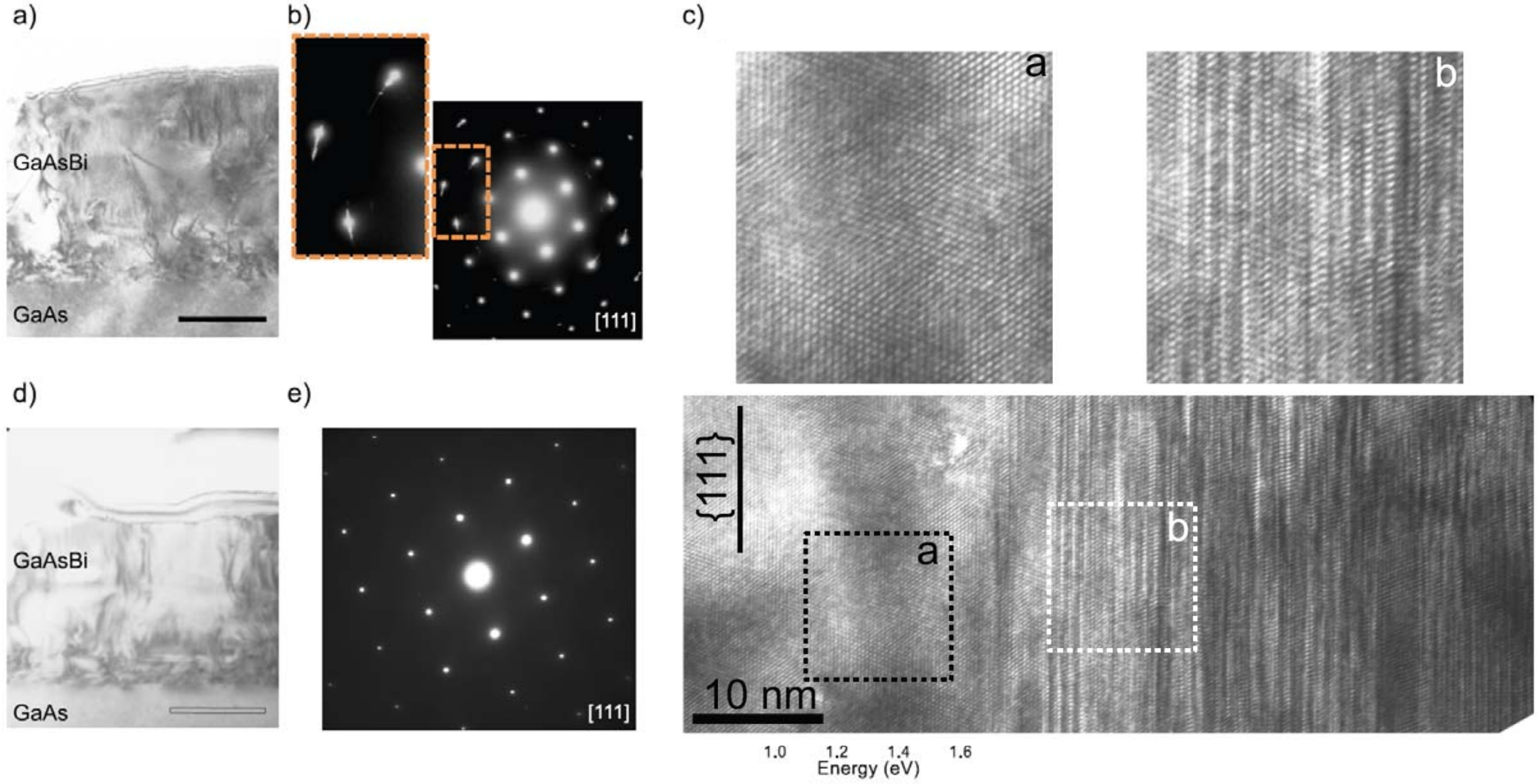


Fig. 1. Bright field TEM images, diffraction patterns and photoluminescence spectra of the as grown sample S1 (a, b and c) and annealed sample S2 (d, e and f). Scale bar corresponds to 500 nm.

Other nano-tools

• Focussed Ion Beam

FEI DUAL BEAM FEI QUANTA 200 3D

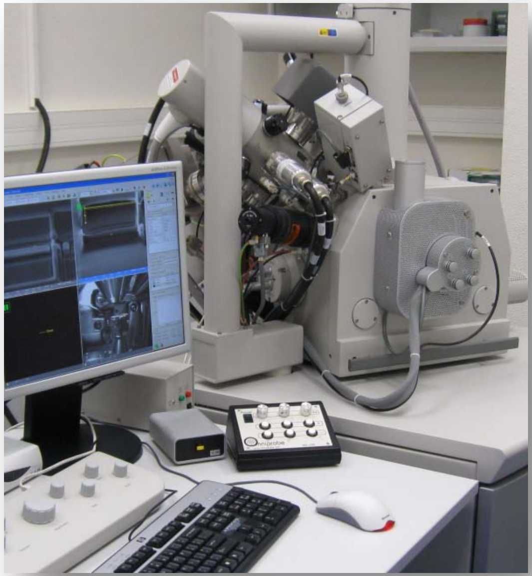
- Nano-machinning

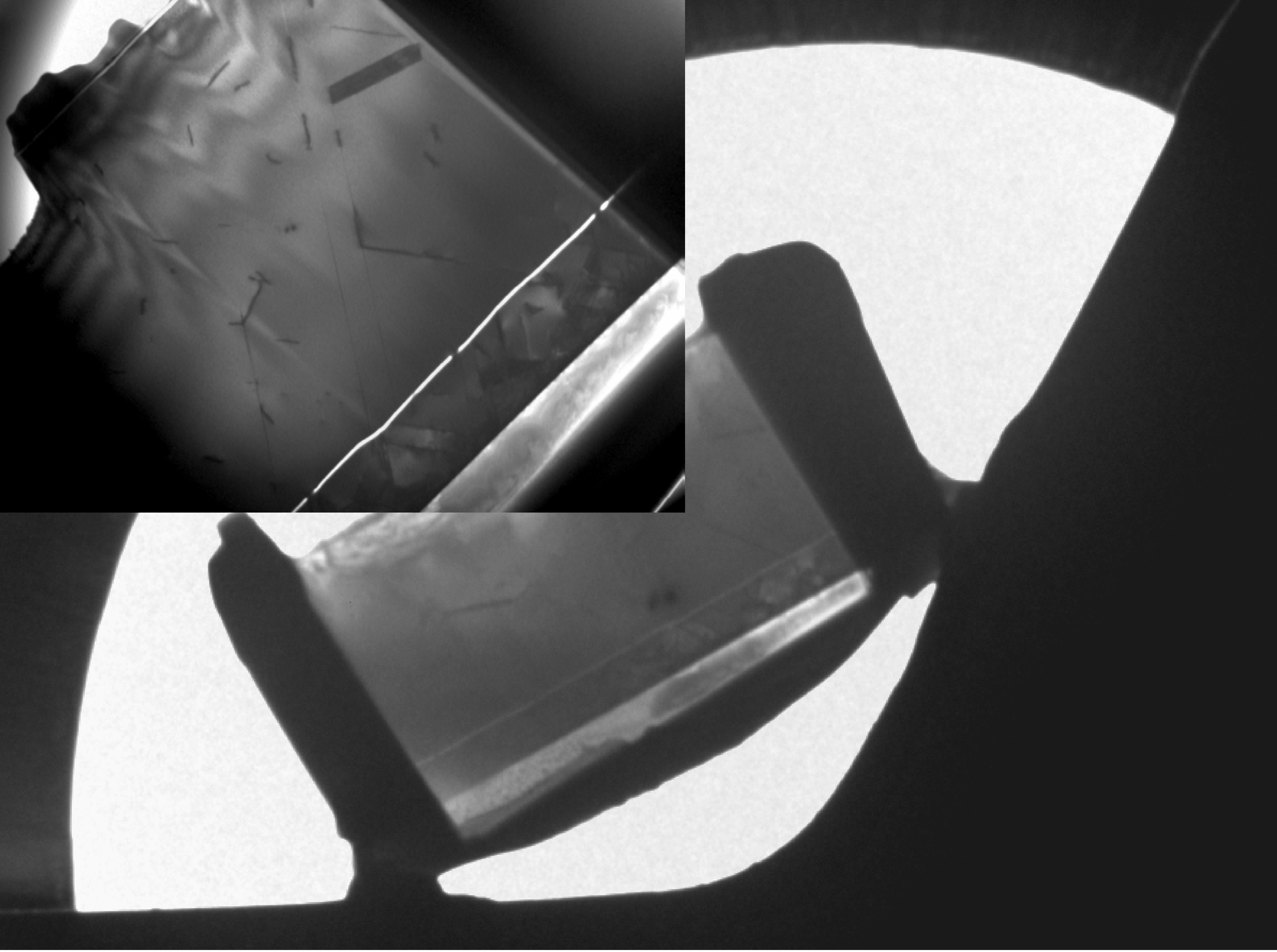
-3D sample preparation for tomopraphy of localized areas.

