Field Evaporation Simulation of a Cross Section ABA Structure

David J. Larson & Brian P. Geiser

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Acknowledgements

- T. Kelly, T. Prosa, D. Reinhard, R. Ulfig, P. Clifton, E. Oltman etc. (Cameca)
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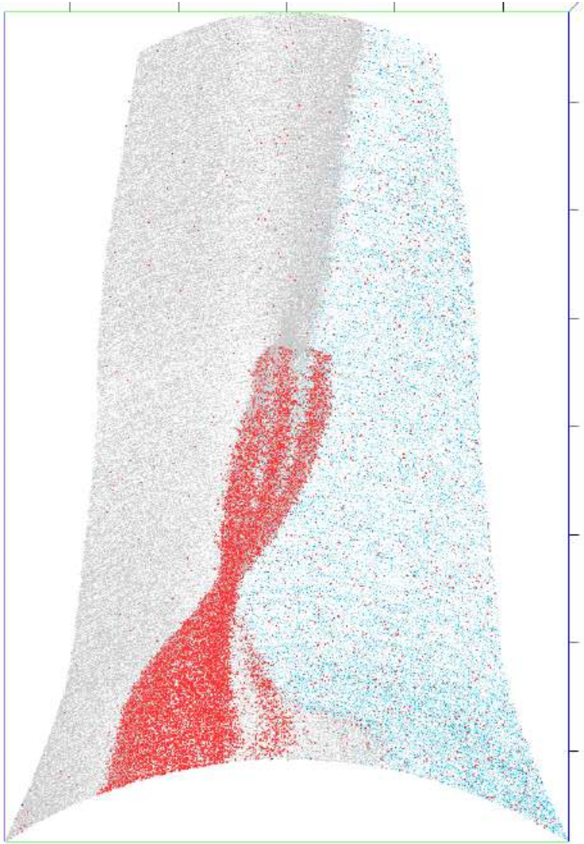
Motivation to Understand APT Reconstruction

From this morning:

“We believe that atom probe tomography is very useful but…reconstruction is still a problem” – Dr. Zhiyong Ma (Intel)



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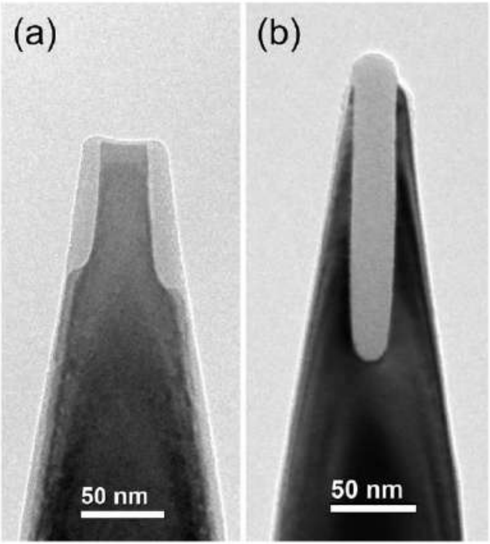
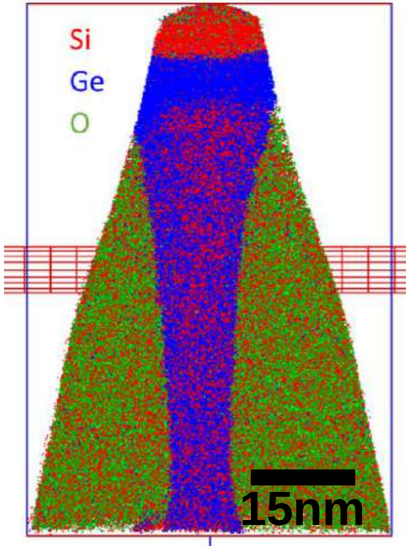
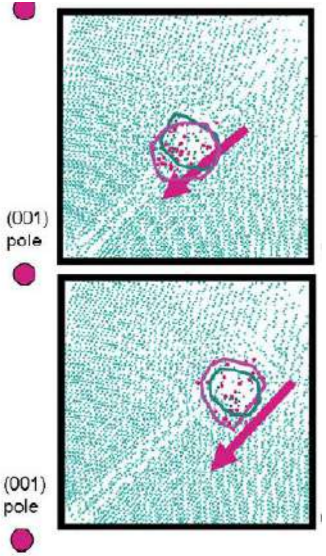
Different Phases Can Cause Issues…



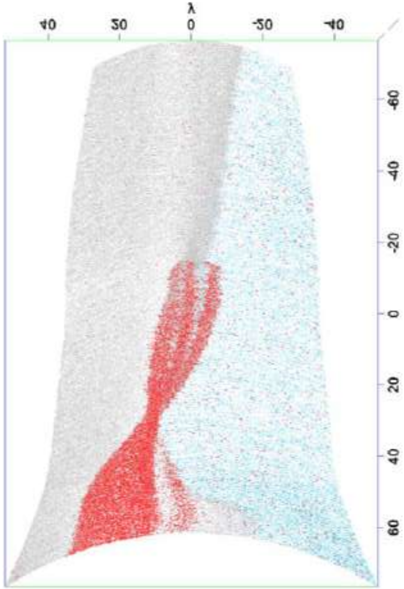
J.H. Lee et al., Micron 58 (2014) 32



A. Franquet et al., Appl. Surf. Sci. 365 (2016) 143
D. Melkonyan et al., Ultramicroscopy 179 (2017) 100

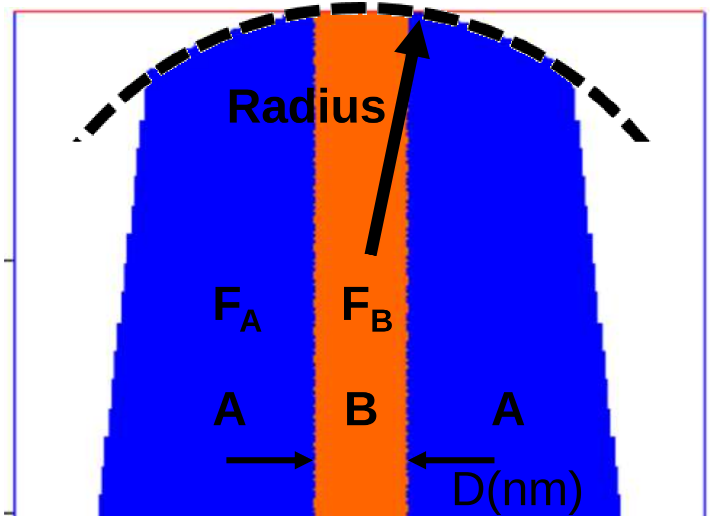


E. Marquis and F. Vurpillot,
Micro. Microanal 14 (2008) 561



- We can find dozens of examples of the issues that occur when trying to reconstruct data containing regions with different evaporation fields
- A few (older) examples
  - Miller MK. The Effects of Local Magnification and Trajectory Aberrations on Atom Probe Analysis. Journal de Physique. 1987;48:565-70.
  - Miller MK, Hetherington MG. Local Magnification Effects in the Atom Probe. Surface Science. 1991;246:442-9.
  - De Geuser F, Lefebvre W, Danoix F, Vurpillot F, Blavette D, Forbord B. An Improved Reconstruction Procedure for the Correction of Local Magnification Effects in Three-Dimensional Atom-Probe. Surface and Interface Analysis. 2007;39:268-72.
  - Vurpillot F, Bostel A, Blavette D. Trajectory Overlaps and Local Magnification in Three-Dimensional Atom Probe. Applied Physics Letters. 2000;76:3127-9.
  - Marquis, E, Vurpillot, F, Chromatic Aberrations in the Field Evaporation Behavior of Small Precipitates. Microsc. Microanal. 14, 561–570, 2008

