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

Ion Current

Exponential rise

Tip rupture

\[ K_n = \nu \times e^{-\frac{Q_n}{kT}} \]
Atom Probe Tomography: Principles

- End of the tip: hemispherical cap radius
- Tip submitted to $F \sim \frac{V}{R}$

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

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

Depends on the elemental nature

$10 \text{ V/nm} < \text{Fe} < 60 \text{ V/nm}$
Ex: Si $\sim 30 \text{ V/nm}$
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
  - $G \sim k/R$

$\Delta x \sim \Delta X / G$
$\Delta y \sim \Delta Y / G$
Principles: Evaporation and projection

Detector resolution < 100 microns

Instrumental lateral resolution < 0.1 nm!

G \approx 10^6

(1 nm \leftrightarrow 1 mm on detector)

Tip

\( x, y \)

\( X, Y \)
Principles:

Depth reconstruction

- $N_A$ atoms detected: $N_A/Q$ atoms evaporated ($Q \approx 60\%$)

\[
V_{evap} \approx S_A \times P
\]

\[
V_{evap} = \frac{N_{at} \times v_{at}}{Q}
\]

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

\[
P \approx \frac{N_{at} \times v_{at}}{QS_A} \approx \frac{N_{at} \times v_{at}}{QS_D} G^2
\]

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

**Instrumental depth resolution**

$< 0.00001 \text{ 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)

Anisotropic resolution

Lateral resolution ~ 0.2 nm

Depth Resolution ~ 0.05 nm

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:

\[ \Phi = 10^{-2} = N \times \nu \times \tau_{\text{evap}} \times e^{\frac{-Q_n}{kT}} \]

Laser = heating

...Field evaporation

Kink site Atoms

100-1000

\[ 10^{12} \text{ Hz} \]

\[ \sim 100 \text{ ps} \]

\[ \sim 0.1-0.5 \text{ eV} \]

\[ kT \sim \frac{Q_n}{10} \]

Pulsed T \sim 100-500 \text{ K} \]

...Atomic diffusion

at the tip surface

\[ N_{\text{jump}} (\text{jump/pulse}) = N \times \nu \times \tau_{\text{jump}} \times e^{\frac{-Q_{\text{jump}}}{kT}} \]

\[ Q_{\text{jump}} \sim 0.5 - 1 \text{ eV} \]

\[ > Q_n \]

(standard conditions)

Probability to field evaporate higher than thermal diffusion
Thermal artifacts:

Non standard conditions

Under high laser Illumination
Atomic diffusion is visible

(example: Tungsten
$I_{\text{laser}} = 2 \times I_{\text{standard}}$

$T \sim 1000 \, \text{K}$)
Test with silicon: (111) double planes are imaged in standard conditions (laser $T_{\text{pulse}} \sim 200 - 300 \text{ K}$)
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)
Delta doped layers: test structure
Width measured in SIMS twice APT value

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

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

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

$F_{e}(B) >> F_{e}(Si)$
Modeling the effect of local electrostatic roughness

Model developed to understand
• depth reconstruction artifacts
• trajectory aberrations
• effects of different $F_e$
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 $\text{Fe}(\text{B}) \sim 1.5 \times \text{Fe}(\text{Si})$ (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)
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)
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)*