Facts and artifacts in Atom probe Tomography

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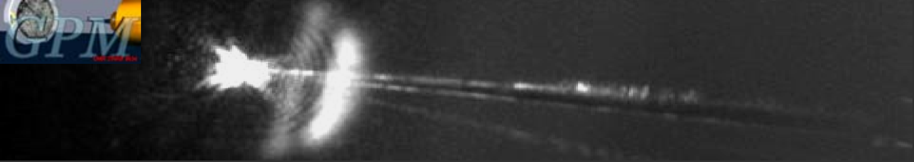
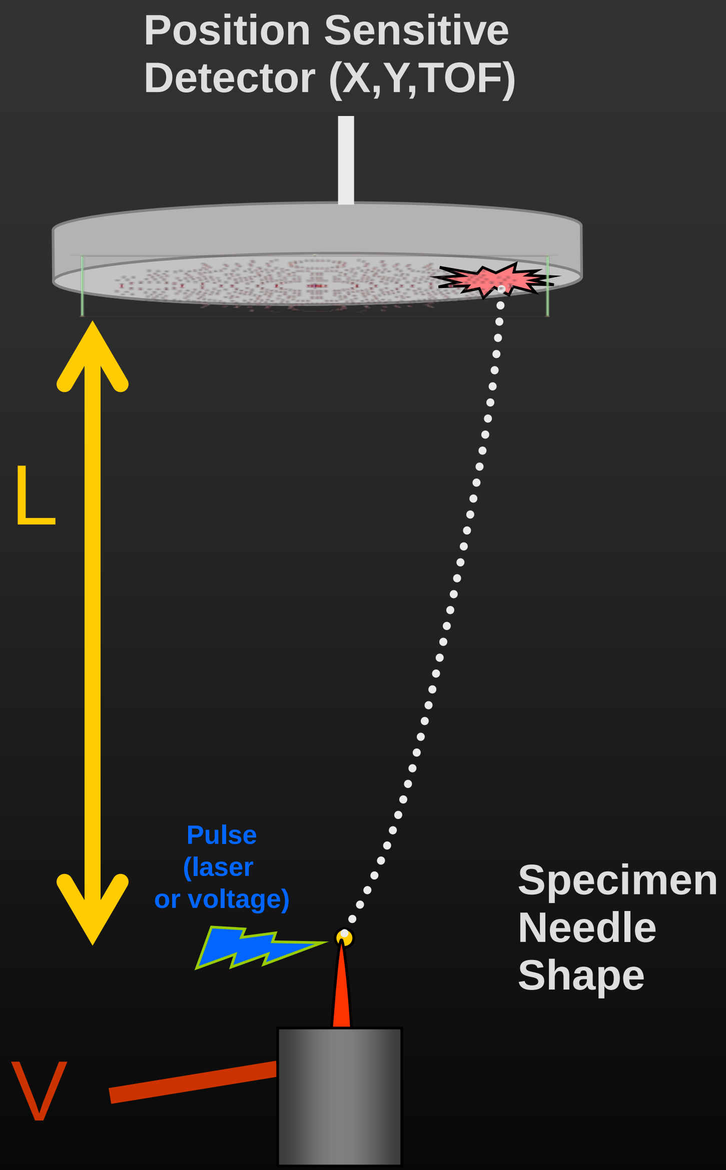
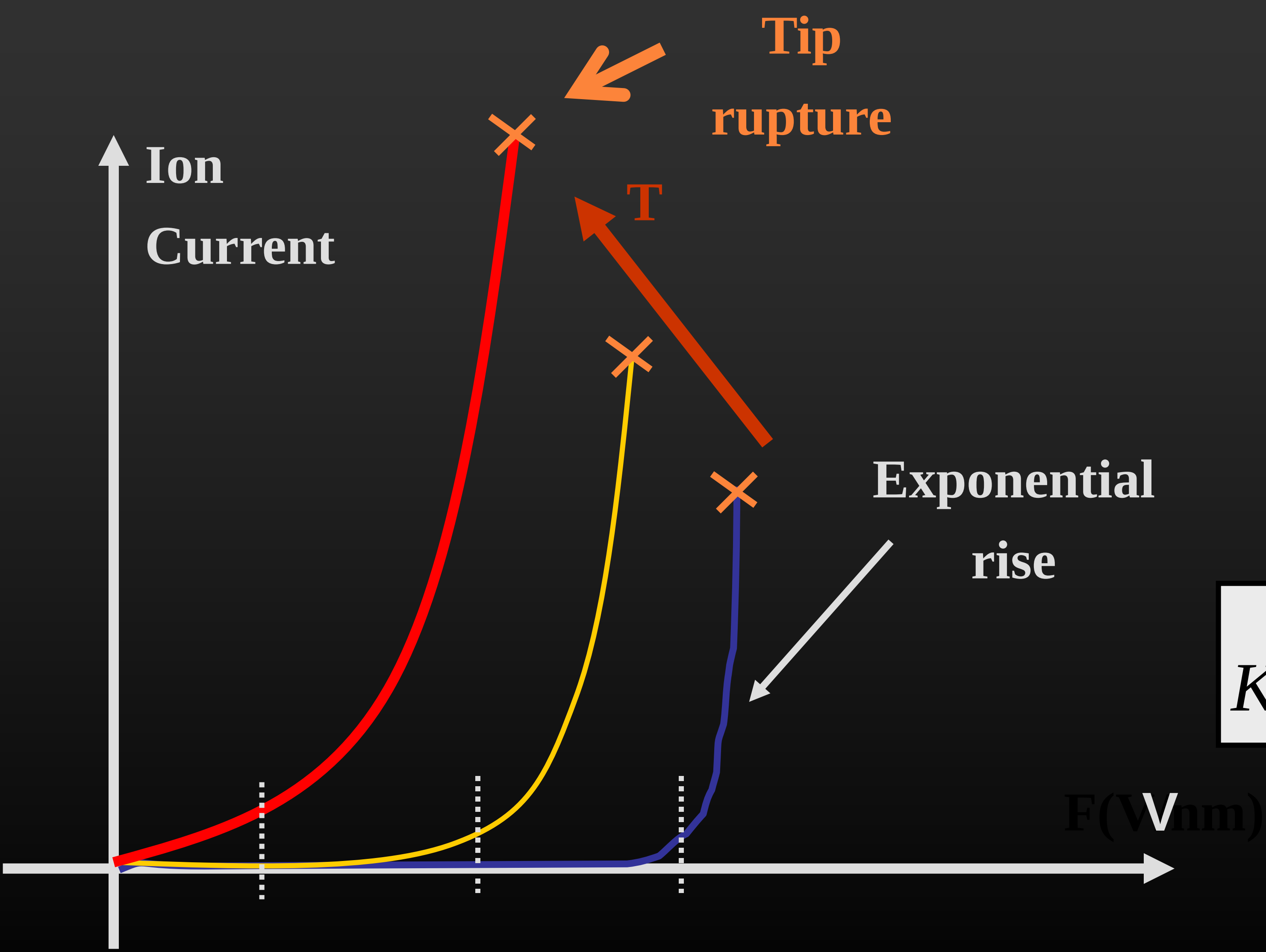


Atom Probe Tomography: Principles

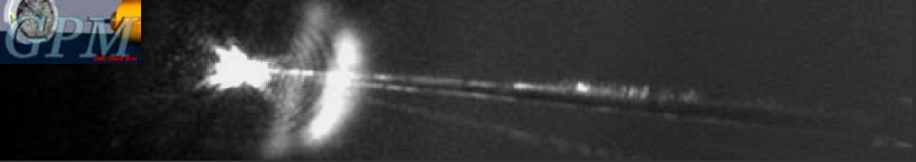


- Tip sample submitted to V (a few kV)
- Tip pulsed field evaporated atom by atom
- Ions projected on a PSD (X,Y, TOF)
- TOF mass spectrometry
- In vacuum P <10^{-10} Torr
- Cooled to <100 K

