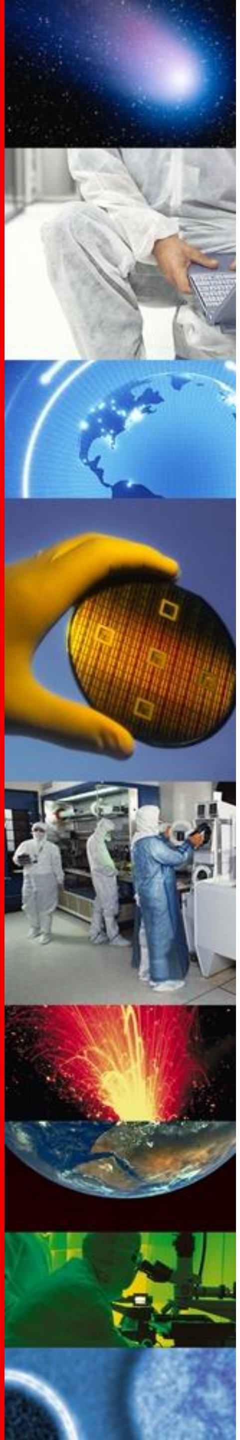

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Spatial Data Reconstruction for Atom Probe Tomography: A Brief Perspective

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<u>For Presentation at:</u>

Atom Probe Tomography: A Special Frontiers Session

Session Chair: Wilfried Vandervorst, IMEC

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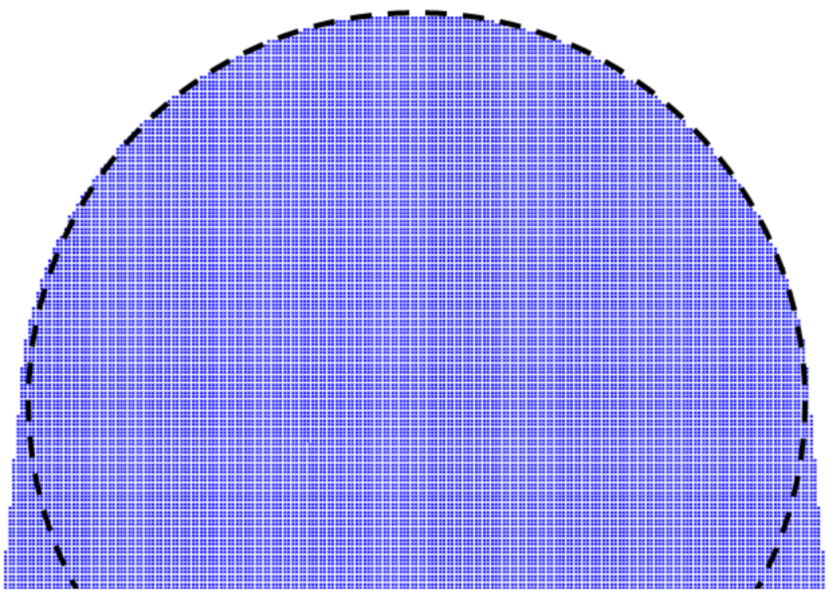
Outline

- Hemispherical Reconstruction
  - Assumptions
  - Calculation of x, y, and z
- Estimation of Field Evaporated Shapes
  - Simulation
  - Experimental Observation
- Limitations & Resulting Inaccuracies
  - Projection
  - Z Increment
- Methods of Correction
  - Density Correction
  - Lattice Rectification
  - Non-Tangential Continuity
  - Variable Image Compression
  - Self-Optimization of Data: *A Priori* and *A Posteriori* to Reconstruction
  - Dynamic Reconstruction
  - Non-Hemispherical Methods

Reconstruction: Two Primary Assumptions

- Atom probe data reconstruction consists of:
  - A magnification transformation (to calculate x and y)
  - A depth transformation (to calculate z)
- The 1995 assumptions* are:
  - The specimen is comprised of a hemisphere on a cone with some shank angle (usually using a tangential constraint)
  - The depth transformation is a constant with respect to x and y
- In 2005, Geiser et al. expanded the method to remove limitations due to small angle approximations