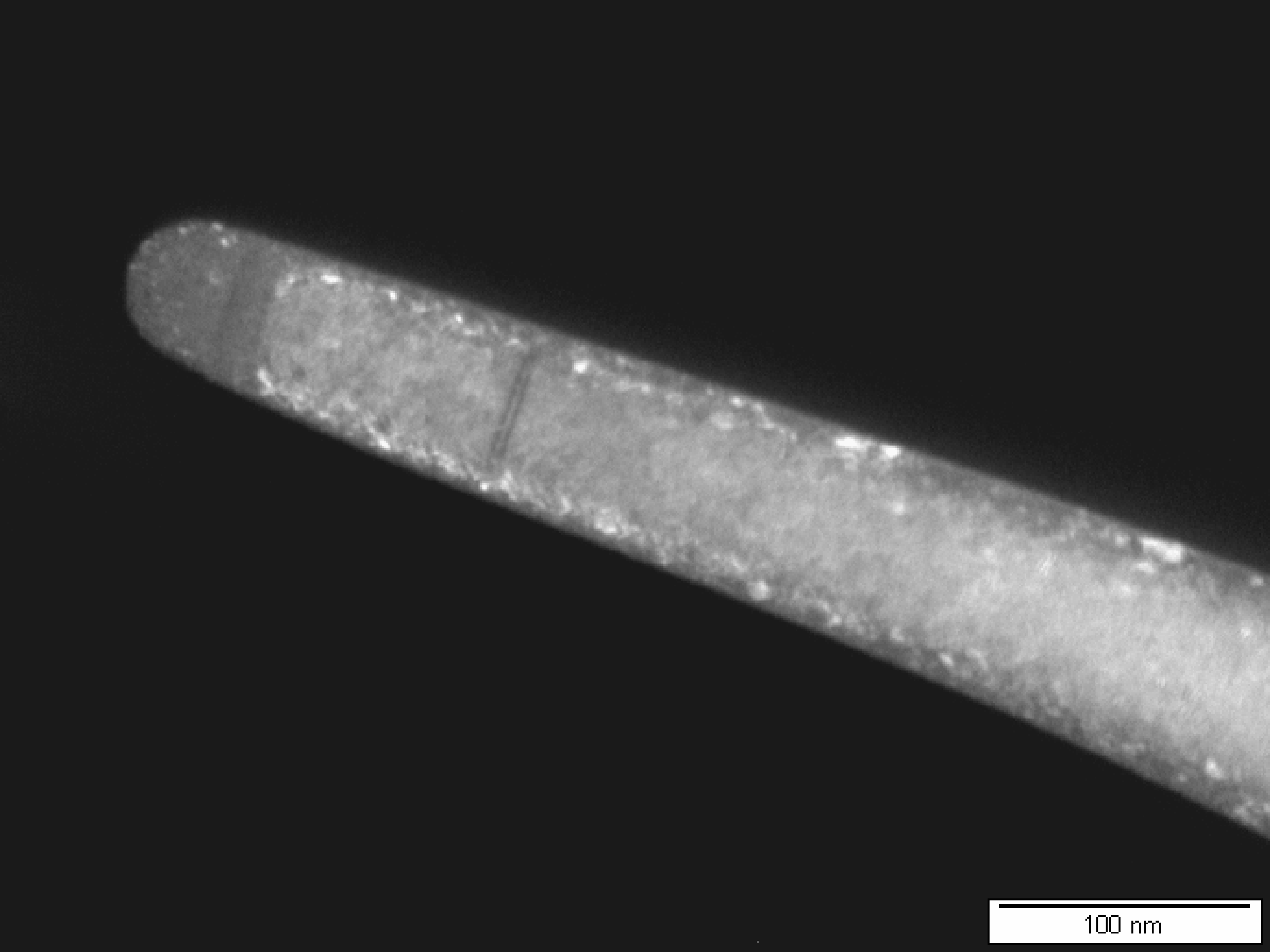
- Substrates nano-patterning

- As ions imaging

-3D tomography






100 nm

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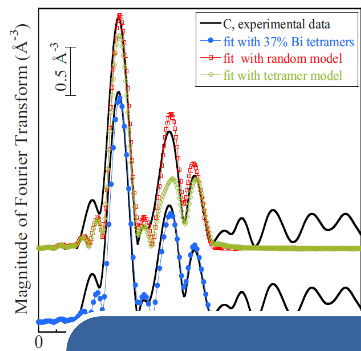
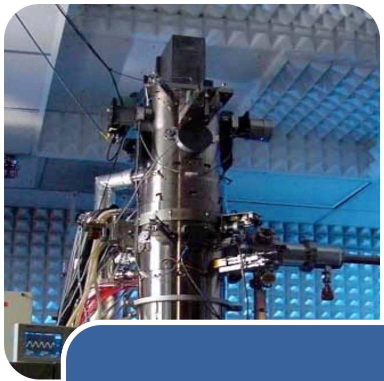
The Motivation

Bi Nanoclusters would explain PL enhancement



There are some experimental evidences



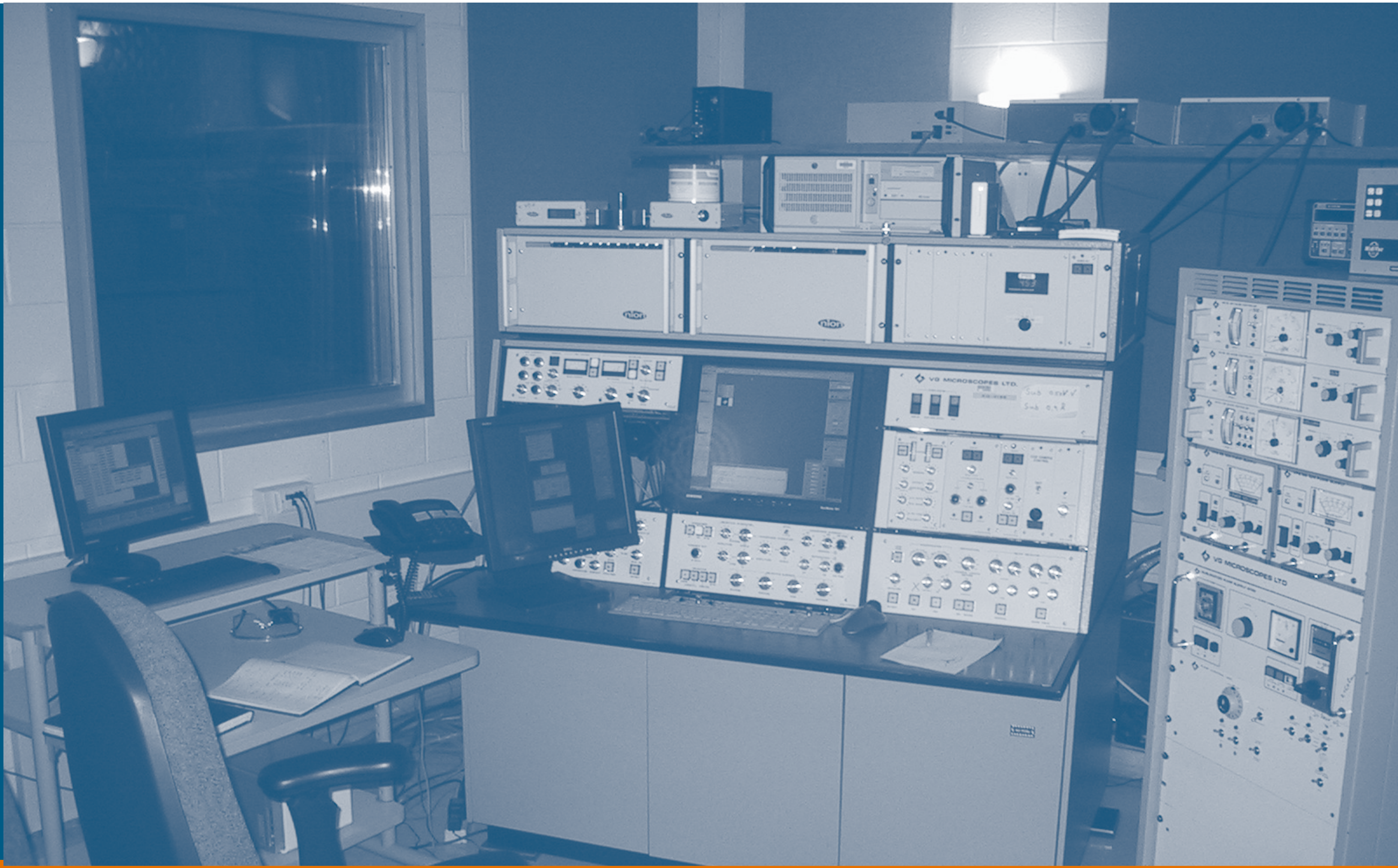
So… ¿can we see them?