Principles : Field evaporation

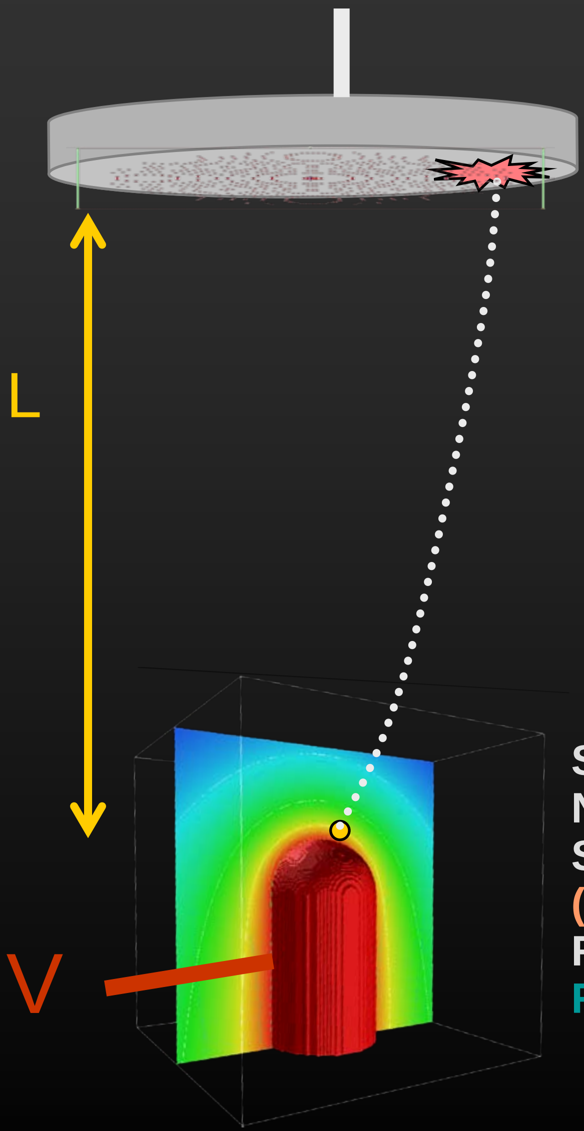


$$K_n = \upsilon \times e^{\frac{-Q_n}{kT}}$$



Atom Probe Tomography: Principles

Position Sensitive Detector (X,Y,TOF)



Specimen Needle Shape (tip) Radius R<100 nm

- End of the tip : hemispherical cap radius
- Tip submitted to F~V/R

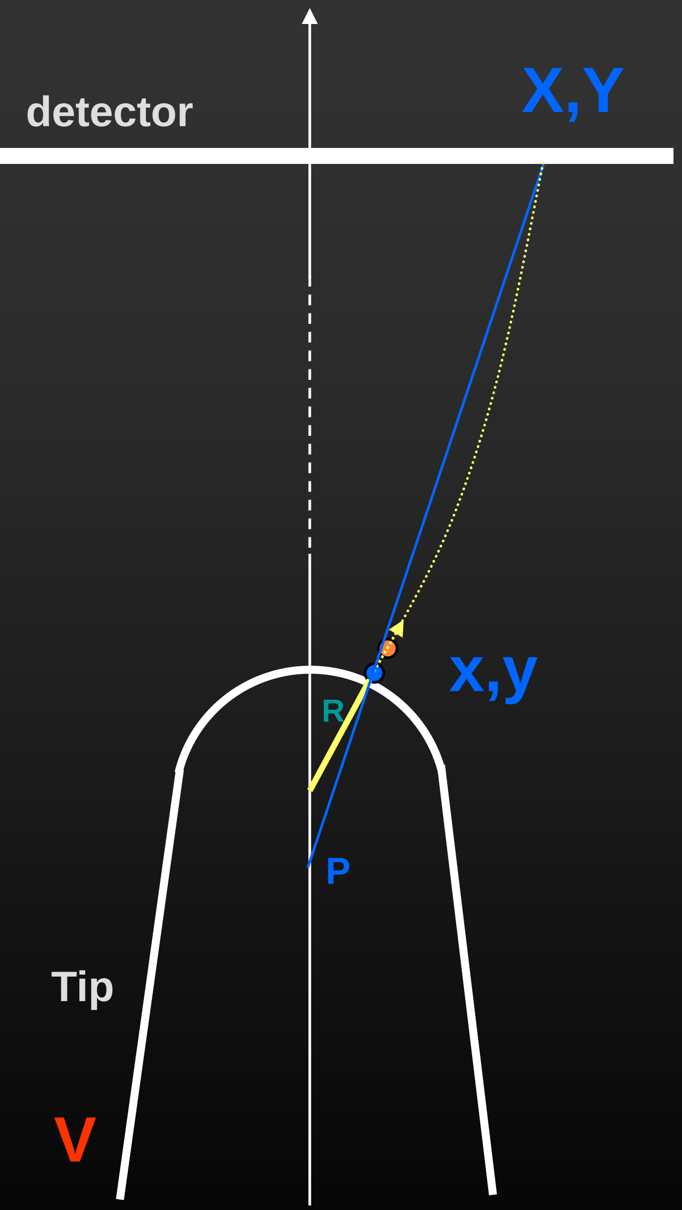
$$K_n = \upsilon \times e^{\frac{-Q_n}{kT}}$$

$$Q_n(F) \approx Q'_{0,n}\left[1-\frac{F}{F_e}\right] \approx 0.1-1eV$$

Depends on the elemental nature

10 V/nm<Fe<60 V/nm
Ex : Si ~30 V/nm

Principles : Evaporation and projection

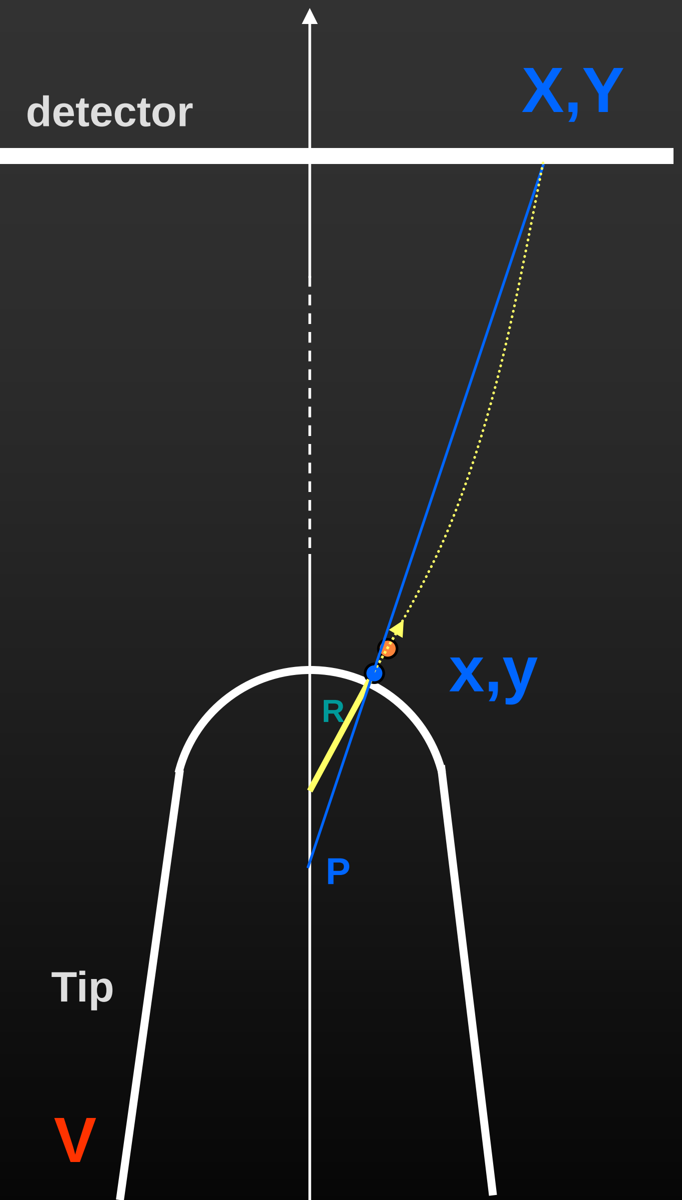


- Ion trajectories determined by electrostatic laws :
  - Depend only on the geometry !!!
    The tip is the lens
  - Do not depend on Voltage, mass, charge …
  - Model : Magnification
  - G ~k/R