Simulation Space

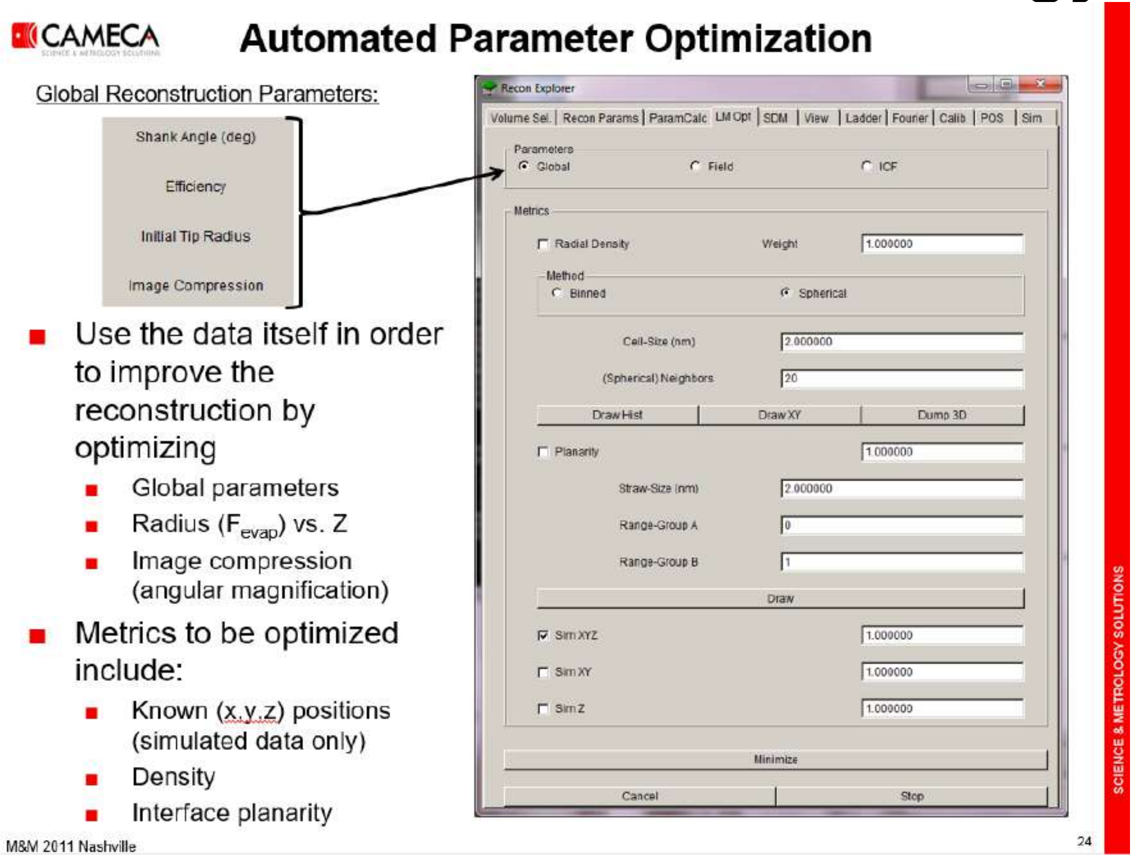


Specimen Radius (nm)	Feature Size D (nm)	Field (B)/ Field (A)
10	2	0.5
20	6	0.6
40		0.71
		0.77
		0.83
		0.87
		0.9
		1.0
		1.2
		1.4
		2.0

- The method to simulate the end-form evolution of atom probe specimens consists of a 3D Poisson simulation using a finite difference algorithm based on previous work
  - B. P Geiser et al., Microsc. Microanal. 15 (2009) 302 and
    F. Vurpillot et al., Appl.Phys.Lett.76(21) (2000) 3127
  - For a recent review see: F. Vurpillot and C. Oberdorfer, Ultramicroscopy 159 (2015) 202
- All simulations used a (full) shank angle of 10deg, using FCC lattice with 0.4nm lattice parameter, simulation lattice 0.2nm with total size of 512x512x1024 cells (plus electrostatic supervolume), 1000 evaporation events/field iteration
- Each simulation takes approximately 1-2 days to run (on high end workstation)
- For further information see B. P. Geiser, D. A. Reinhard and D. J. Larson, Mat. Char (2018) in press.

Reconstruction Methodology

- We do not want the measurements to be biased by reconstruction quality
- We have reconstructed all data using automated optimization of the reconstruction parameters
- One of the options in this developmental code is to use the known original atom positons of simulated data
- Optimal parameters are determined by minimizing the different between original and reconstructed atom positions



Automated Parameter Optimization

Global Reconstruction Parameters:

Shank Angle (deg)
Efficiency
Initial Tip Radius
Image Compression

- Use the data itself in order to improve the reconstruction by optimizing
  - Global parameters
  - Radius (F_{evap}) vs. Z
  - Image compression (angular magnification)
- Metrics to be optimized include:
  - Known (x,y,z) positions (simulated data only)
  - Density
  - Interface planarity

Recon Explorer

Parameters: ● Global ○ Field ○ ICF

Metrics

☐ Radial Density Weight 1.000000
Method: ○ Binned ● Spherical
Cell-Size (nm) 2.000000
(Spherical) Neighbors 20
☐ Planarity 1.000000
Straw-Size (nm) 2.000000
Range-Group A 0
Range-Group B 1
☑ Sim XYZ 1.000000
☐ Sim XY 1.000000
☐ Sim Z 1.000000

M&M 2011 Nashville

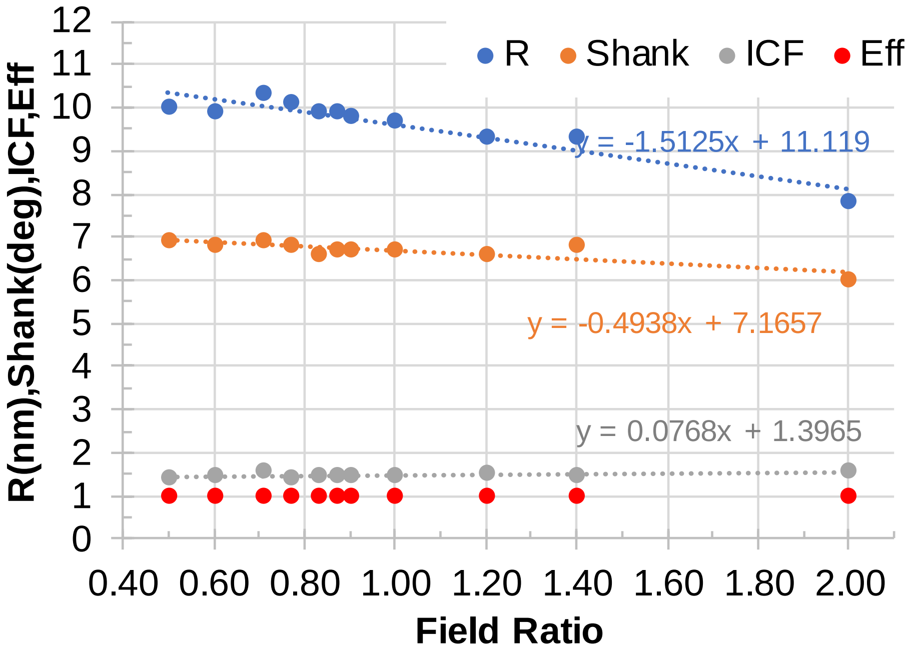
24

D J Larson, B. P. Geiser, T J Prosa and T F Kelly
Microscopy and Microanalysis 17(S2) (2011) 724