PHYSICAL REVIEW B 78, 035325 (2008)

Spatial correlation between Bi atoms in dilute $GaAs_{1-x}Bi_x$: From random distribution to Bi pairing and clustering

G. Ciatto,[1,*] E. C. Young,[2] F. Glas,[3] J. Chen,[4] R. Alonso Mori,[4] and T. Tiedje[2]

Methodology and materials



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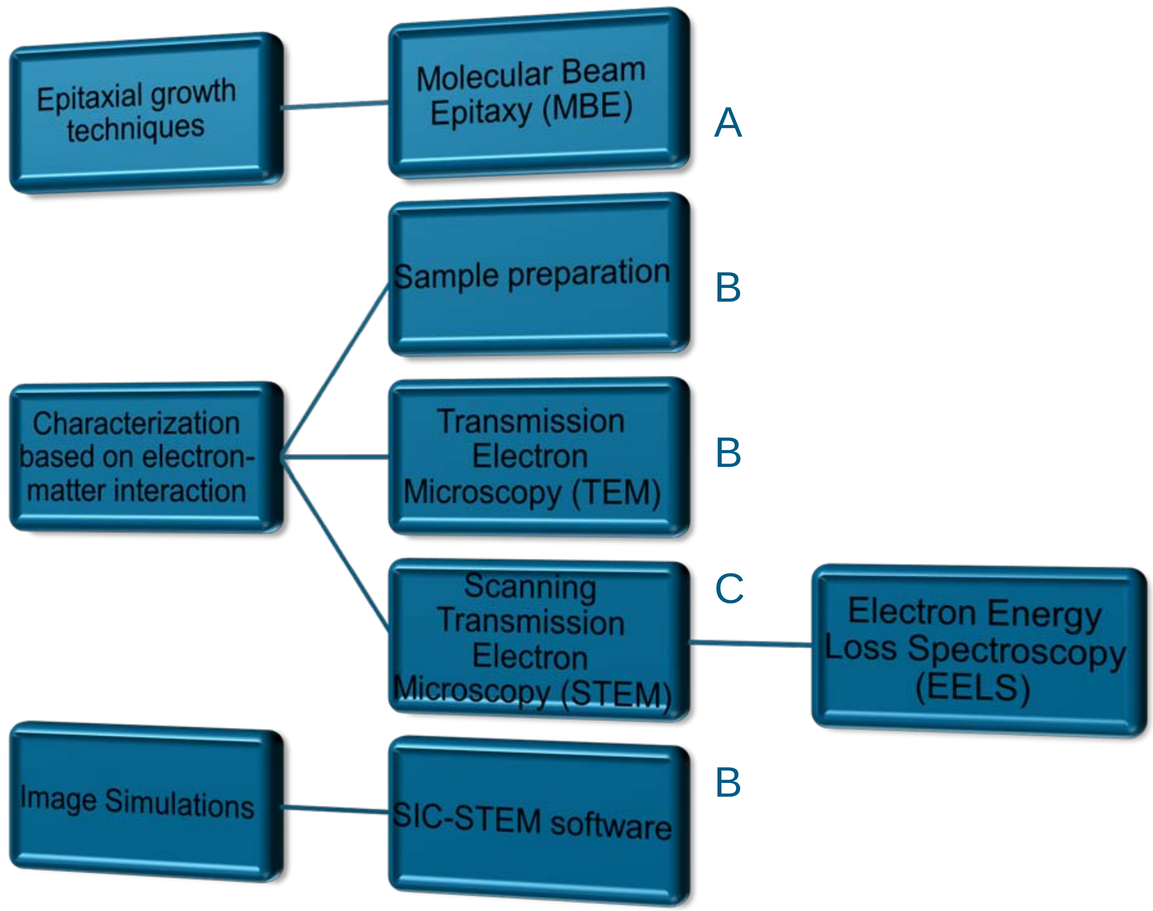
Experimental techniques



A The University of Nottingham

B UCA Universidad de Cádiz

C Oak Ridge National Laboratory

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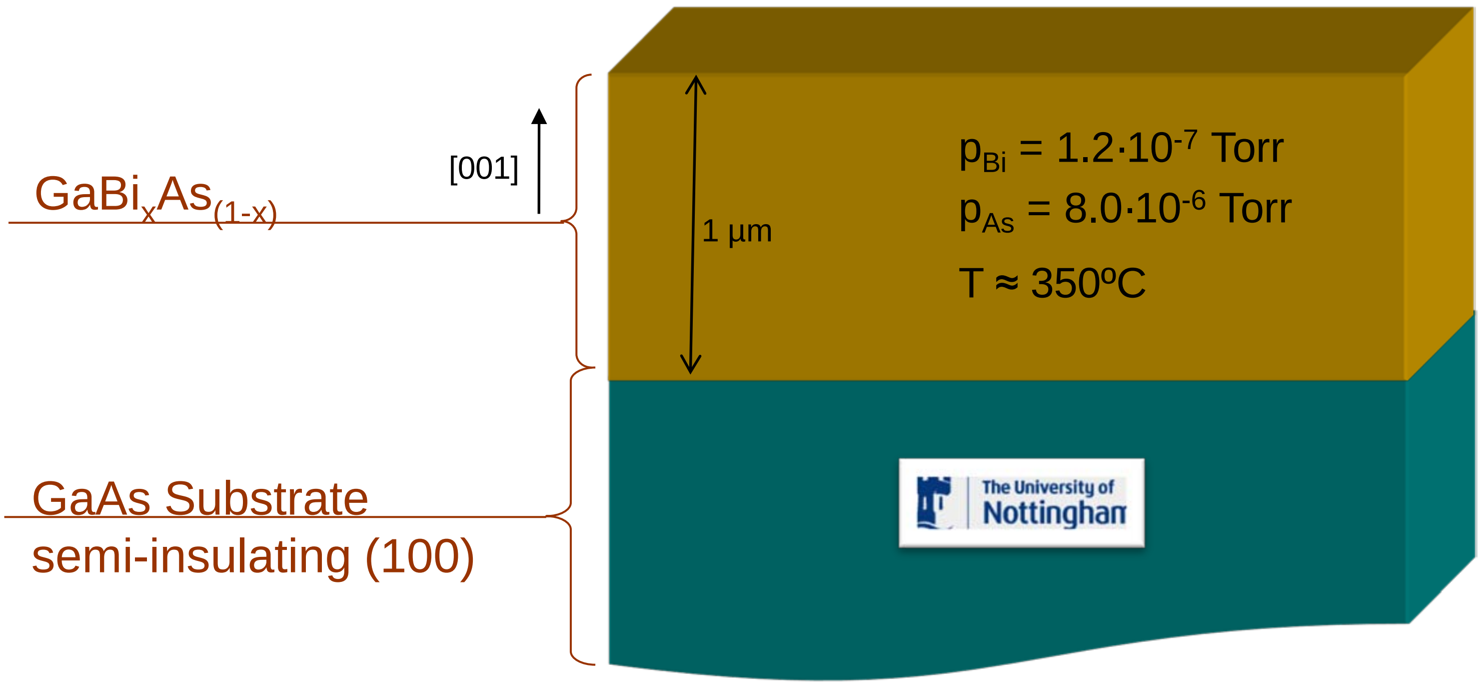
The sample