$\Delta x \sim \Delta X / G$

$\Delta y \sim \Delta Y / G$

Principles : Evaporation and projection

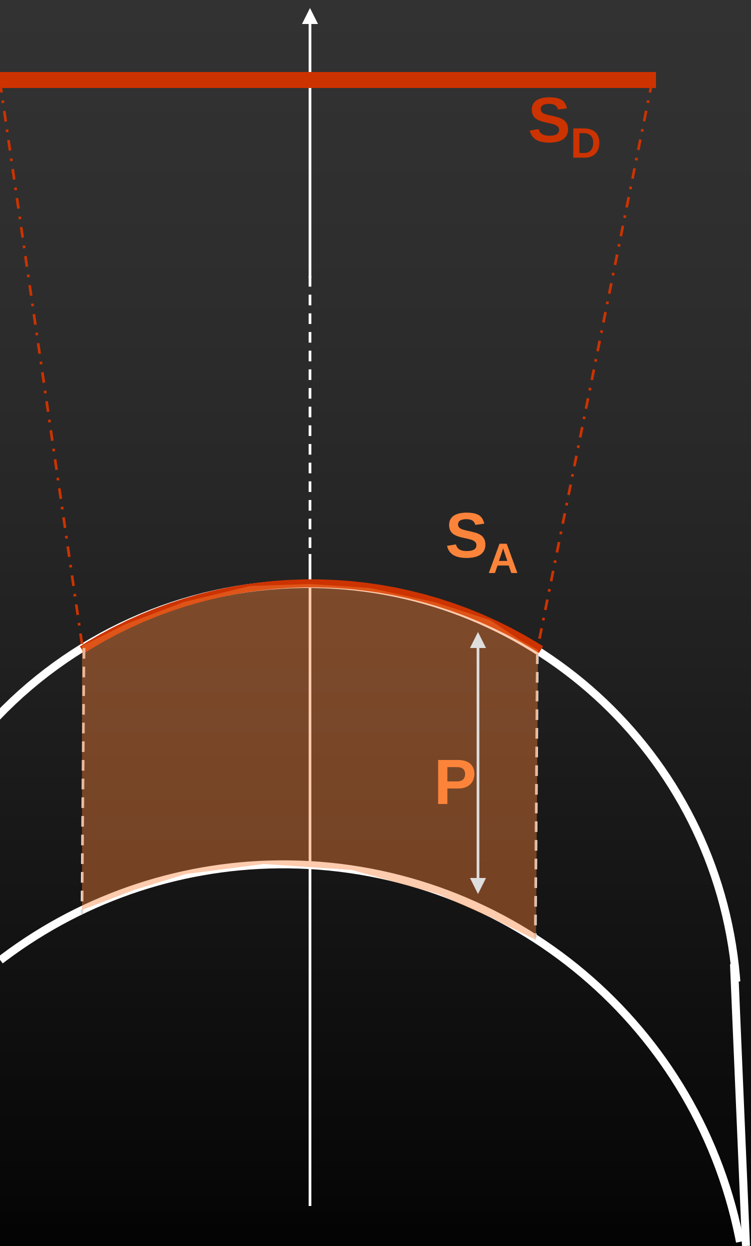


G~10^6

(1 nm <->1 mm on detector)
Detector resolution<100 microns

Instrumental lateral resolution
<0.1 nm !

Principles : Depth reconstruction



- N_A atoms detected : N_A/Q atoms evaporated (Q~60%)

$$V_{evap} \approx S_A \times P$$

$$V_{evap} = \frac{N_{at} \times \overline{v_{at}}}{Q}$$

v_{at} = volume occupied by 1 atom in tip

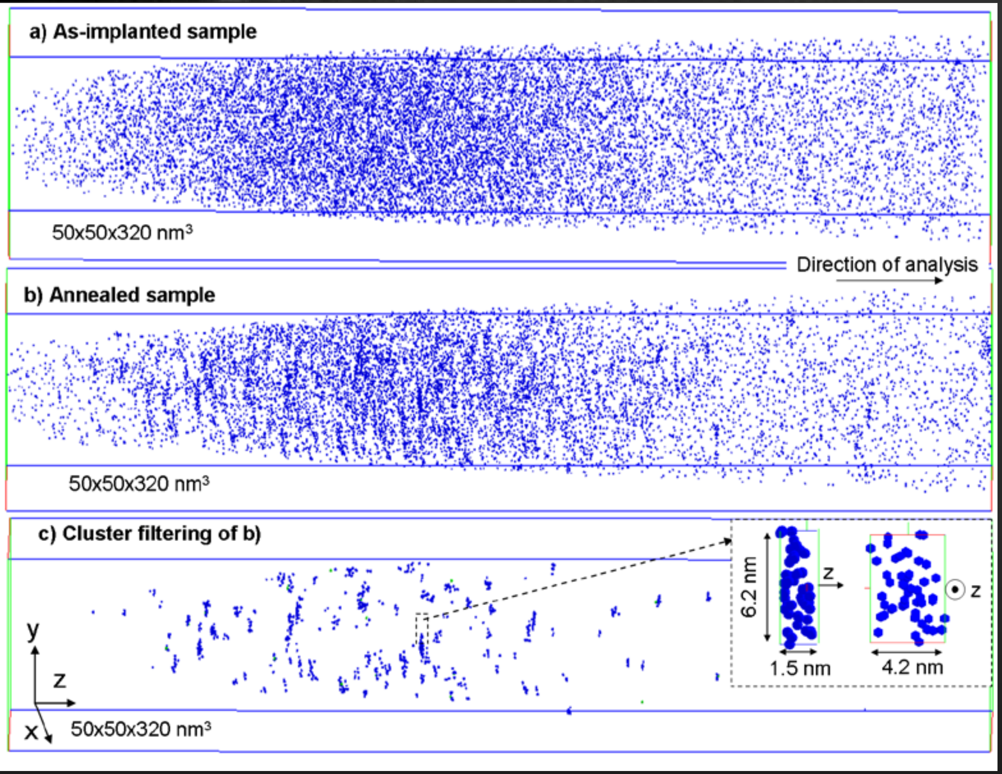
$$P \approx \frac{N_{at} \times \overline{v_{at}}}{QS_A} \approx \frac{N_{at} \times \overline{v_{at}}}{QS_D} G^2$$

- For 1 atom $p \sim 10^{-5}$ nm

$$p \approx \frac{\overline{v_{at}}}{QS_A} \approx \frac{\overline{v_{at}}}{QS_D} G^2$$

Instrumental depth resolution <0.00001 nm !!!!!

Performances ?