General Reconstruction Procedure**

1. Project Transverse coordinates to tip coordinates:

$$\left(x_{Ion}, y_{Ion}\right) = M^{-1}\left(x_{Det}, y_{Det}, R_{Tip}\right)$$

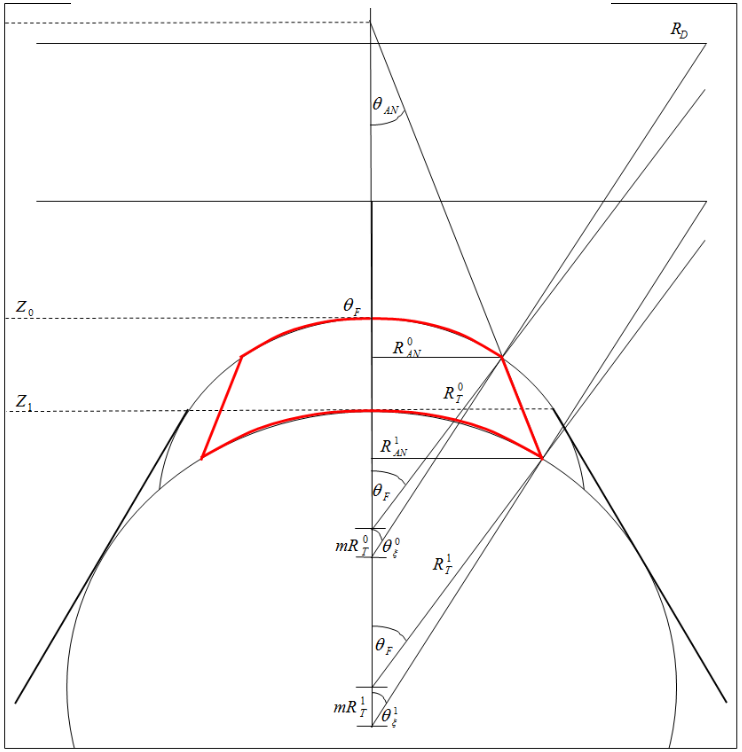
2. Calculate a position dependent Z correction:

$$z_{Ion} = Z_{Tip} + Z_P\left(x_{Ion}, y_{Ion}\right)$$

3. Evolve the Tip Model:

a. $$Z_{Tip} = Z_{Tip} + \frac{Vol_{Ion}}{\varepsilon\left(\frac{dVol}{dZ_{Tip}}\right)}$$

b. $$R_{Tip} = R_{Tip} + \left(\frac{dR_{Tip}}{dZ_{Model}}\right) dZ_{Model}$$

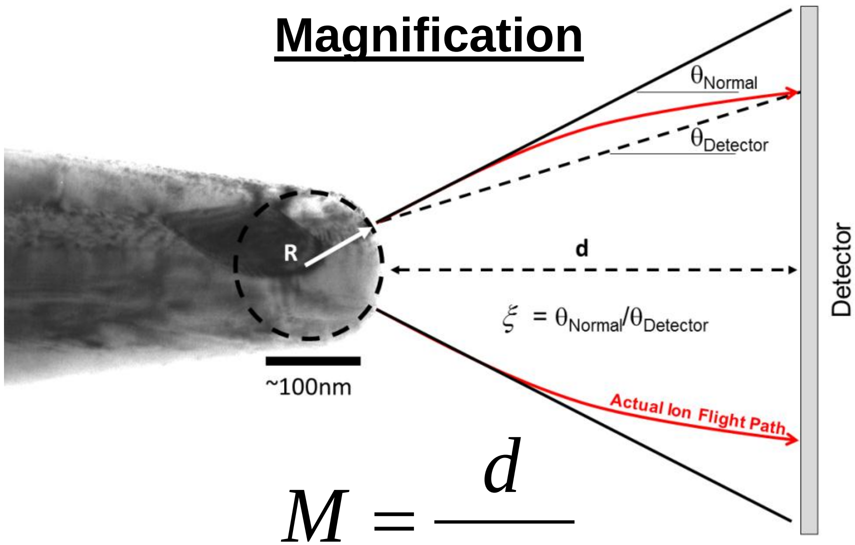


* Bas et al, *Appl. Surf. Sci.* 87/88 (1995) 298

** B. P. Geiser et al., *Microscopy and Microanalysis* 15(S2) (2009) 292

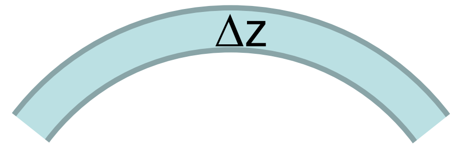
Reconstruction: How to Calculate x, y, and z