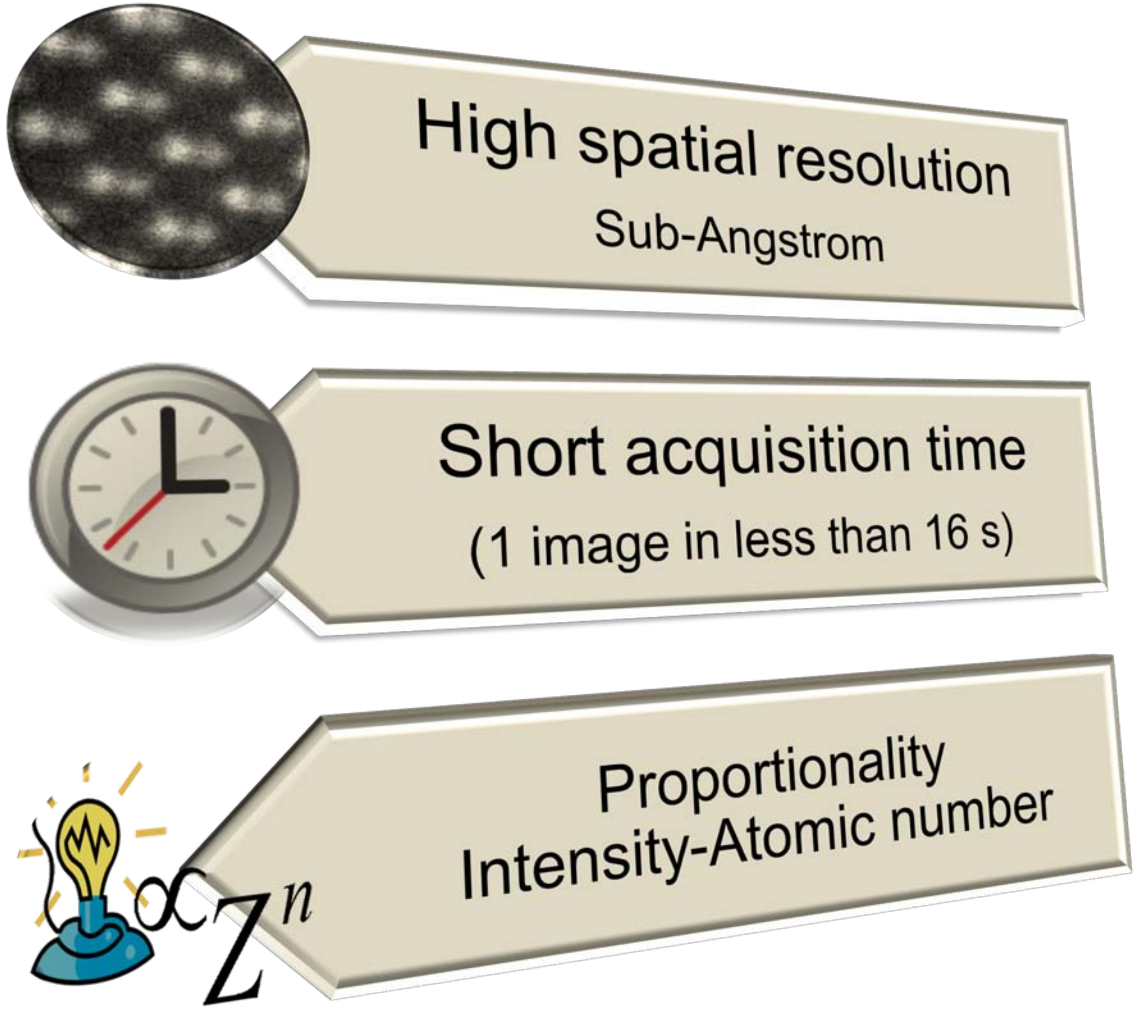


Region of near stochiometric growth

HRXRD → $x \approx 0.03$

Henini et al. APL **91**, 251909 (2007)

Why HAADF?



High spatial resolution
Sub-Angstrom
Short acquisition time
(1 image in less than 16 s)
Proportionality
Intensity-Atomic number
∝Z^n

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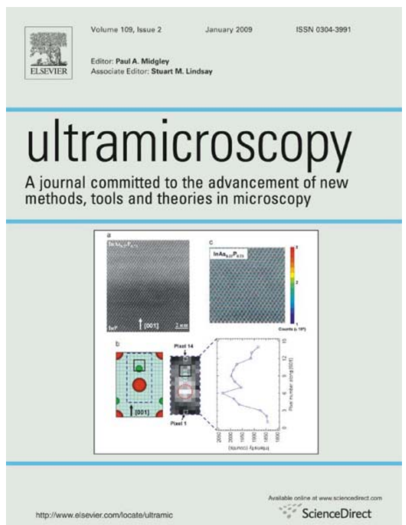
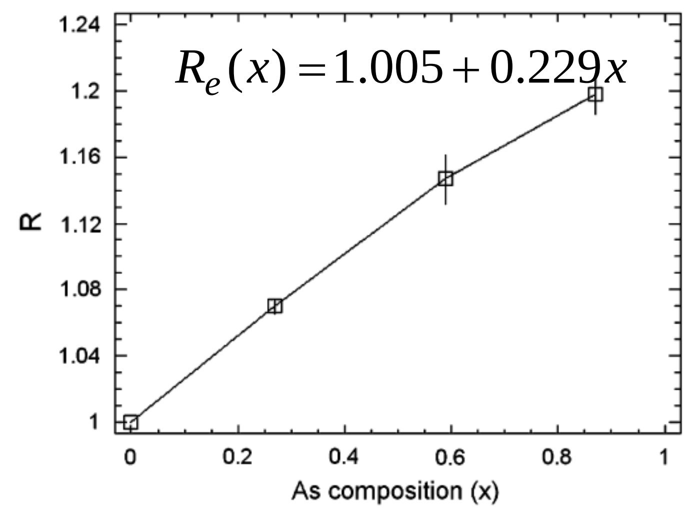
Why HAADF?

- **For a ternary alloy:**
  - **Linear relationship**

    Intensity quotient (R) vs. Composition.

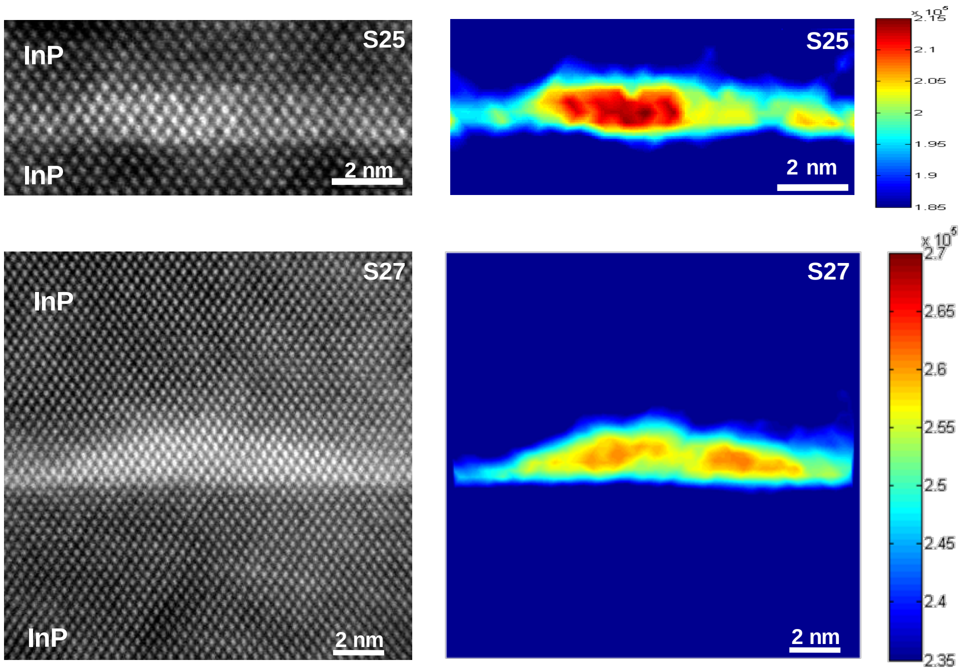




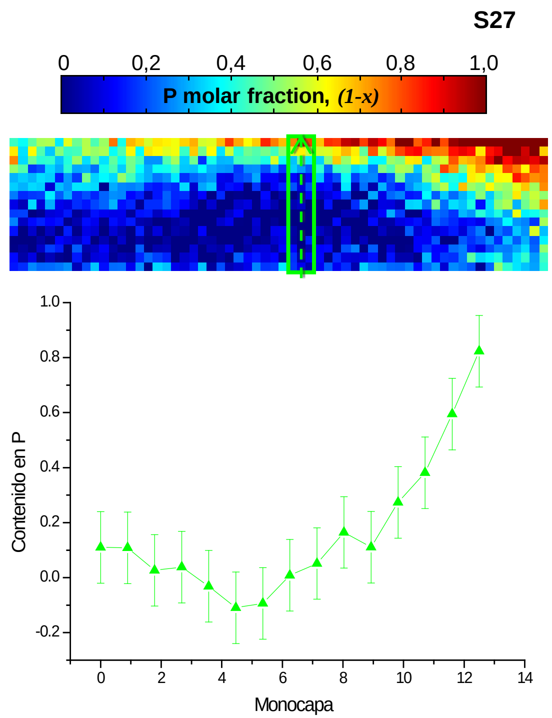
Column-by-column compositional mapping by Z-contrast imaging
S. I. Molina et al. Ultramicroscopy 109 (2009) 172–176