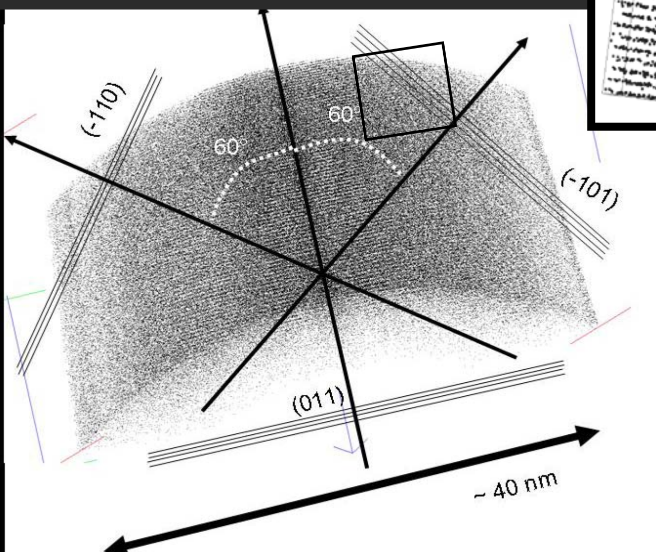
Nanometer objects are observed unambiguously

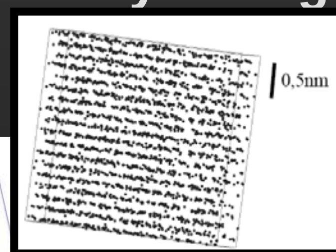
Spatial resolution of the Atom Probe Tomography

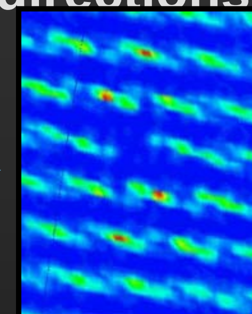
Best spatial resolution observed in Pure metal such as Tungsten

…

Atomic planes in several crystallographic directions

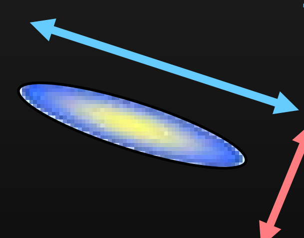






Mean atomic distribution around atom positions (~3D RDF)

Lateral resolution ~ 0.2 nm



Anisotropic resolution

Depth Resolution ~ 0.05 nm

F. Vurpillot et al., J. Micros., 216 (2004) 234

Depth resolution

degraded by

quantum nature of atom (<0.01 nm)

field penetration at the tip surface (<0.01 nm) *(semiconductors ??)*

Change in evaporation order … *(temperature, laser pulsing)*

Depth reconstruction artifacts (??)

Lateral resolution

degraded by

the quantum nature of atom in position

the quantum nature of atom in velocity

the transverse velocity due to temperature

thermal diffusion at the tip surface

field/thermal diffusion at the tip surface

Base Temperature <100 K but Laser = heating

Trajectory aberrations (??) → **Electrostatic dependence**

Thermal artifacts :

Laser = heating

…Field evaporation

Kink site Atoms 100-1000

10^{12} Hz

~100 ps

~0.1-0.5 eV

$$\Phi = 10^{-2} = N \times \upsilon \times \tau_{evap} \times e^{\frac{-Q_n}{kT}}$$

kT ~ Q_n/10

Pulsed T ~100-500 K

…Atomic diffusion at the tip surface

$$N_{jump}(jump/\,pulse) = N \times \upsilon \times \tau_{jump} \times e^{\frac{-Q_{jump}}{kT}}$$

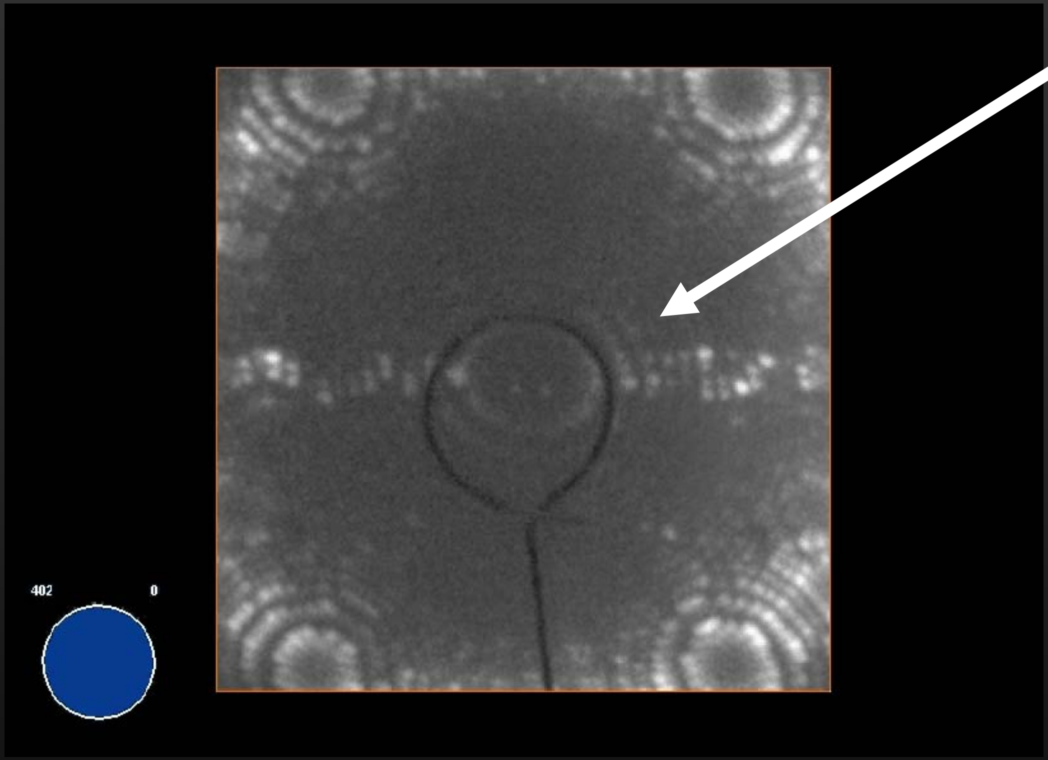
Q_{jump} ~ 0.5 -1 eV

> Q_n

(standard conditions)

Probability to field evaporate higher than thermal diffusion

Thermal artifacts :



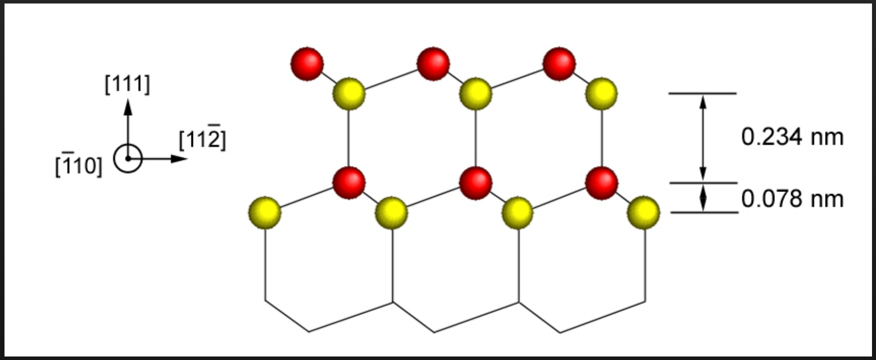
Under high laser Illumination Atomic diffusion is visible

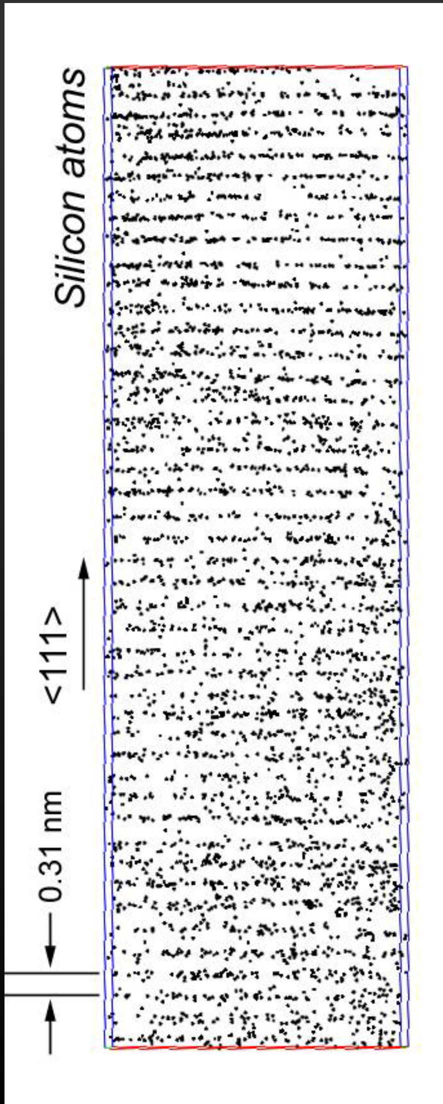
(example: Tungsten I_{laser} =2x $I_{standard}$