Magnification



$$M = \frac{d}{\xi \cdot R}$$

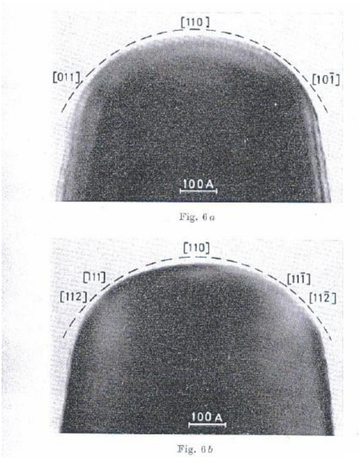
Depth



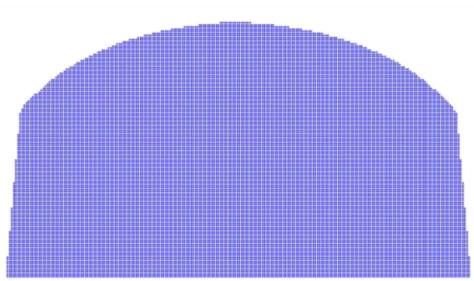
$$\Delta z = \frac{\Omega d^2}{A \varepsilon \xi^2 R^2}$$

- Magnification is the key calculation for the xy transformation from detector space to specimen space
  - d is distance between specimen and detector
  - ξ is the image compression
  - R is the average radius of the specimen
- A z increment must be calculated in order to transform from ion arrival number to z in specimen space
  - Ω is the atomic volume
  - A is the detector area
  - ε is the efficiency

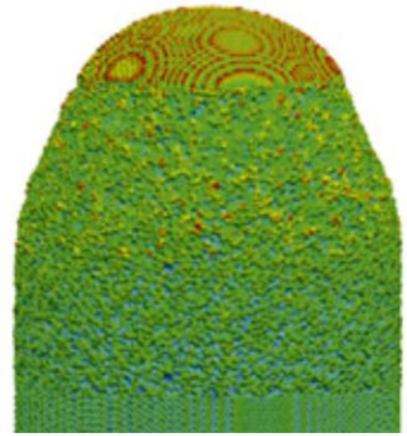
Examples of Specimen Shapes…



B. Loberg and H. Norden, Arkiv for Fysik 39 (1968) 383
T. Wilkes et al., Metallography 7 (1974) 403



B. P. Geiser et al., *Micro. Microanalysis* 15(S2) (2009) 302



C. Oberdorfer and G. Schmitz, *Ultramicroscopy* (2013) in press

D. J. Larson et al., *Ultramicroscopy* 111 (2011) 506

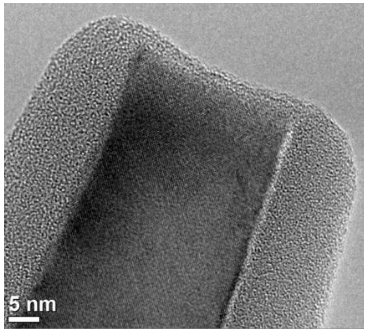
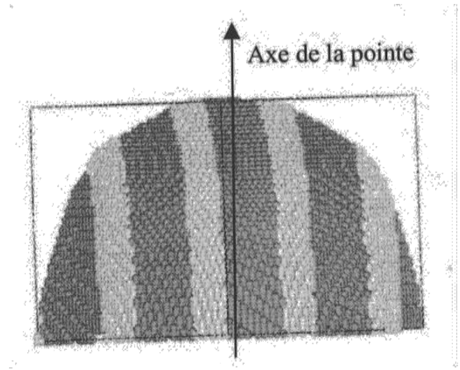
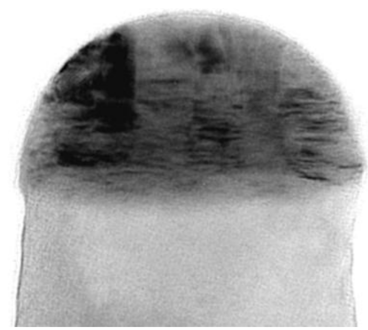


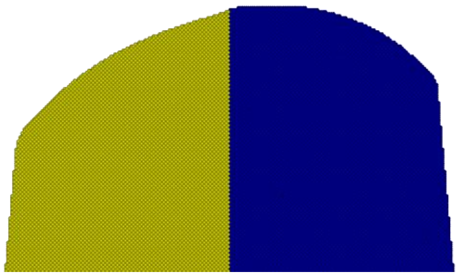
Image courtesy J. Lee (Samsung)



F. Vurpillot, *Ph.D. Thesis* (2001) Université de Rouen



D. J. Larson et al., *J. Microscopy* 243 (2011) 15



D. J. Larson et al., *Micro. Microanalysis* 18 (2012) 953

- Field evaporated specimen shapes often deviate substantially from hemispherical
- This conclusion is based on observations from both electron microscopy and simulation