Automated Parameter Determination

Radius=10nm
D=2nm

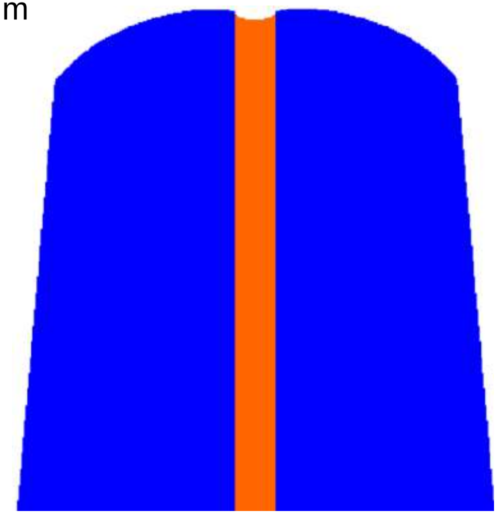
Precipitate Field	R	Shank	ICF	Eff
0.50	10.0	6.9	1.41	1
0.60	9.9	6.8	1.45	1
0.71	10.3	6.9	1.58	1
0.77	10.1	6.8	1.39	1
0.83	9.9	6.6	1.46	1
0.87	9.9	6.7	1.45	1
0.90	9.8	6.7	1.46	1
1.00	9.7	6.7	1.46	1
1.20	9.3	6.6	1.50	1
1.40	9.3	6.8	1.45	1
2.00	7.8	6.0	1.58	1
Average	9.6	6.7	1.5	1.0
Sigma	0.68	0.25	0.06	0.00



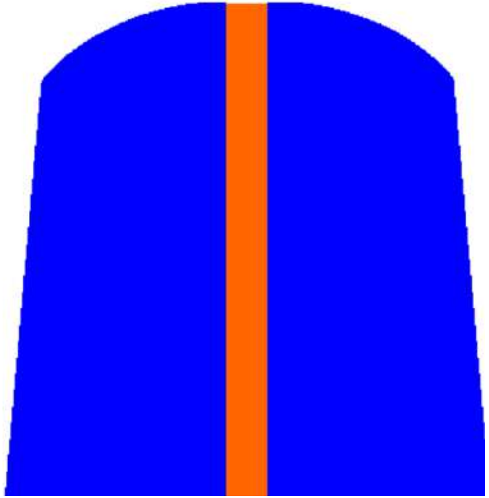
- Generally pretty happy with the automated results
- We are not seeing strange efficiencies or image compression
- R and shank values are quite close or within reasonable proximity to the known simulation starting values

Field Evaporated Shapes

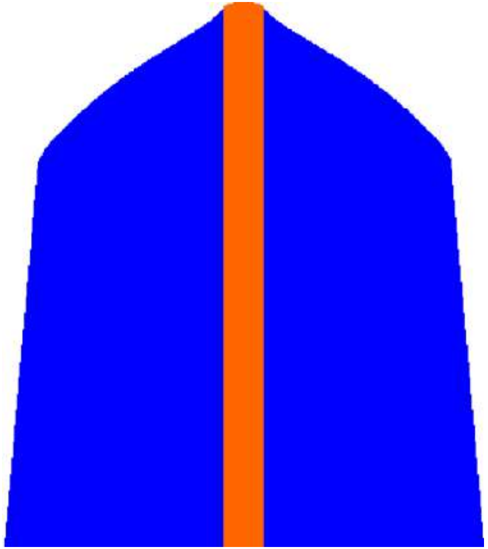
Radius=40nm
D=6nm



F_{BA}=0.5



F_{BA}=0.83



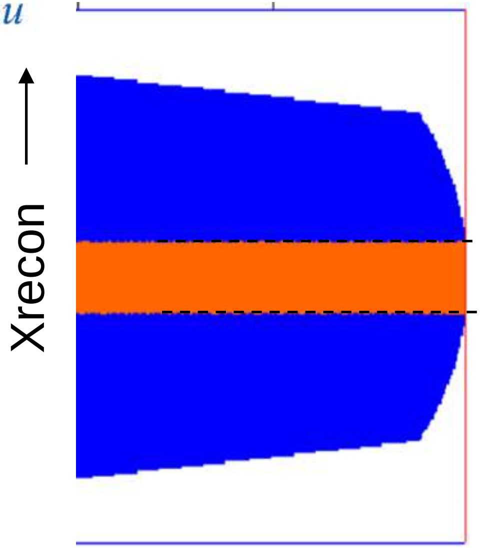
F_{BA}=2.0

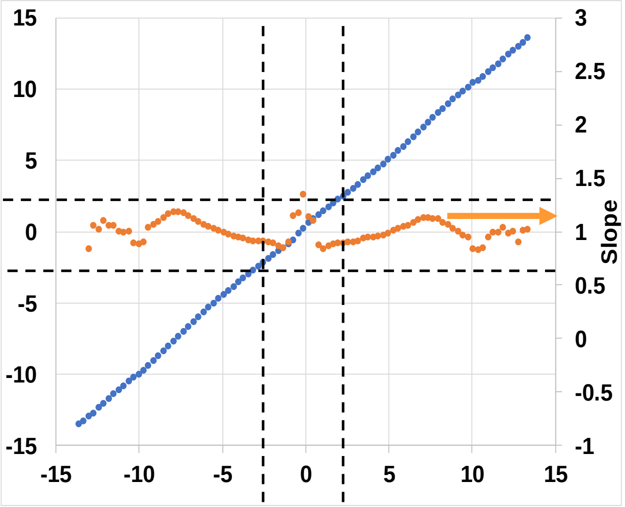
The various shapes are as one might expect* appear after simulated field evaporation of the specimen

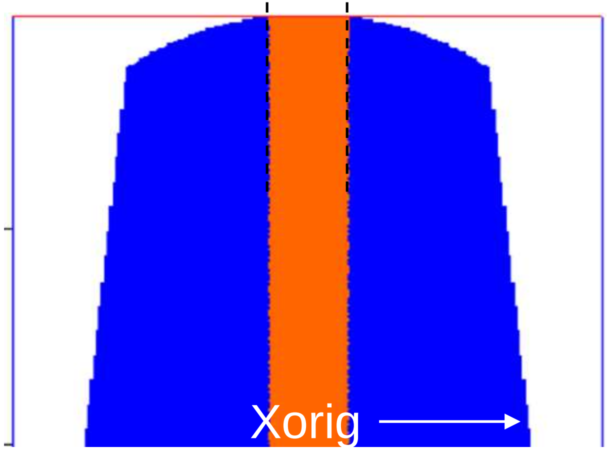
* M. K. Miller, J. de Phys. Colloq. 48 (1987) C6-565
O.Dimond, Part II Thesis, University of Oxford (1999)
F. Vurpillot et al., Appl. Phys. Lett 76 (2000) 3127
F. Vurpillot et al, Microsc. Microanal. 10 (2004) 384
C. Oberdorfer and G. Schmitz, Microsc. Microanal 17 (2011) 15
D. Melkonyan et al., Ultramicroscopy 179 (2017) 100