T~1000 K)

Spatial resolution of the laser Atom Probe Tomography in semiconductors

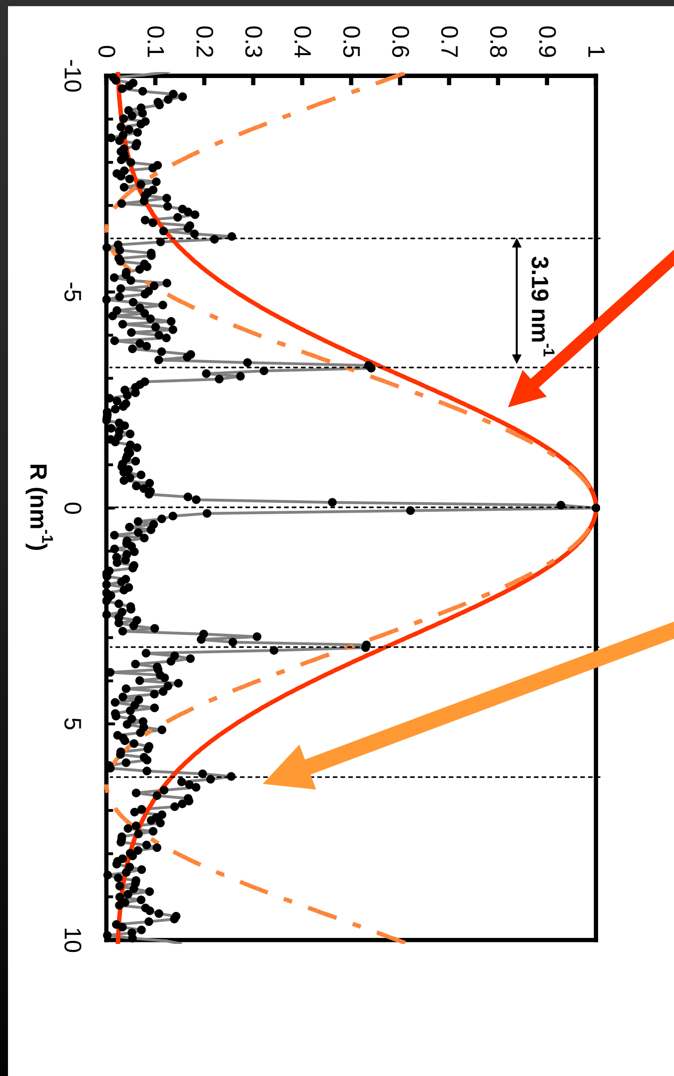
Test with silicon : (111) double planes are imaged in standard conditions (laser T_{pulse}~200 -300 K)





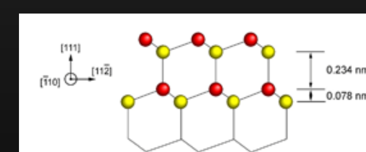
Spatial resolution of the laser Atom Probe Tomography in silicon

In Fourier space



Spread :
Depth
Resolution ~0.1 nm

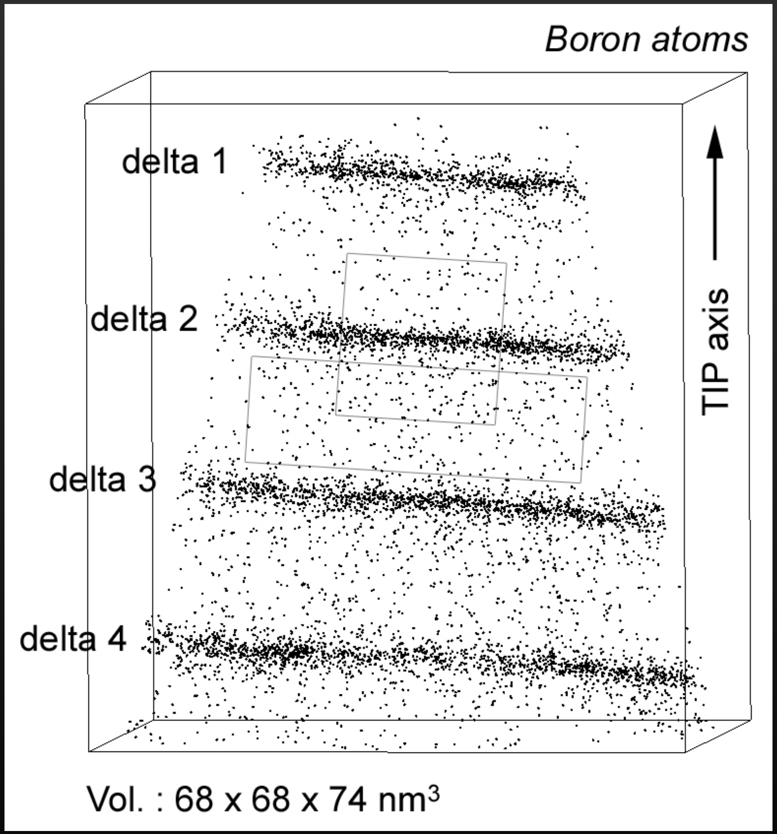
(Double plane sur-structure : <222>extinction)
Peak at<222> !??

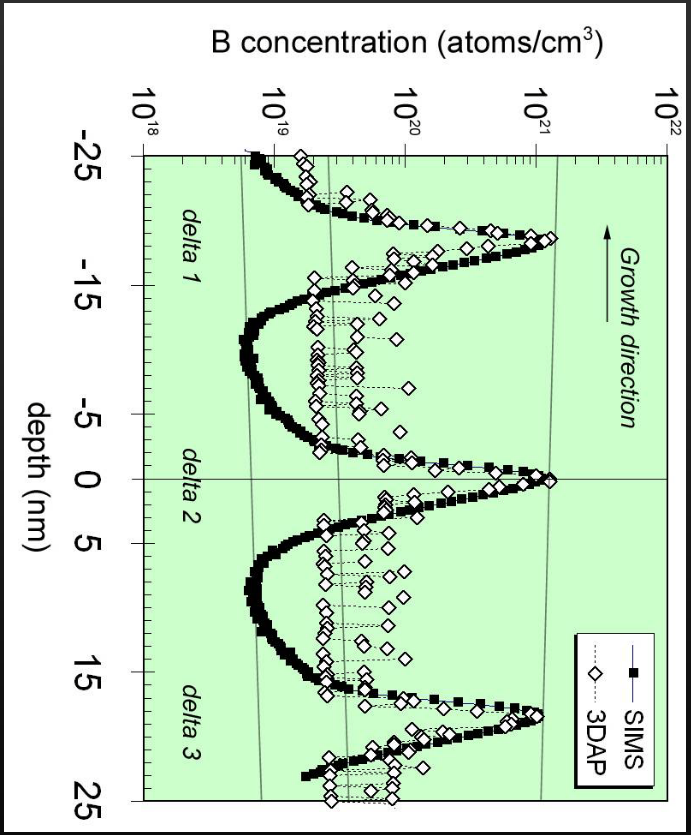


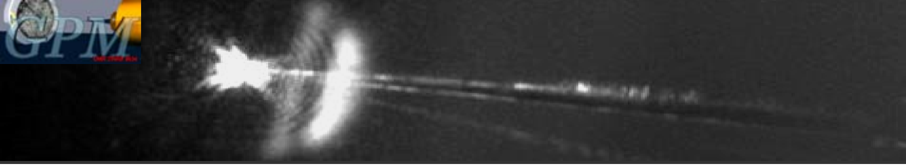
Correlated evaporation of the double layer (field penetration in silicon)