Quantitative Compositional analysis

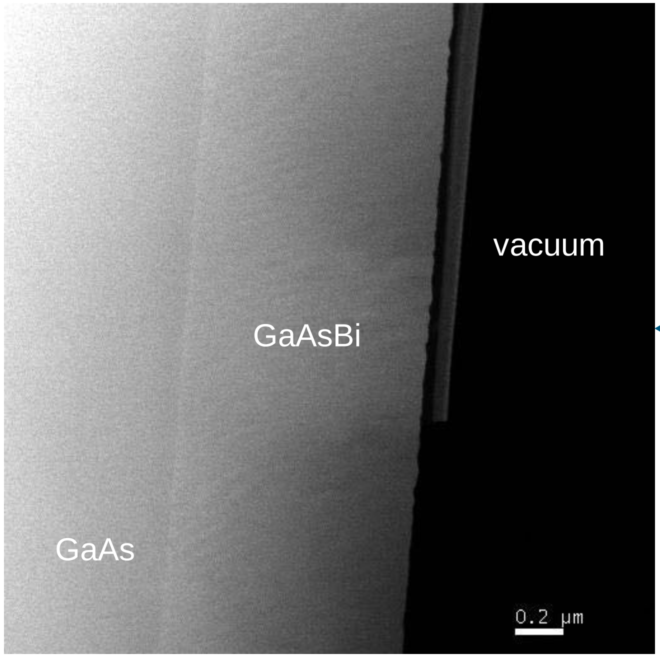
HAADF

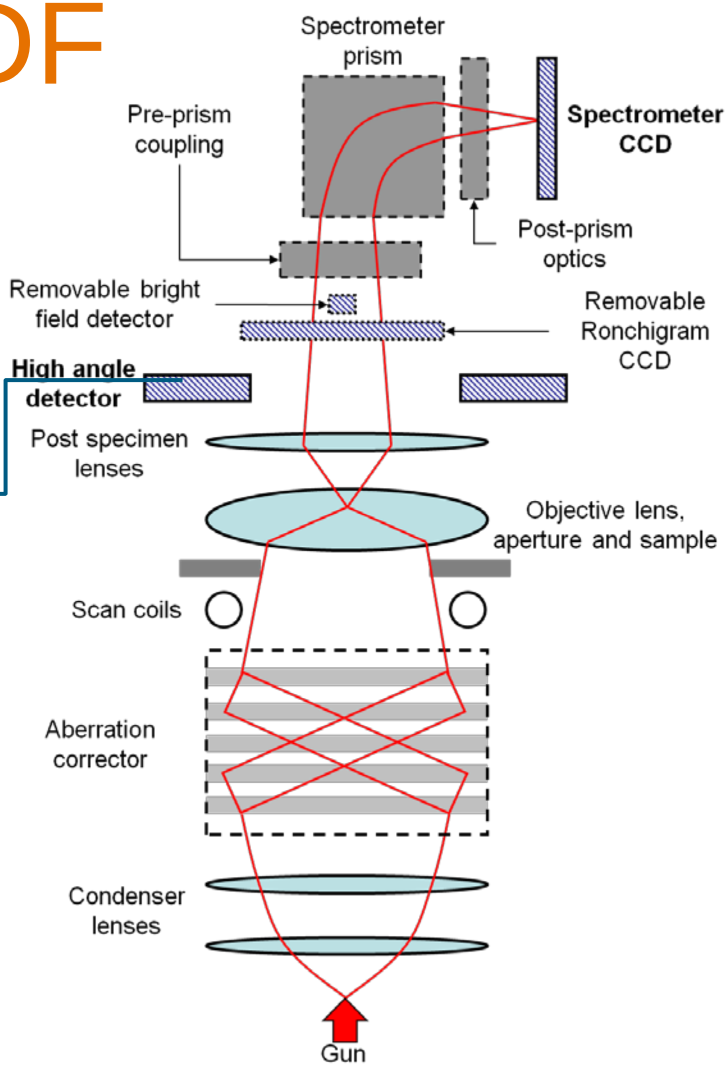


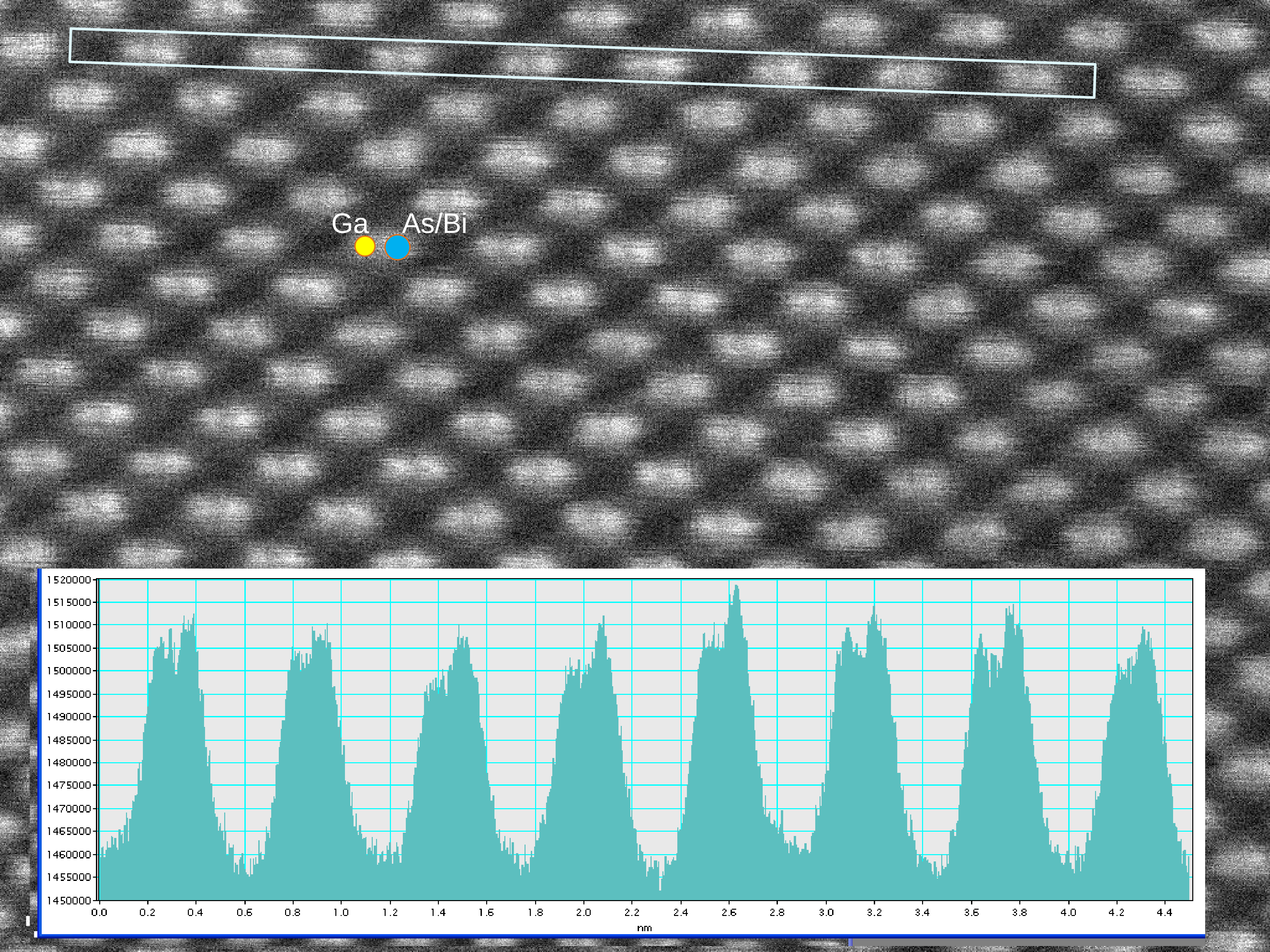
EELS



STEM - HAADF


vacuum
GaAsBi
GaAs
0.2 μm


Spectrometer prism
Pre-prism coupling
Spectrometer CCD
Post-prism optics
Removable bright field detector
Removable Ronchigram CCD
High angle detector
Post specimen lenses
Objective lens, aperture and sample
Scan coils
Aberration corrector
Condenser lenses
Gun


Ga
As/Bi
nm

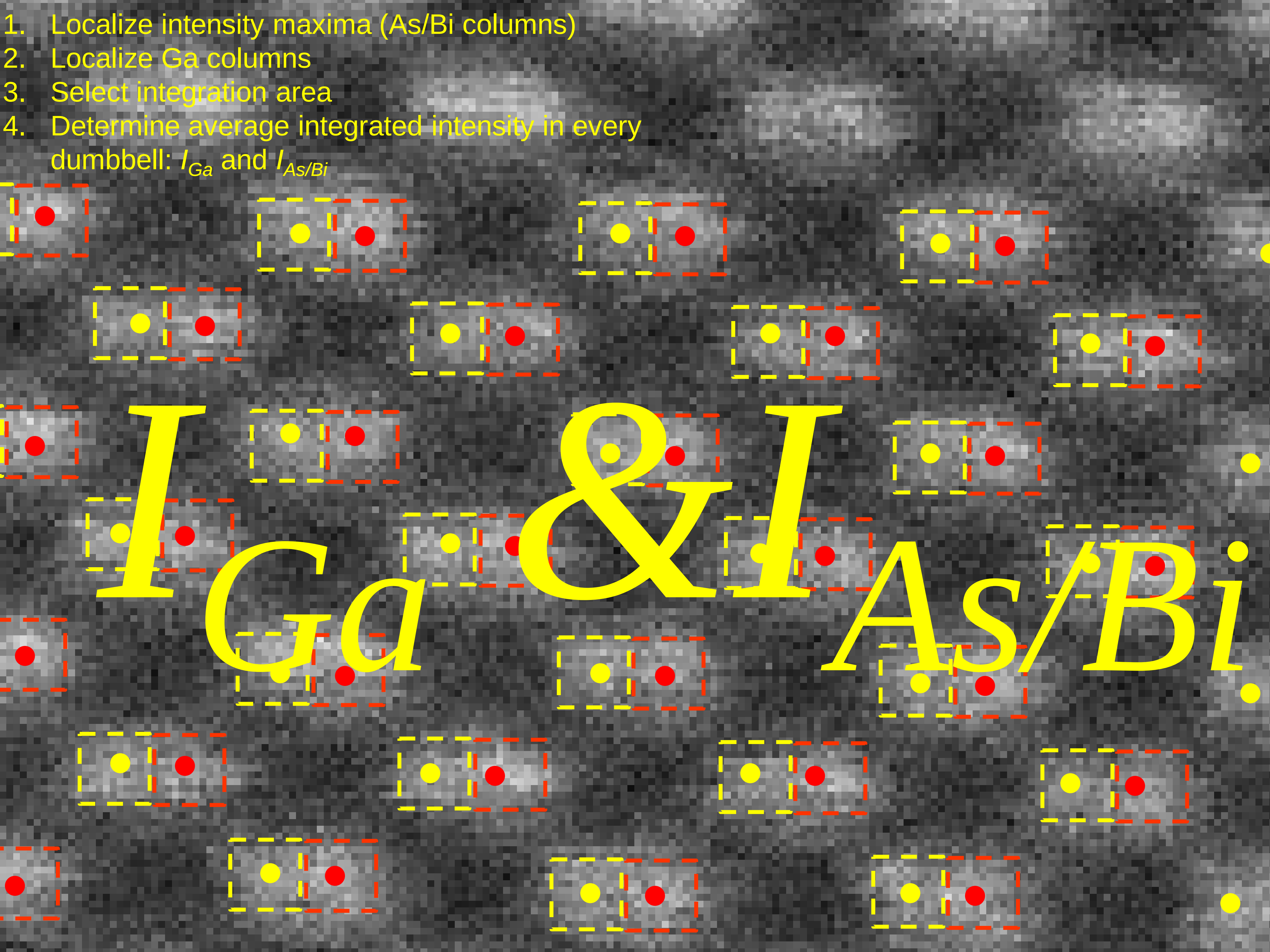
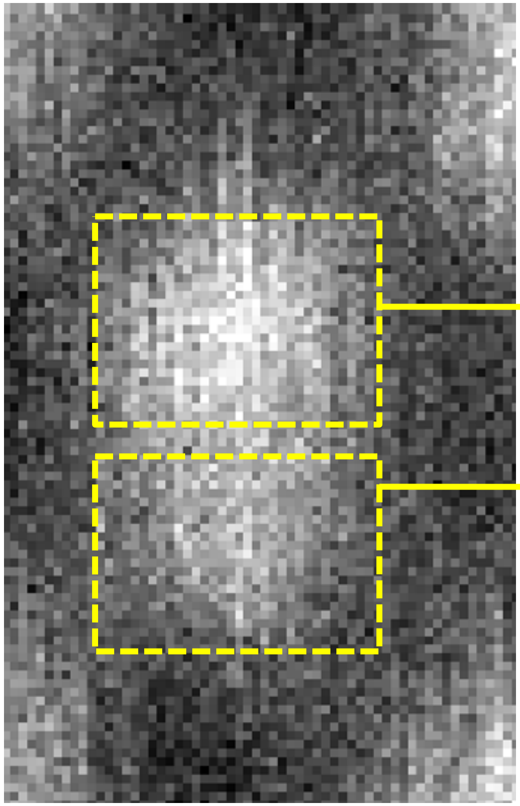