Methodology

Radius=20nm
D=6nm
F_{BA}=1.0





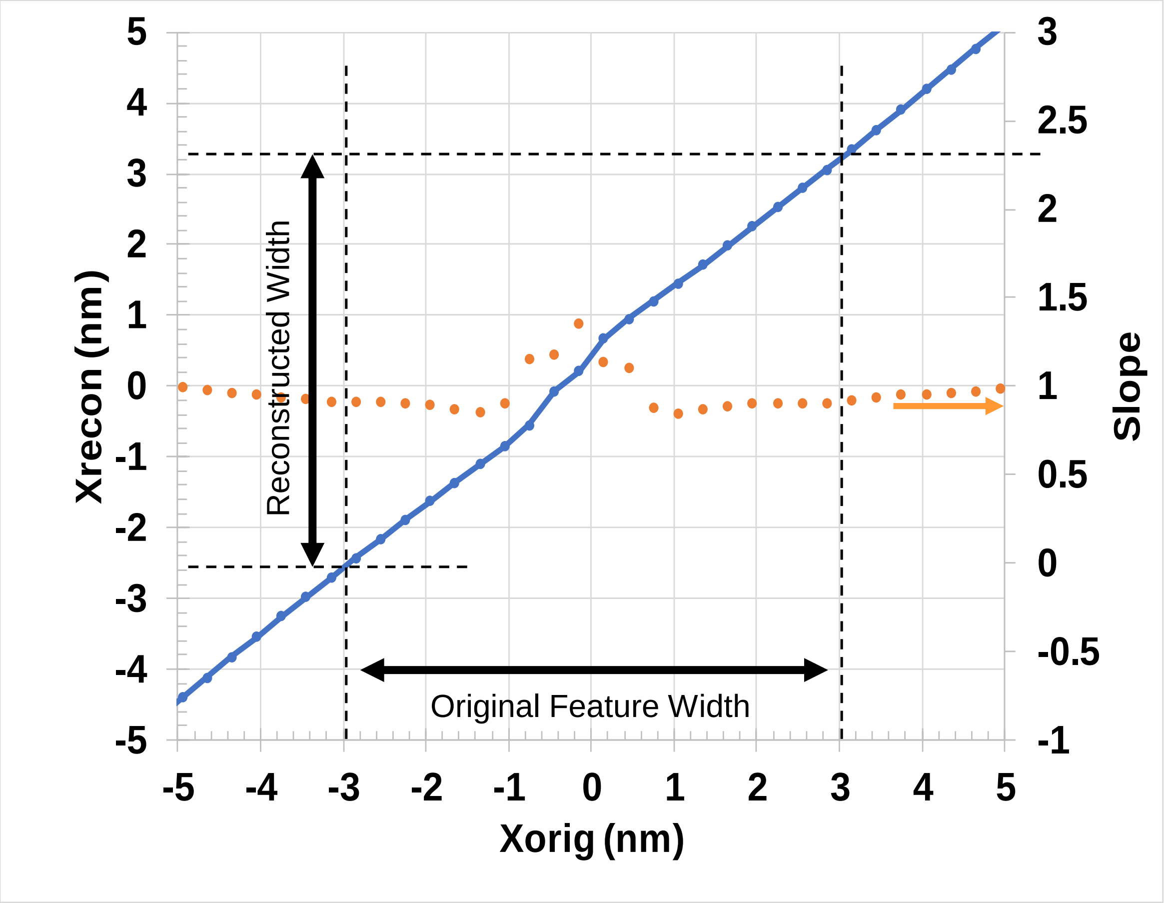


- Following reconstruction of the data from each simulated cell, we created a curve of original x position vs. reconstructed x position – these are the blue points shown at upper right
- The ideal slope of this curve is unity
- The brown points plot the slope (right hand axis)

Methodology

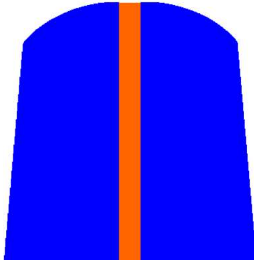
Radius=20nm
D=6nm
F_{BA}=1.0

- Plot of Xorig vs Xrecon gives us the effective reconstructed width of the feature
- The slope (orange points) of these data (effectively a magnification) is ideally unity
- Reconstructed width is ~5.5nm, average slope in feature region is ~0.96



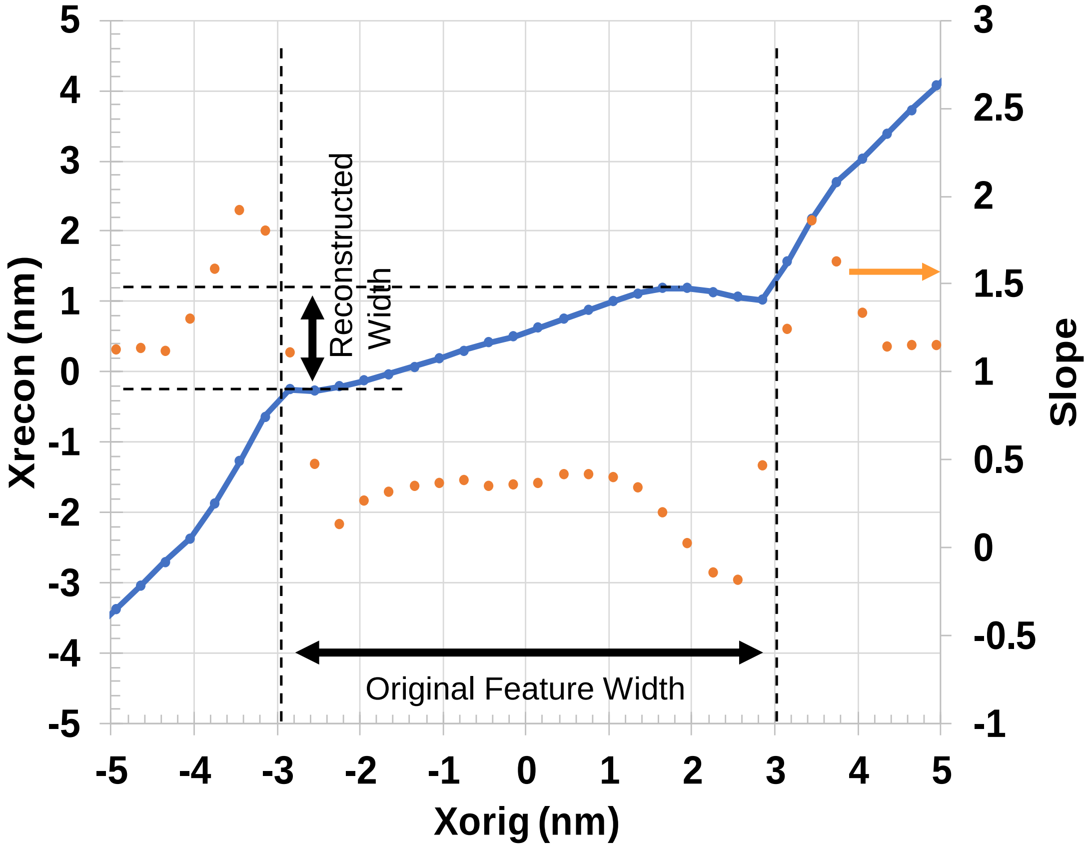
Methodology

Radius=20nm
D=6nm
F_{BA}=0.83



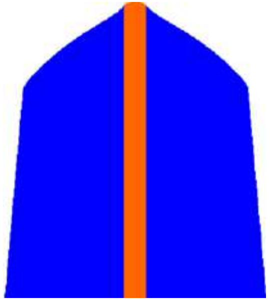
Let’s examine a more interesting case…

- For the case of F_{BA}=0.83…
- Reconstructed width 1.5nm, average slope in feature region is ~0.2