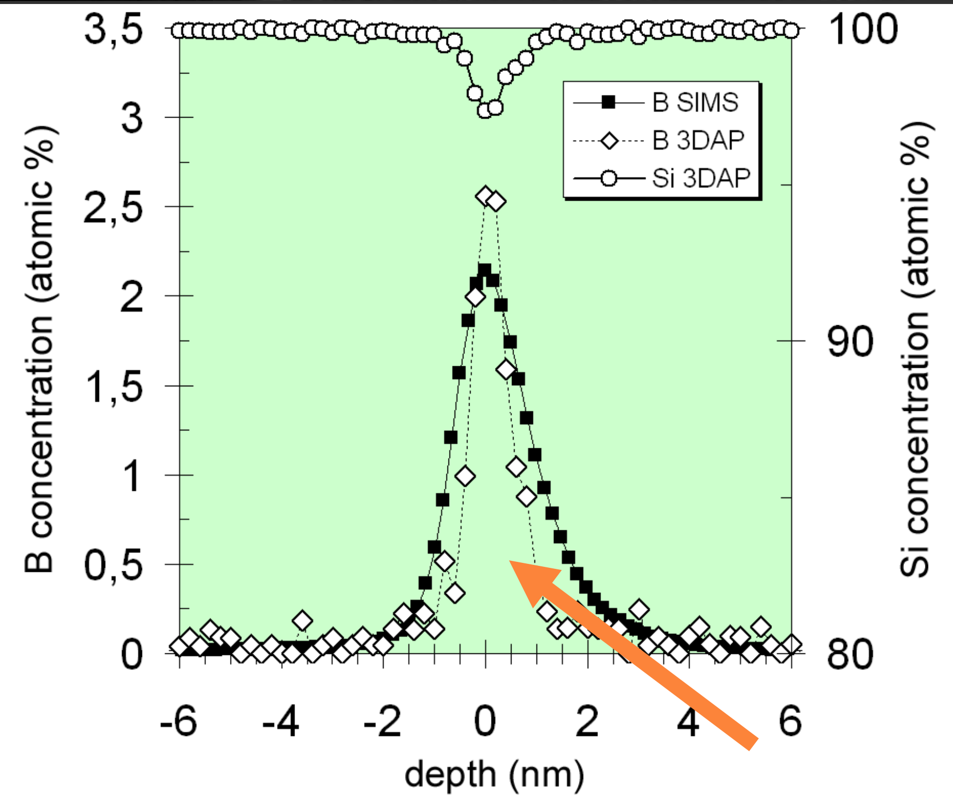
Spatial resolution of the laser Atom Probe Tomography in semiconductors

Delta doped layers : test structure







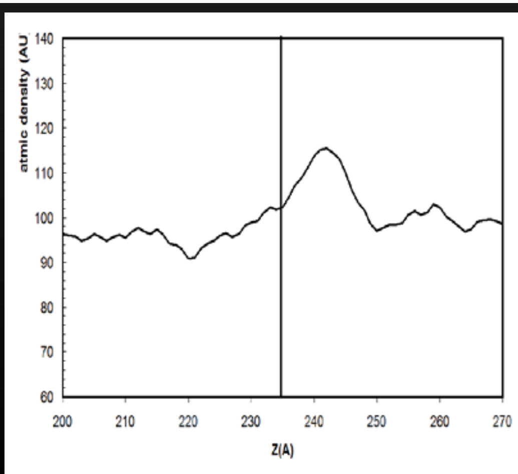


$$C_B^{SIMS} = 2.14 \times e^{-\frac{d^2}{2\times 0.74^2}}$$

$$C_B^{3DAP} = 2.6 \times e^{-\frac{d^2}{2\times 0.39^2}}$$

Width measured in SIMS twice APT value

Atomic density In depth



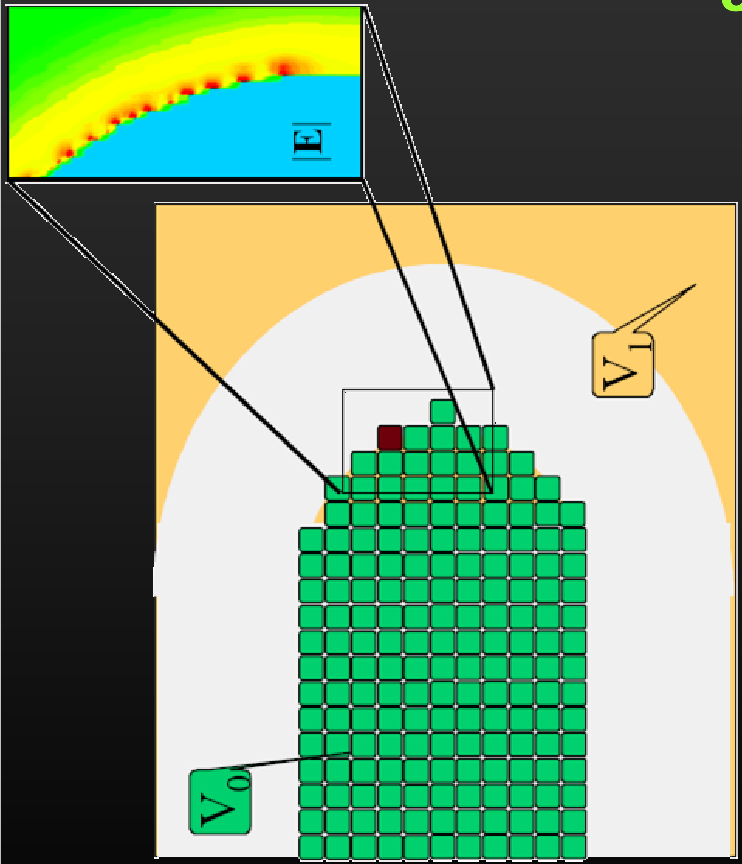
Theory width ~0.2 nm (1 atomic layer)
0.9 nm FWHM ??
Fact or artifact ??