1. Localize intensity maxima (As/Bi columns)
2. Localize Ga columns
3. Select integration area
4. Determine average integrated intensity in every dumbbell: I_{Ga} and $I_{As/Bi}$
I_{Ga} & $I_{As/Bi}$

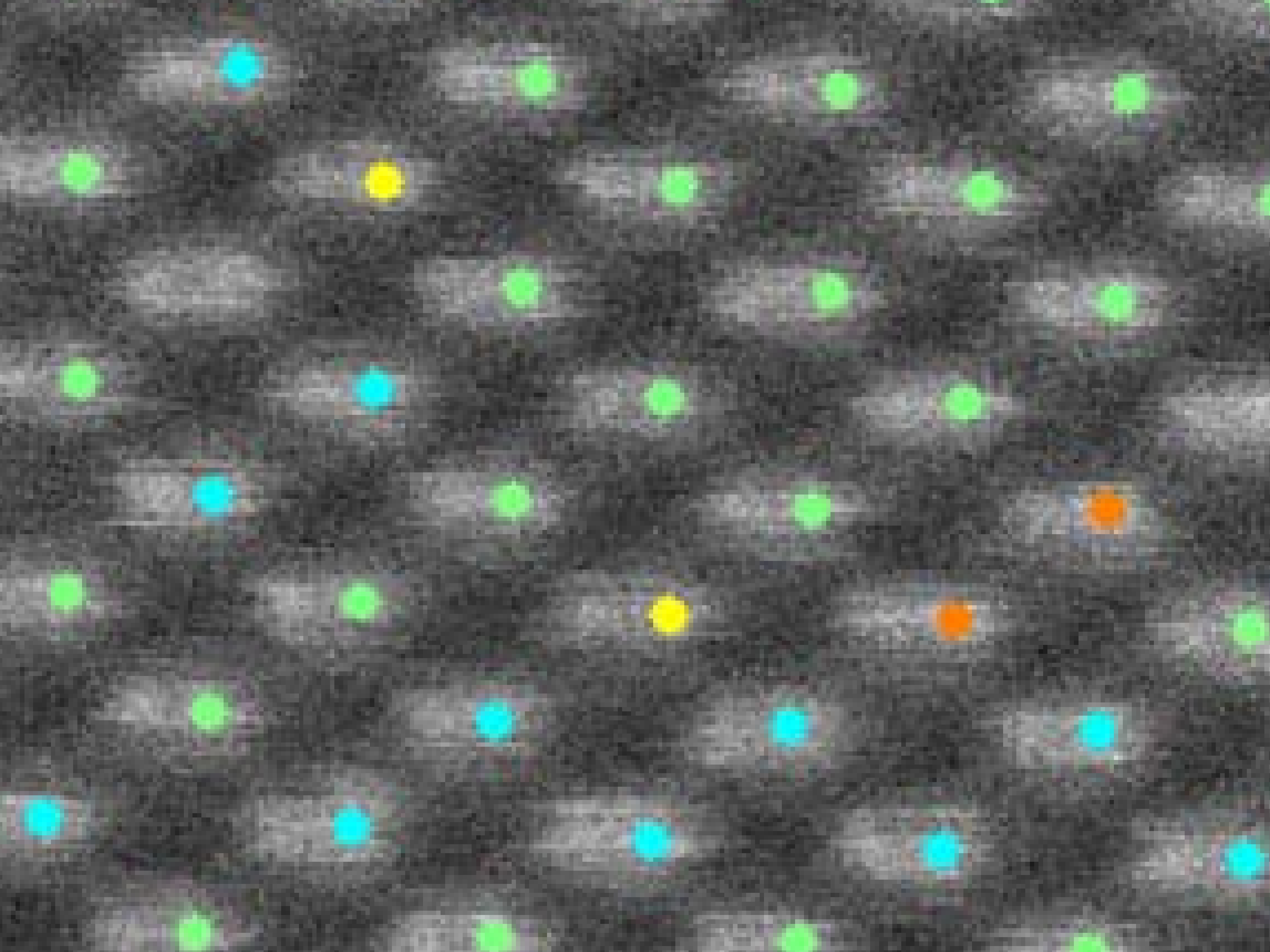
Image processing

• Determining *R* factors:

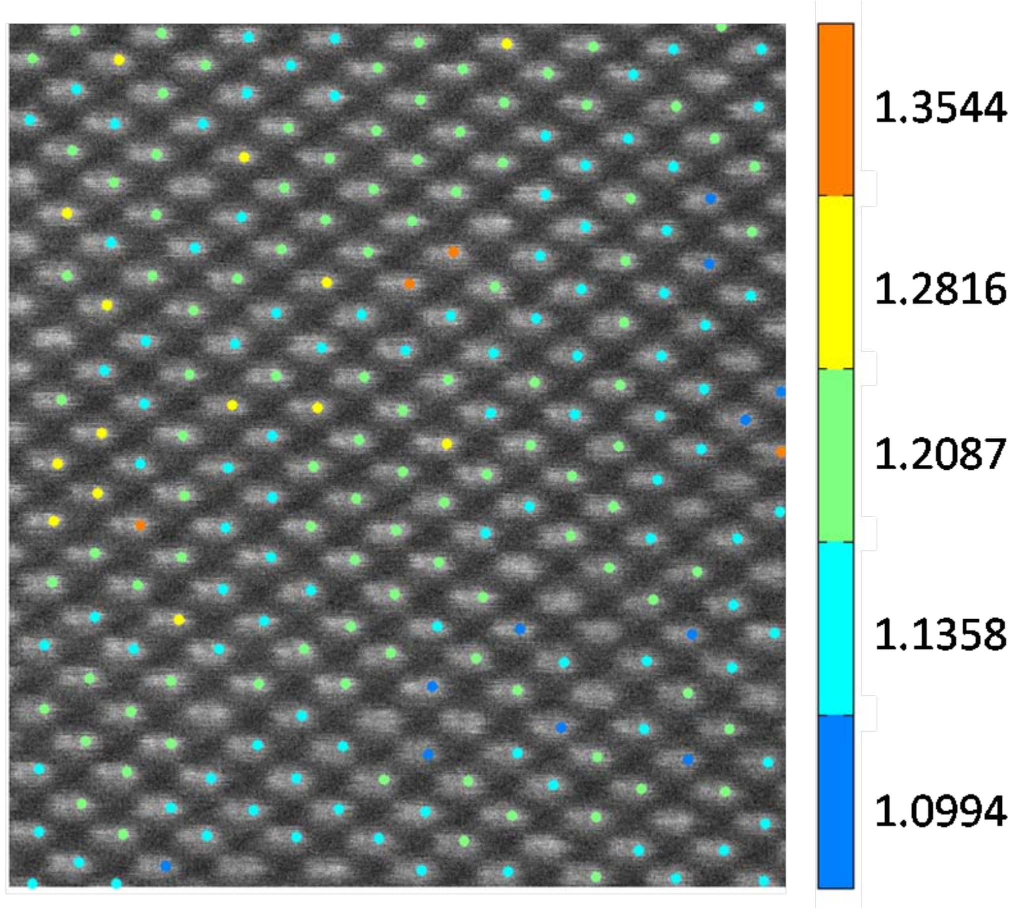


$$\frac{I_{As/Bi}}{I_{Ga}} = R(x)$$

Minimize variations due to:
• Same local thickness
• Same amorphous layer
• Same experimental image conditions