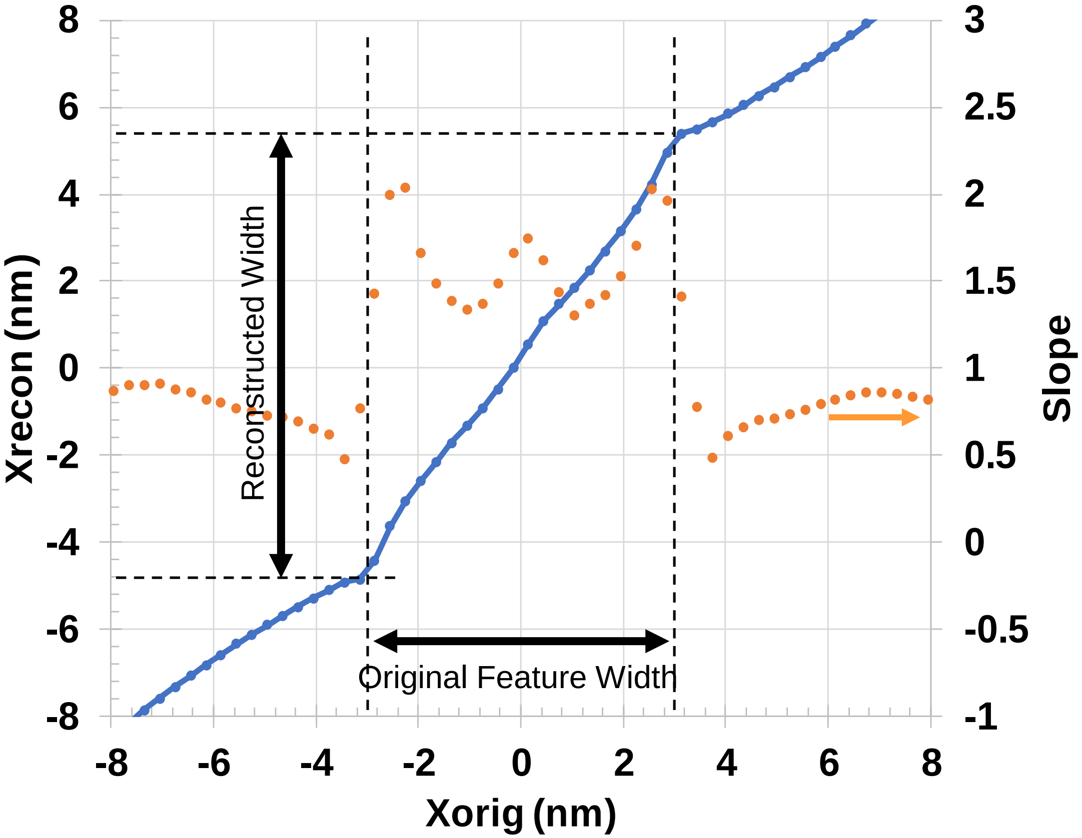


Methodology

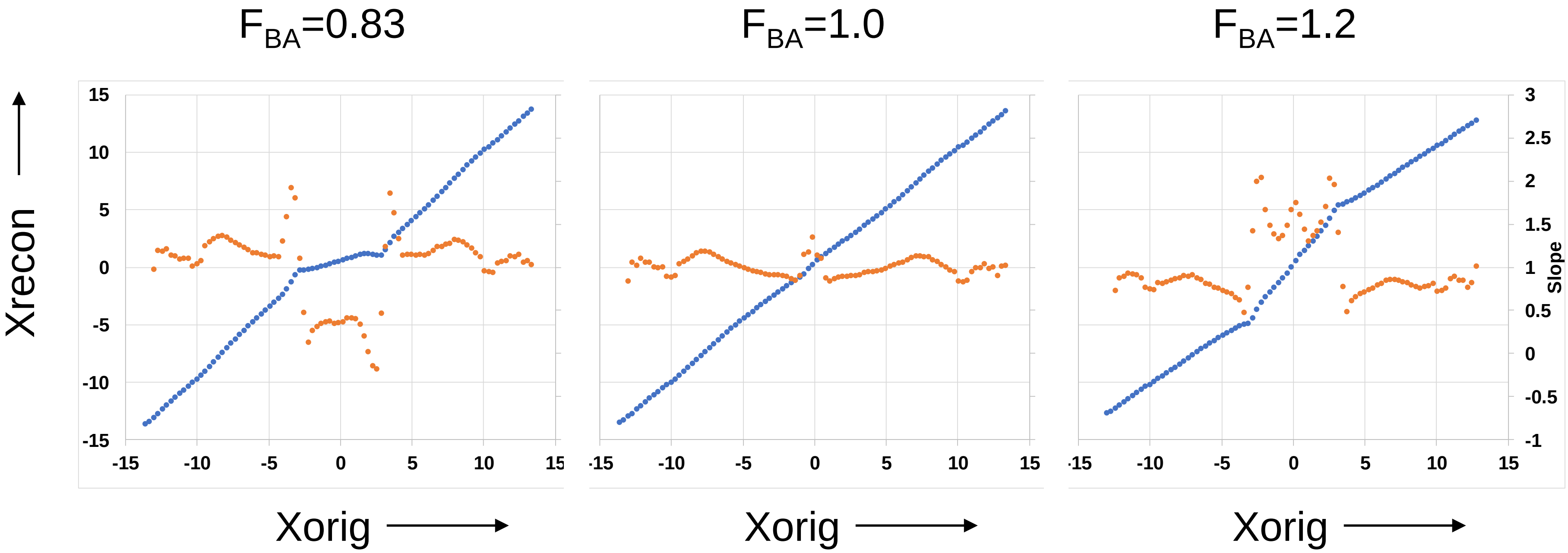
Radius=20nm
D=6nm
F_{BA}=1.2



- For the case of F_{BA}=1.2…
- Reconstructed width 8.5nm, average slope in feature region is ~1.5