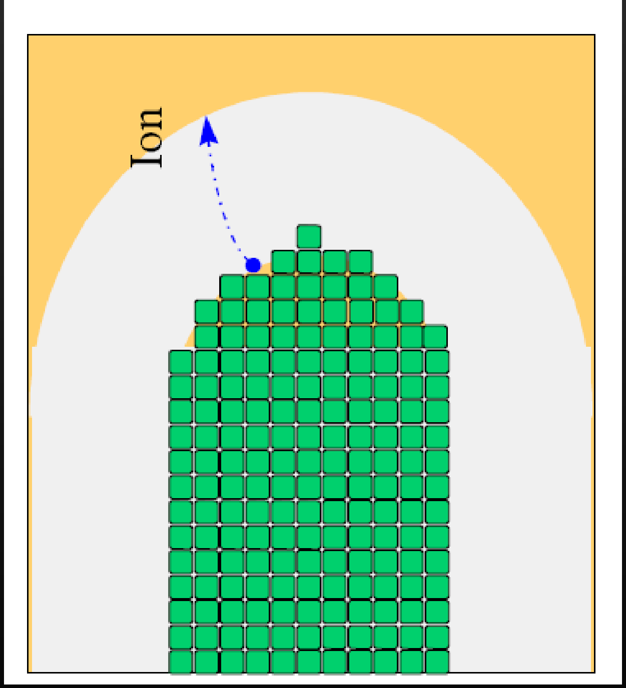
$F_e(B) >> F_e(Si)$

Modeling the effect of local electrostatic roughness

Model developed to understand

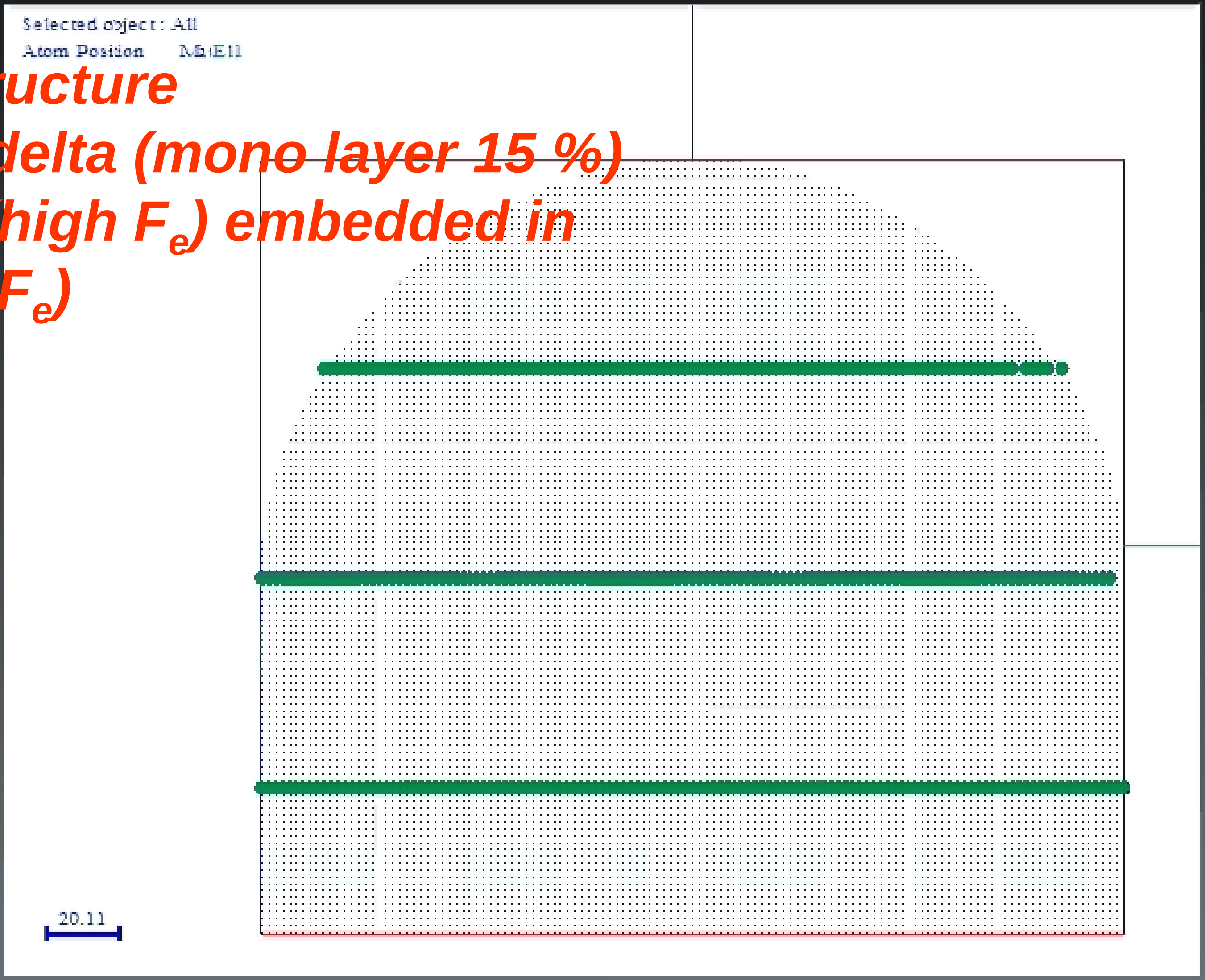
- *depth reconstruction artifacts*
- *trajectory aberrations*
- *effects of different F_e*



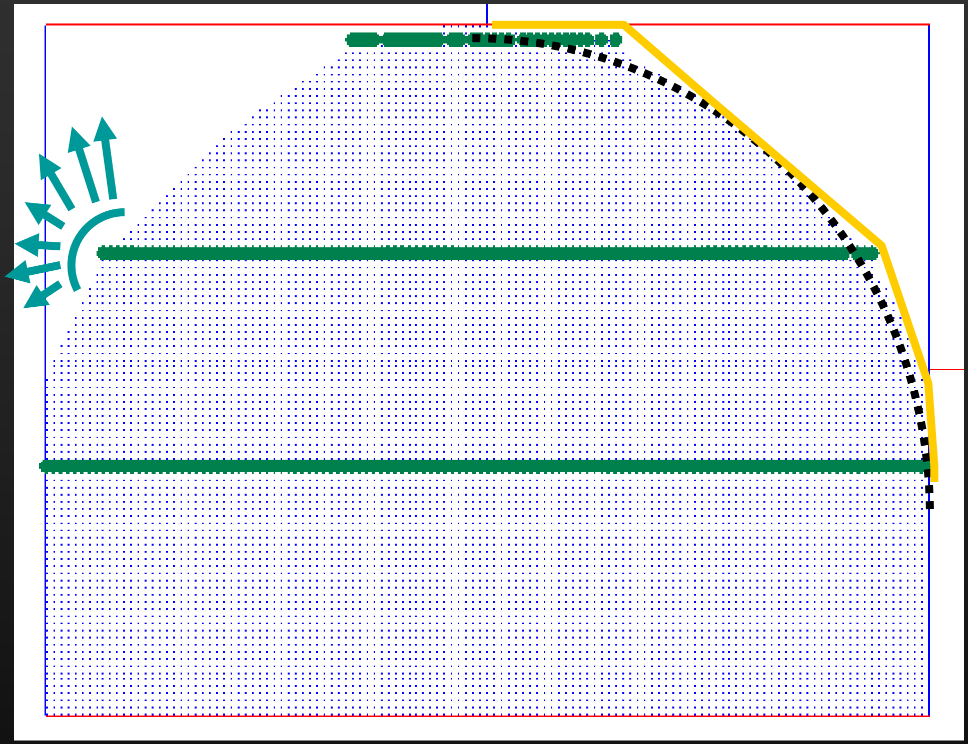


Delta – B doped layer
B evaporation field ??

CFC structure with B delta (mono layer 15 %) layers (high F_e) embedded in Si (low F_e)



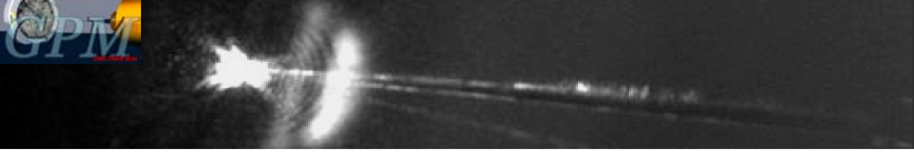
Delta – B doped layer
B evaporation field ??