Plotting R



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Analysis

- **In order to relate *R* with *x* (Bi content):**

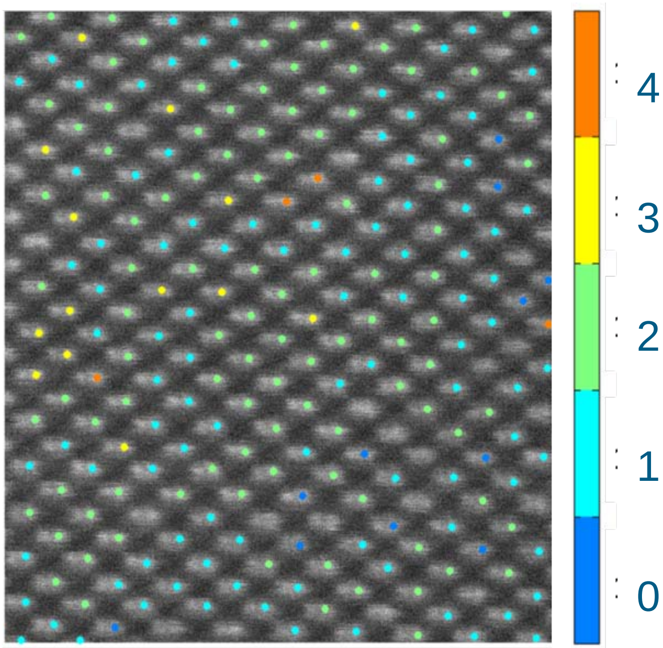
$$\sum_{i=1}^{N} R_i = N + a\sum_{i=1}^{N} x_i$$

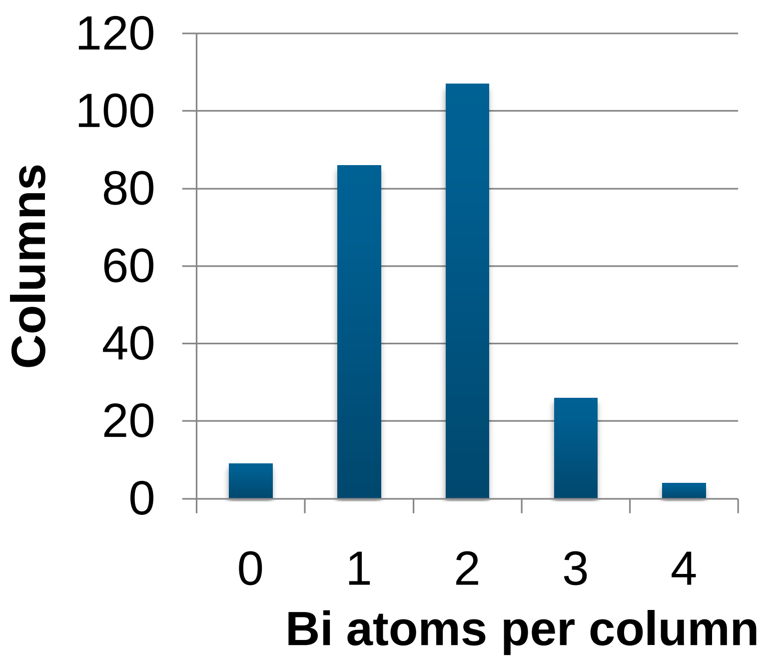
N, the number of atomic columns,
x_i = Bi percentage per column,
Σx_i=2.65% total Bi percentage

- **Fitting equation:**

$$R = 1.0629 + 0.0729x$$

Results





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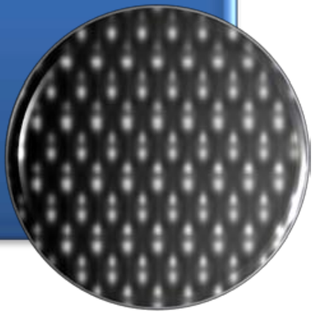
The next step…

Solving the Schrödinger stationary equation

$$\frac{\hbar^2}{2m_0}\Delta|\Psi\rangle+[E_t-\hat{V}]|\Psi\rangle=0$$

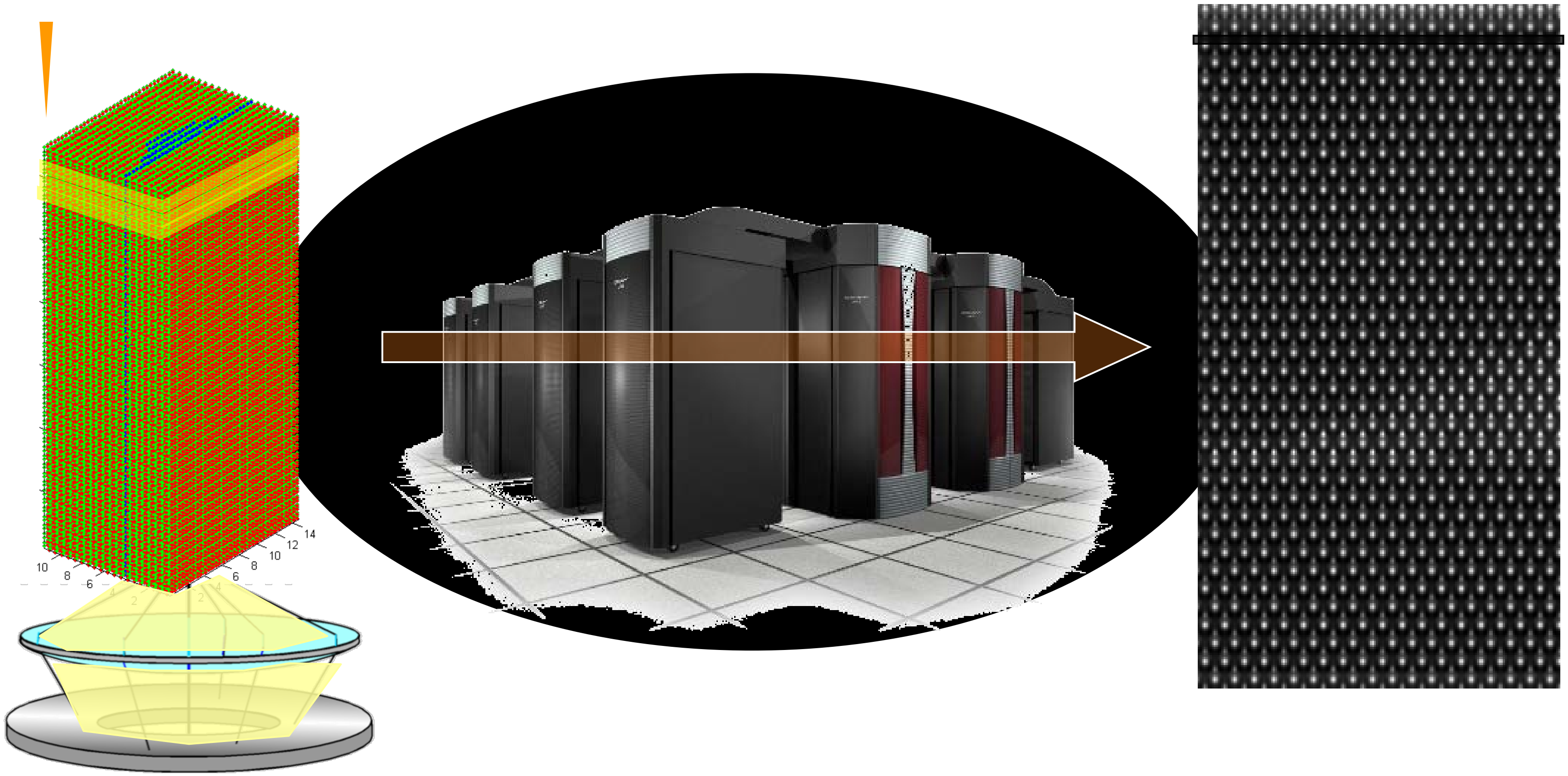
by FFT multislice method (Ishizuka's code)