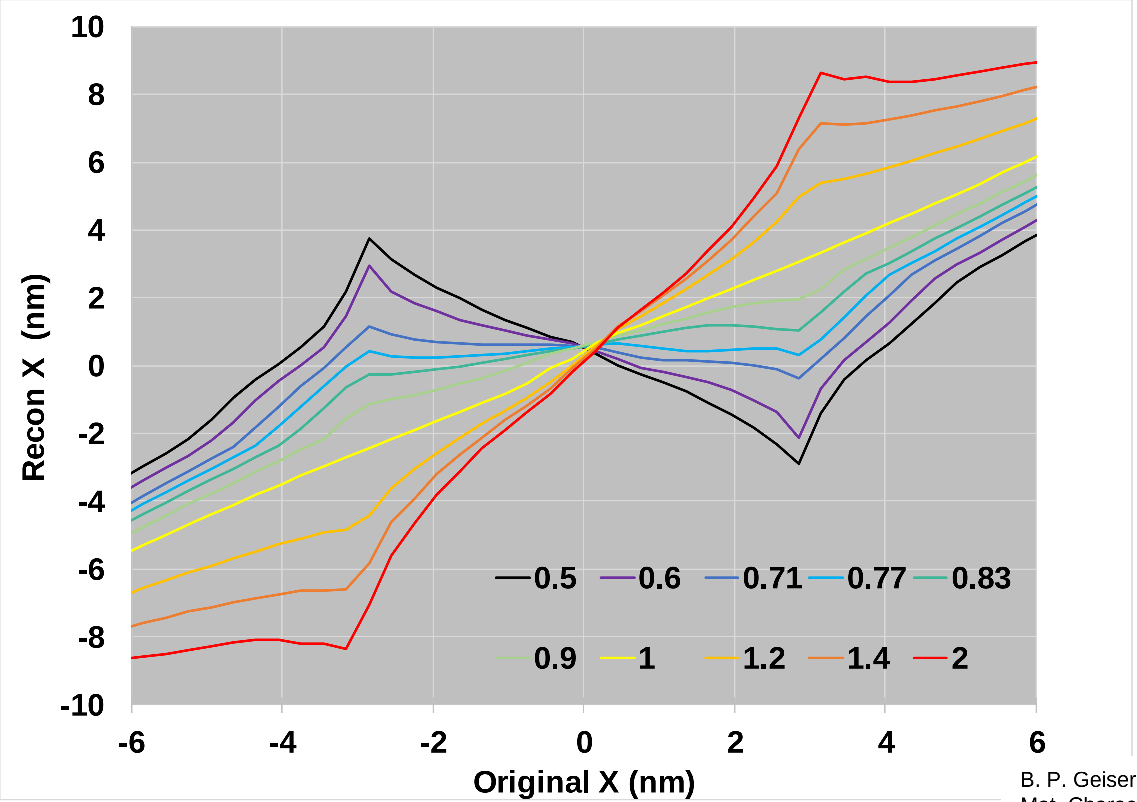
$F_{AB} = 0.83/1.0/1.2$



- R=20nm, D=6nm

Analysis Methodology

Radius=20nm
D=6nm
F_{BA}=ALL

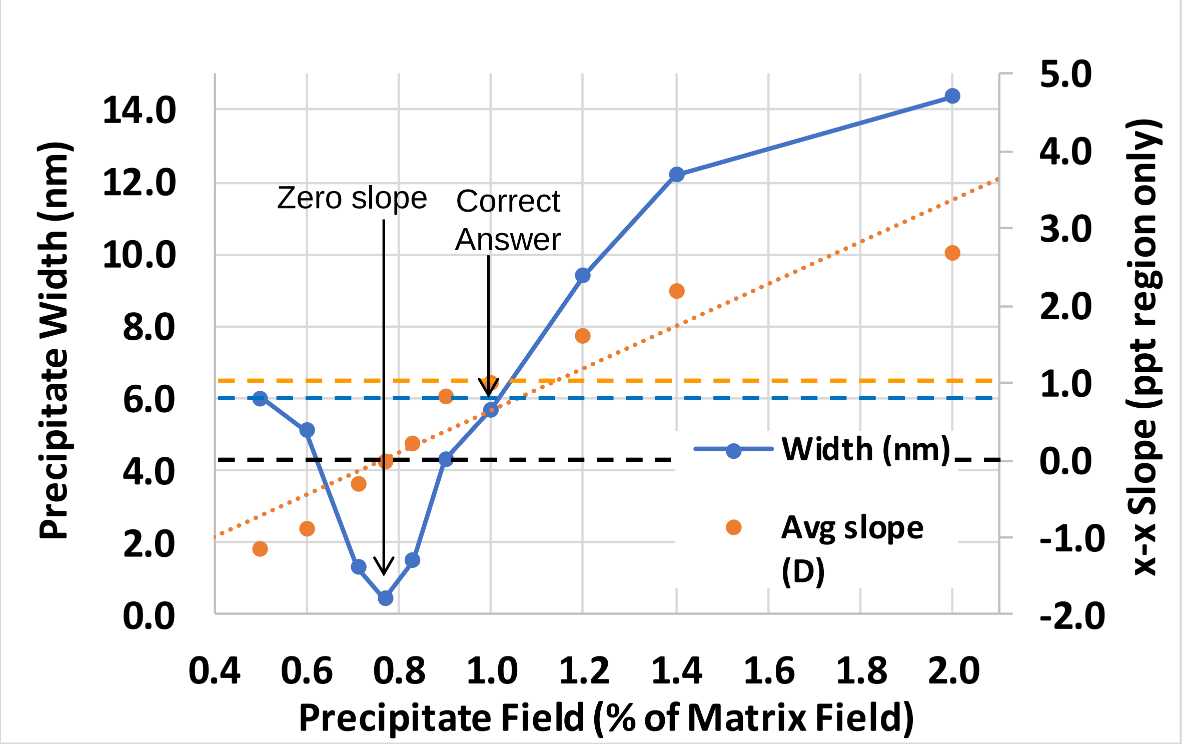


B. P. Geiser, D. A. Reinhard and D. J. Larson, Mat. Characterization (2018) in press.

If we calculate the plots for all values of F_{BA}, we get the above, from which we can calculate a effective feature width and slope for each curve

Apparent Feature Widths & Slopes

Radius=20nm
D=6nm
F_{BA}=ALL

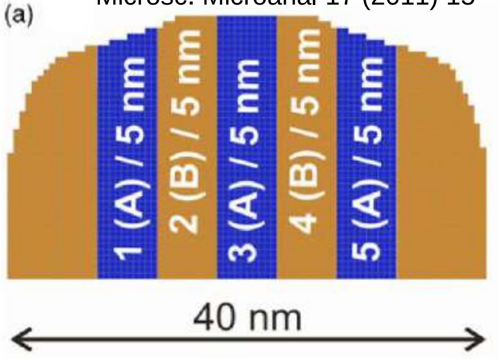


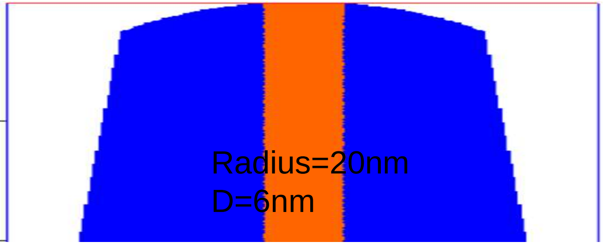
Dashed lines show desired width and slope

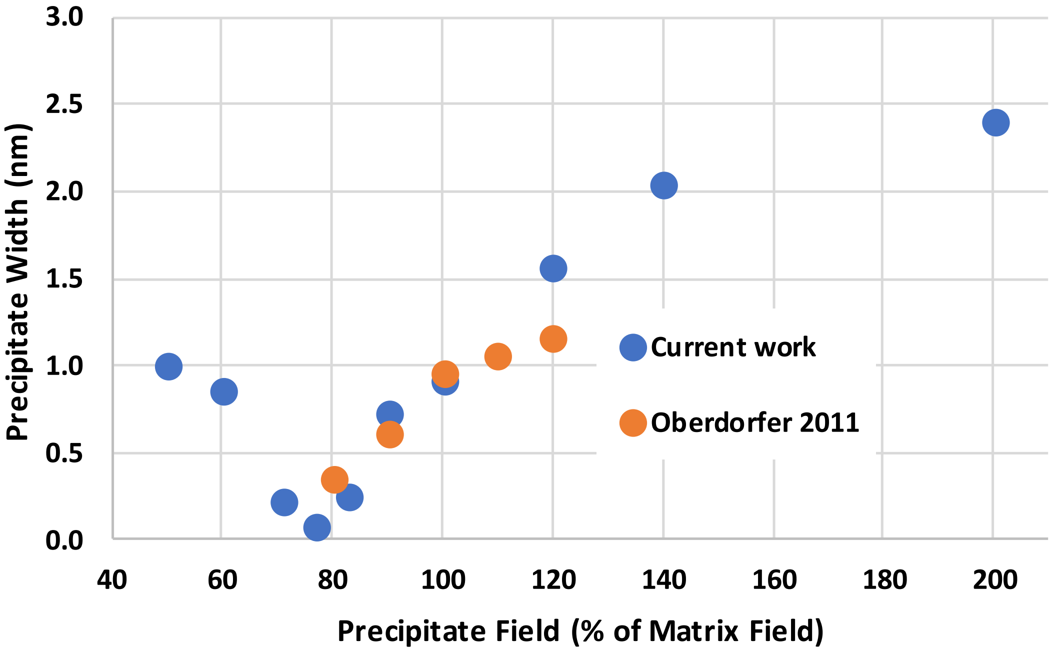
We can compile curves like this for all combinations (66) of specimen radius and feature size