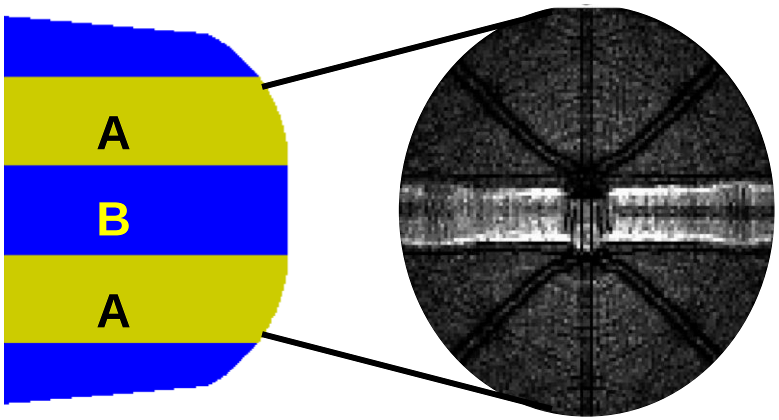
Limitations of the Primary Assumptions

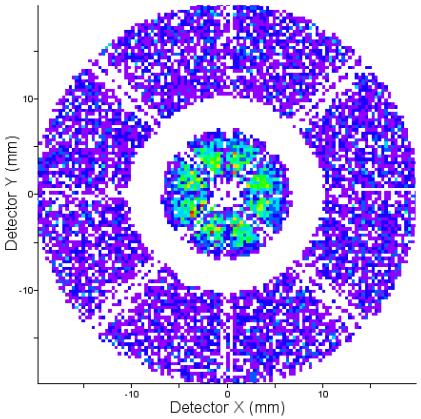
Magnification (XY Projection)

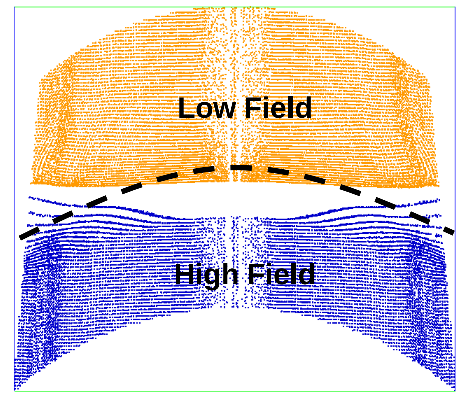
$$M = \frac{d}{\xi \cdot R}$$

Depth (Z Increment)

$$\Delta z = \frac{\Omega M^2}{A\varepsilon}$$







- The assumed reconstruction radius is contained in both equations: Magnification & Depth
- Anisotropic (in evaporation field) regions in x and y (above left) may result in expansion or compression in the reconstruction
- Differing evaporation fields also produce hit density variations which are <u>not</u> the result of xy projection errors (above right), but are simply uneven field evaporation from certain regions on the specimen surface

Methods of Improvement/Correction

Correction Method	Reference
Density Correction	F. Vurpillot, D.J. Larson and A. Cerezo, Surface and Interface Analysis 36 (2004) 552, F. DeGeuser et al., Surface and Interface Analysis 39 (2007) 268
Lattice Rectification	M. Moody et al., Microscopy & Microanalysis 17 (2011) 226
Radius Evolution	F. DeGeuser et al., Surface and Interface Analysis 39 (2007) 268, D. J. Larson et al., Ultramicroscopy 111 (2011) 506
Non-Tangential Continuity	D. J. Larson et al., Microscopy and Microanalysis 17(S2) (2011) 740
Variable Image Compression	D. J. Larson et al., Journal of Microscopy 243 (2011) 15
Self-Optimization of Data: *A Priori* and *A Posteriori* to Reconstruction	B. P. Geiser et al., Microscopy and Microanalysis (2013) in press, D.J. Larson et al., Microscopy and Microanalysis 17(S2) (2011) 724, F. Vurpillot et al., Ultramicroscopy 111(8) (2011) 1286
Dynamic Reconstruction	B. Gault et al., Ultramicroscopy 111(11) (2011) 1619
Non-Hemispherical Methods	D. J. Larson et al., Microscopy and Microanalysis 18(5) (2012) 953, D. Haley, Journal of Microscopy 244 (2011) 170.

Summary & Future Developments

- Compared to 20 years ago, the bottlenecks in atom probe methodology have shifted away from specimen preparation and data collection (in terms of time and effort) with two of the major problem areas now being reconstruction quality and specimen yield
- Major advances have been made in some areas:
  - Specimen preparation using FIB
  - Data collection rate
  - Laser-assisted field evaporation
- Two assumptions that limit the current reconstruction methodology are 1) a constant magnification projection onto hemisphere and 2) a uniform depth increment over the field of view
- Contemporary developments in reconstruction methods are focused both on improvements to the current model as well as new methods that are unconstrained by the above assumptions

Acknowledgements

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