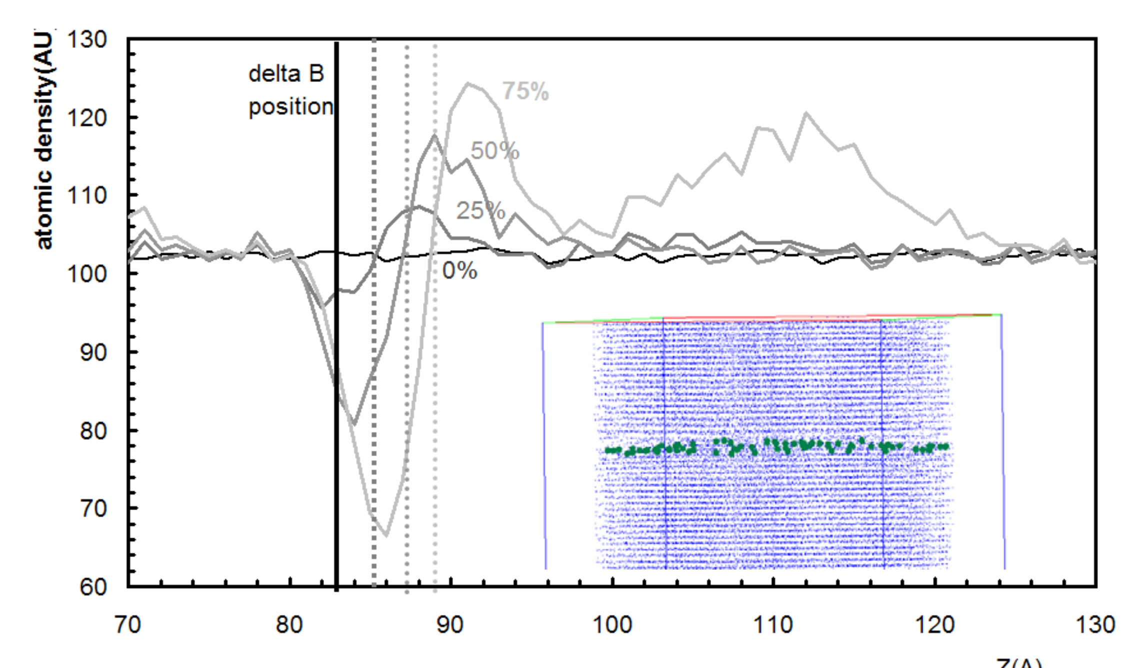


Two effects :

Local magnification due to local radius at the Surface

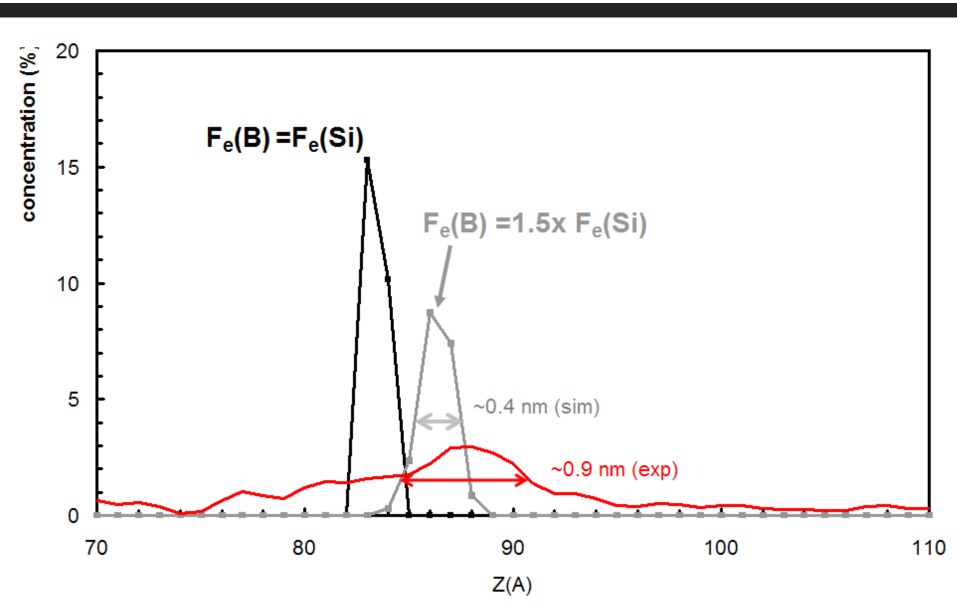
Tip is not spherical !!! Reconstruction artifact





Density artifact observed
With $F_e(B)$~1.5 x $F_e(Si)$

(agreement with theoretical value)



0.2 nm width degraded to 0.4 nm Still < 0.9 nm …

Actual width certainly about 0.5 nm

Conclusion

Main source of artifacts in APT :

Evaporation field difference between species

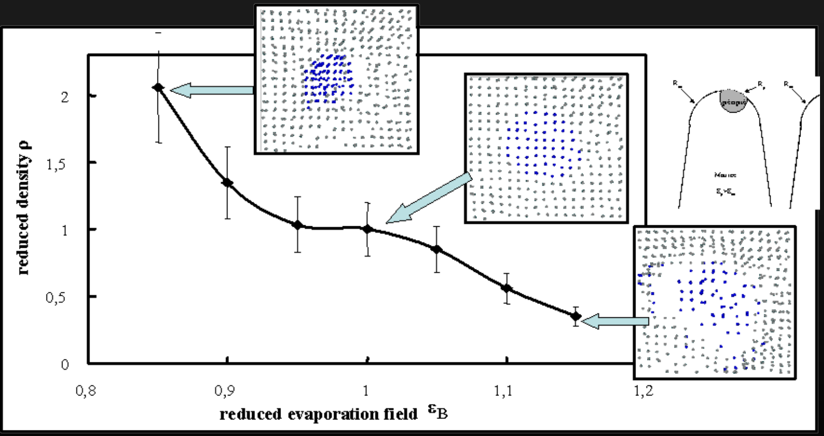
In pure specimen : spatial resolution in the 0.1nm range

in random solid solution : degradation of the spatial resolution

In multi-phases alloys :

local magnification effects

(care if density variations)

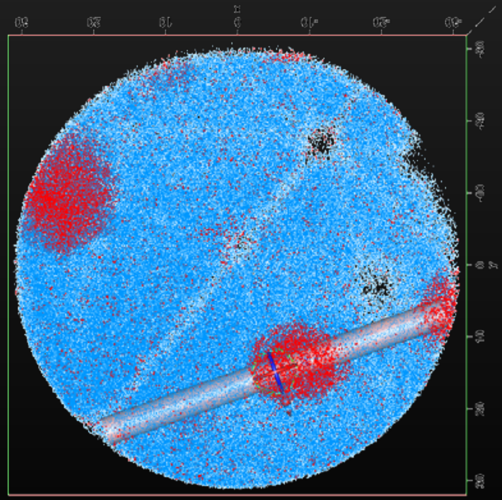


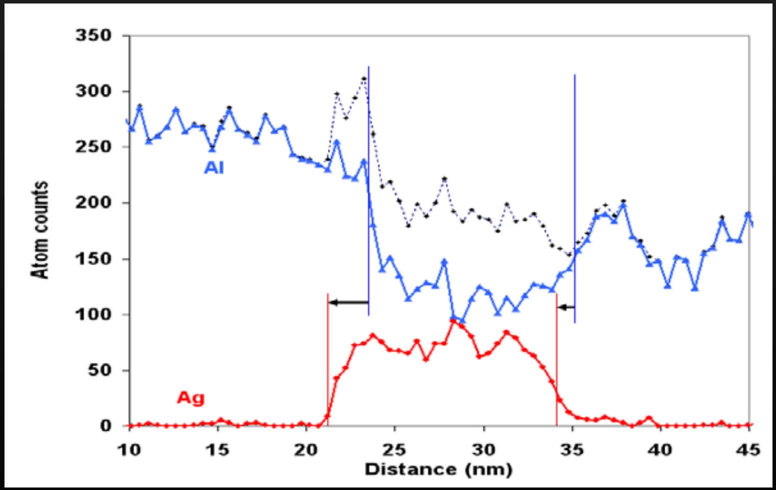
Si particles in SiO_2

Conclusion

Artifacts are worst laterally and with heterogeneous structures !!!!!

- *local magnification effects (density variations)*
- *Trajectory overlaps*
- *Chromatic aberrations*
- *resolution can be degraded to 2-3 nm (laterally)*





Conclusion

Artifacts are worst laterally and with heterogeneous structures !!!!!

- *local magnification effects (density variations)*
- *Trajectory overlaps*
- *Chromatic aberrations*
- *resolution can be degraded to 5 nm (laterally)*