Comparison to Previous Work*

* C. Oberdorfer and G. Schmitz, Microsc. Microanal 17 (2011) 15



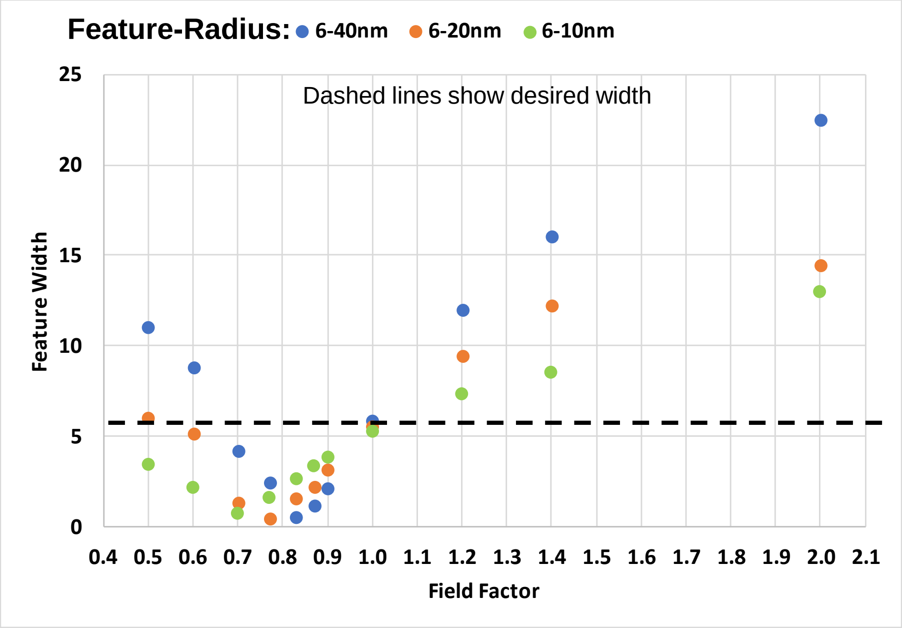




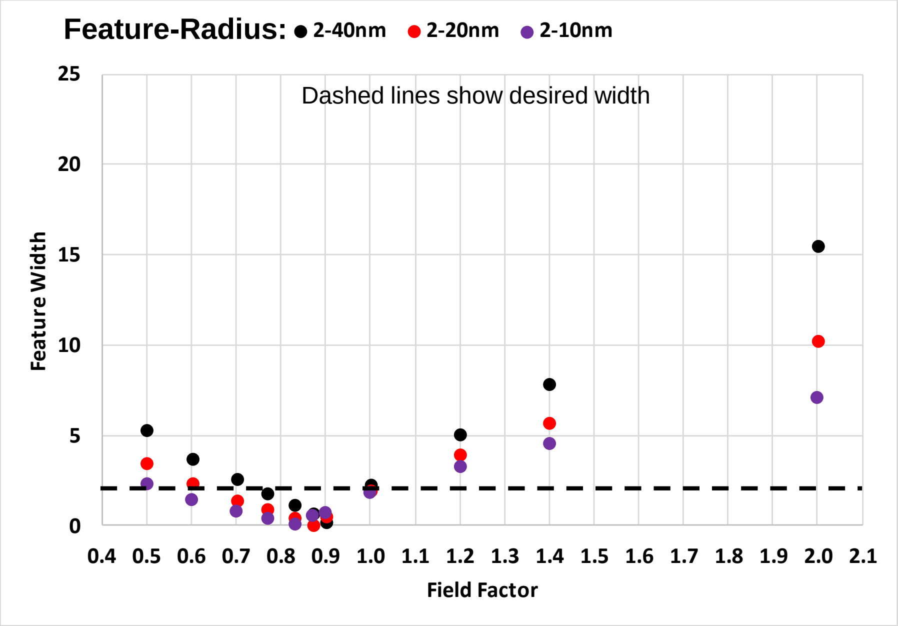
- Although not the same simulation starting point, there is reasonably good agreement between the data
- Previous work however did not explore the effects of changing the feature size or the specimen radius and also used only a limited range of field ratios – <u>did not get to the inflection point</u>
  - R=20nm only
  - Feature size 5nm
  - Zero shank (no radius change)

Width Comparisons

Feature Size 6nm

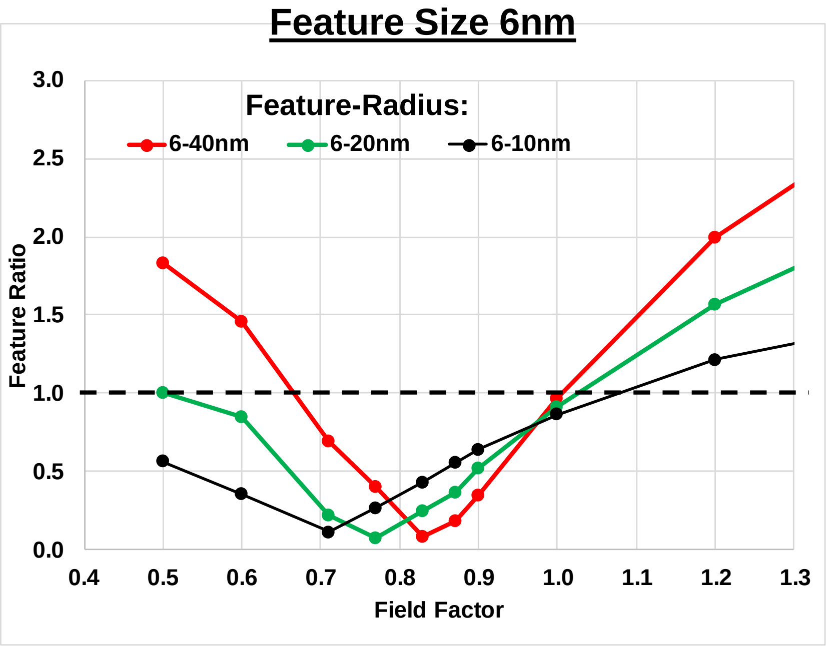


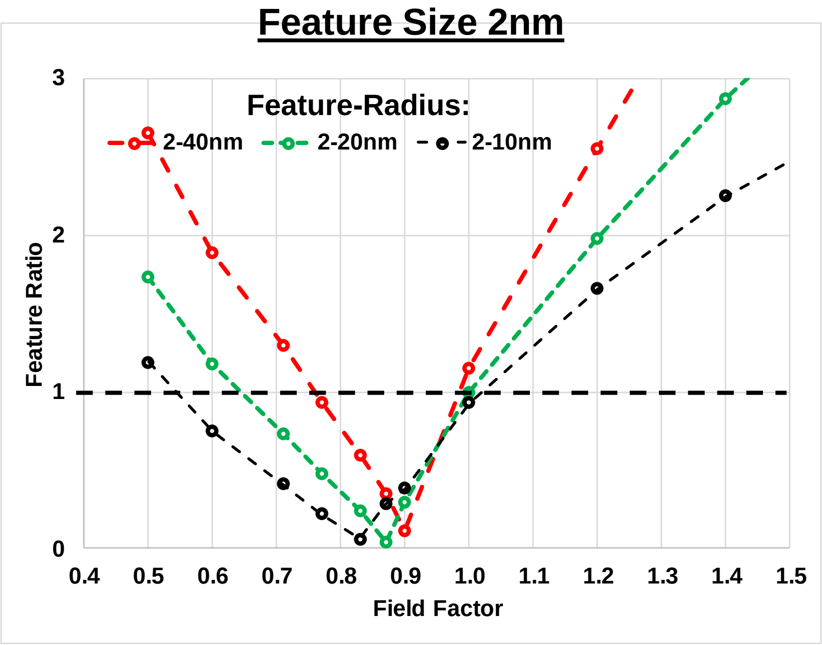
Feature Size 2nm



- Very close to the nominal feature width is obtained for the F_{BA}=1.0 cases
- The zero slope crossover point (minimum feature width) is observed to shift with changes in specimen radius and feature width