STEM image simulations



The SICSTEM software

A Paralell HAADF-STEM Simulation Sw

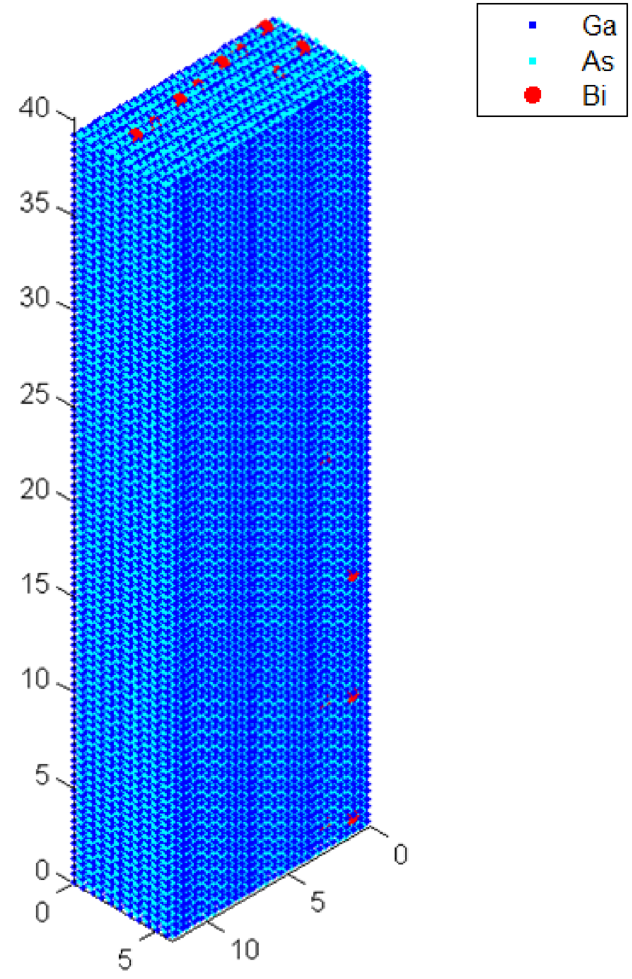


Cádiz University supercomputer

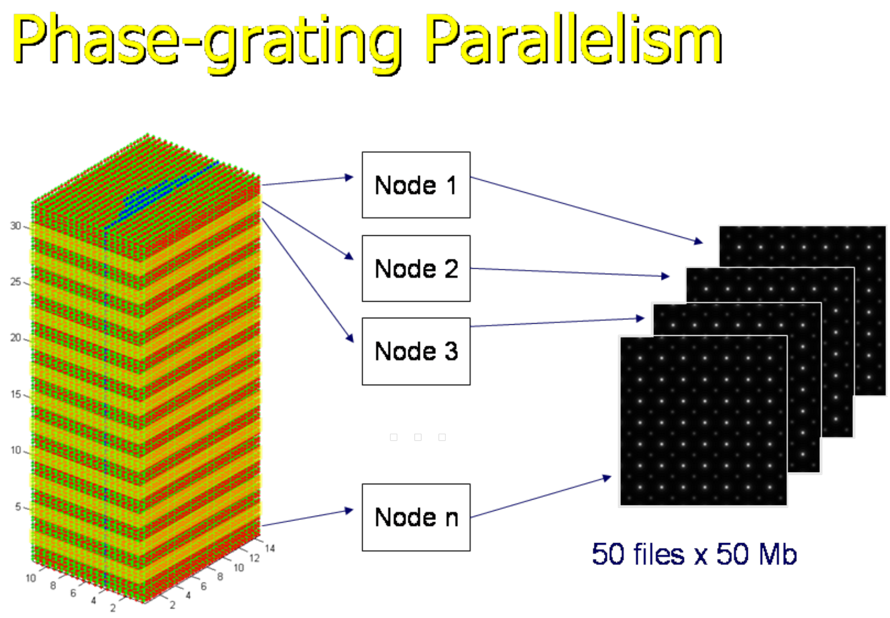
- Hewlett-Packard (2007)
  - 320 Xeon Woodcrest cores running at 3GHz
  - 3.75 Tflops (position 327 in Top500 last year)
  - Each node 8 or 16 Gb RAM
  - Total RAM = 700 GB
  - 2.5 TB disk capacity

Create the supercell

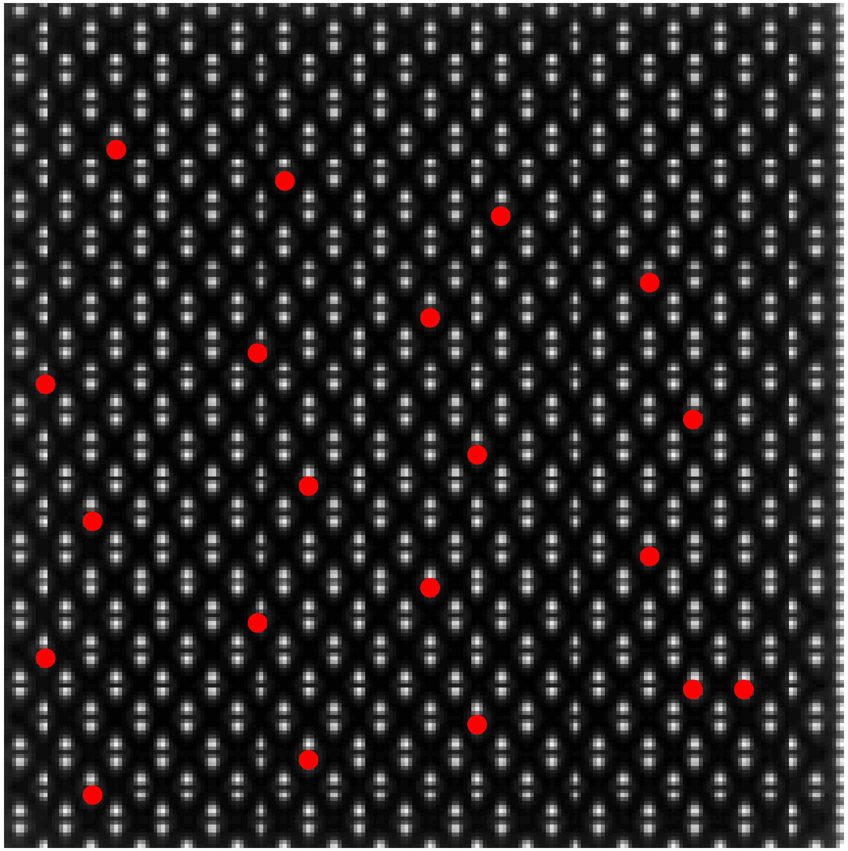
- **56,000 atoms**
- **5x6x40 nm**



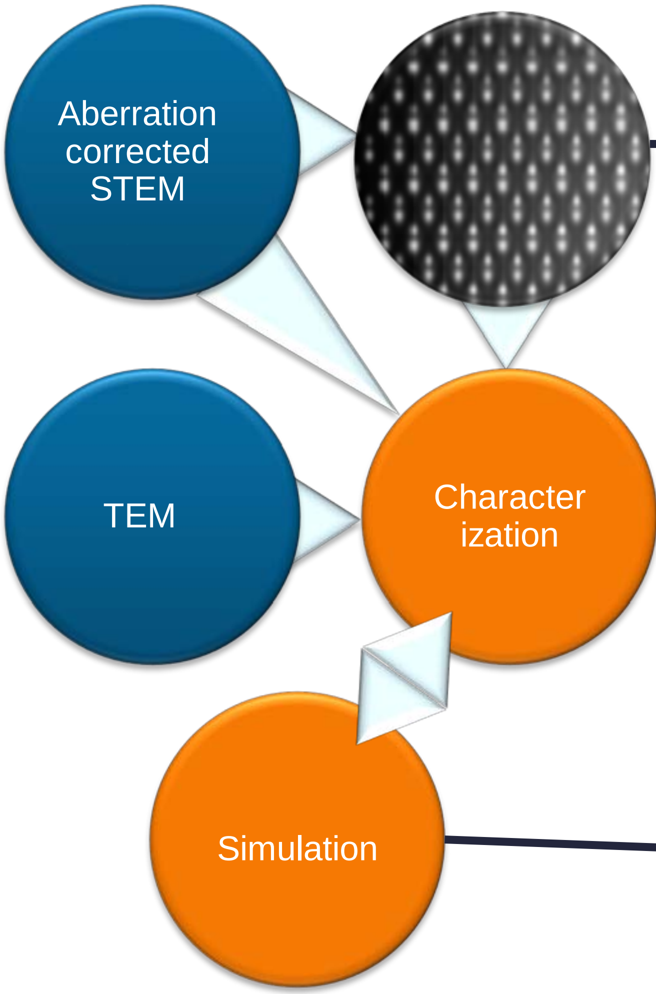
- **Aprox. time for simulation: 50 hours.**
- **High resolution: 182 pix/nm**



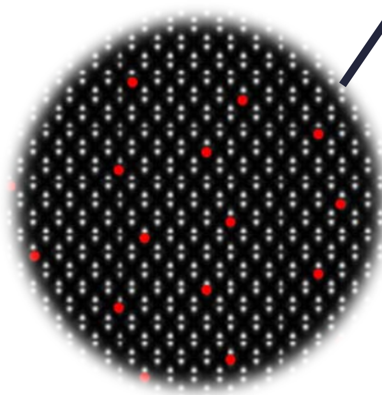
GaAsBi 40 nm - 3 Bi Atoms in red



Summary and Conclusions



Using HAADF-STEM images, a quantitative composition analysis with atomic column resolution is achievable in GaBiAs layers.



In order to corroborate the results and know the limits of this technique, image simulation is being processed using SIC-STEM software.


¡Muchas gracias!
Cádiz old town.