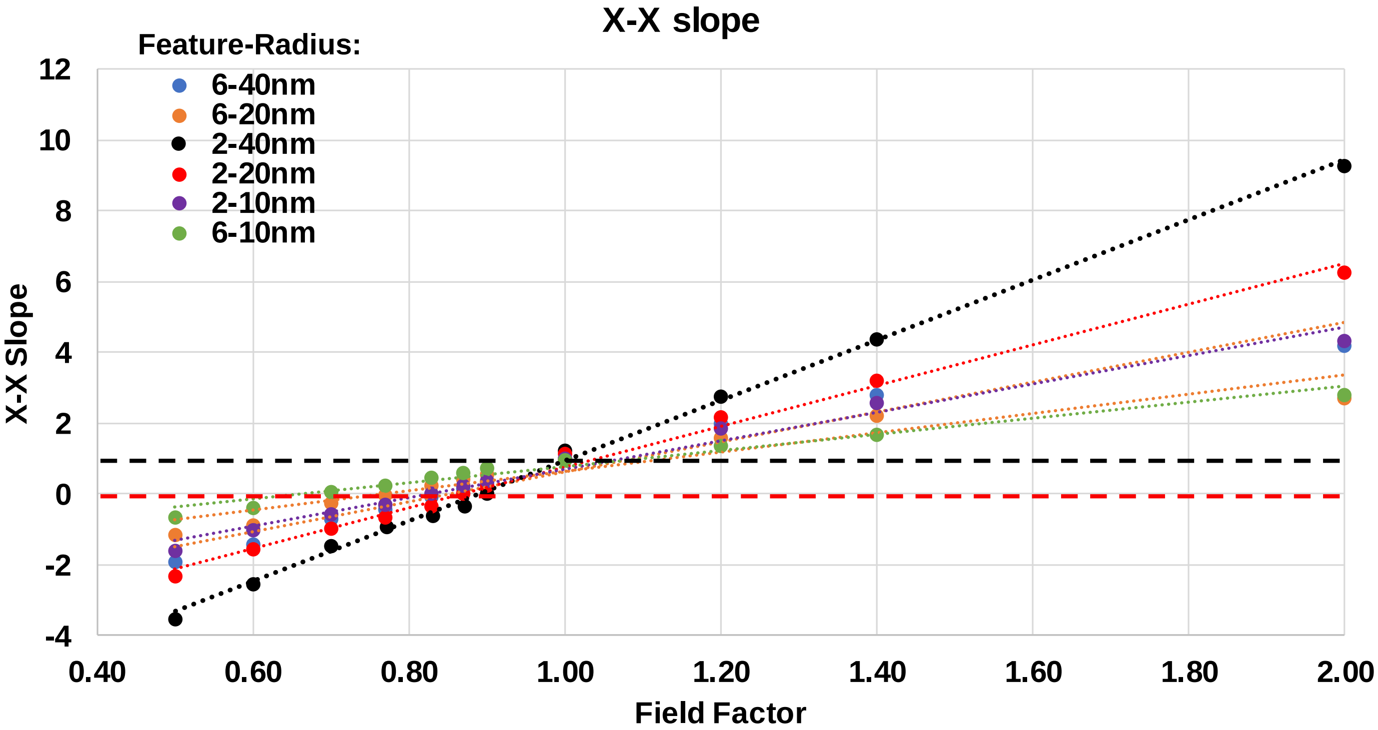
Normalized Width Comparisons





- Crossover to negative slope point shifts to the right (worse) for increasing specimen radius and for decreasing feature size
- The second of these trends appears slightly more substantial

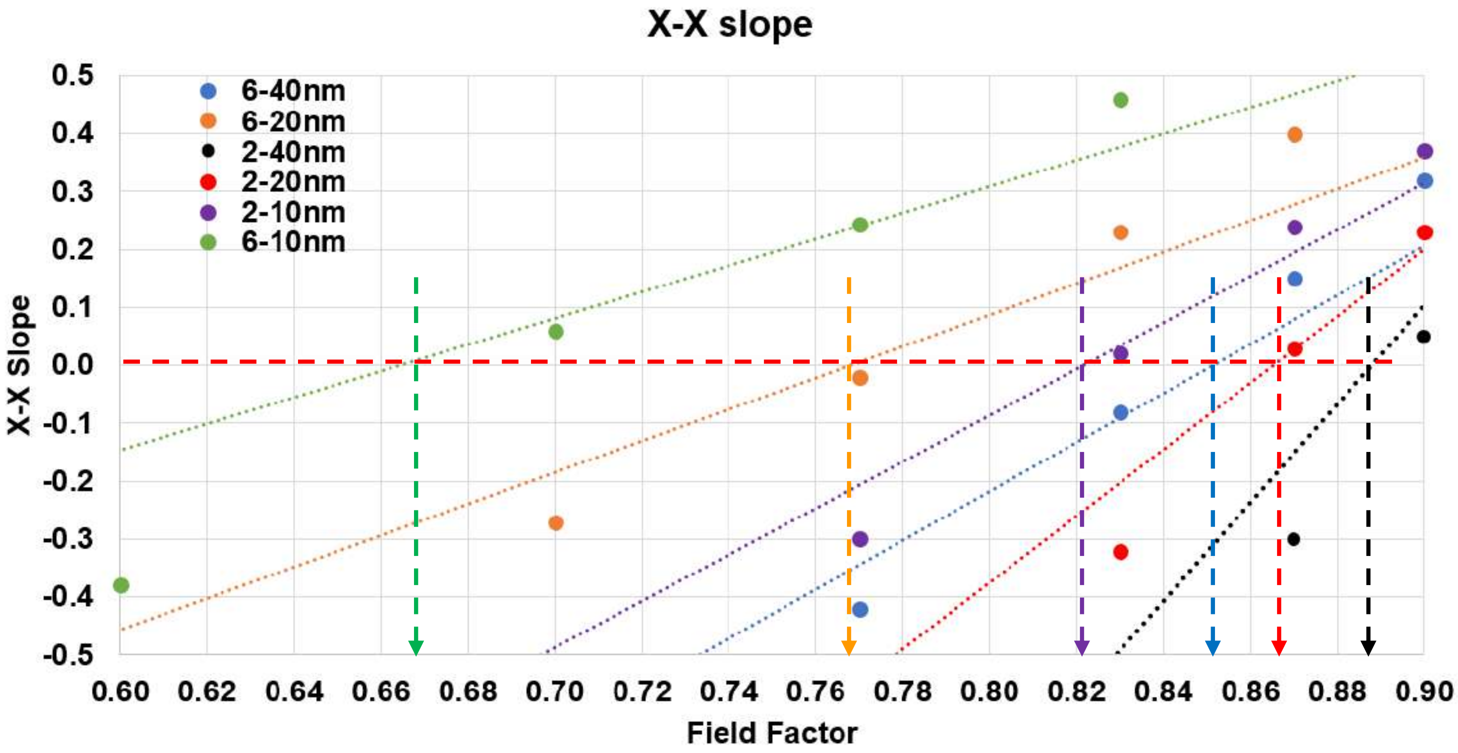
Slope Comparison



Dashed lines show desired slope (unity) and crossover slope for ion crossing (zero)

- Comparison of slopes (magnification) for all data
- Smallest feature and largest radius shows the most deviation
- Blow up the zero slop cross over region…

Zero Slope Points



Dashed red line show crossover slope for ion crossing (zero)

We can generate an estimate of the zero slope cross over phase space as a function of specimen radius and feature size

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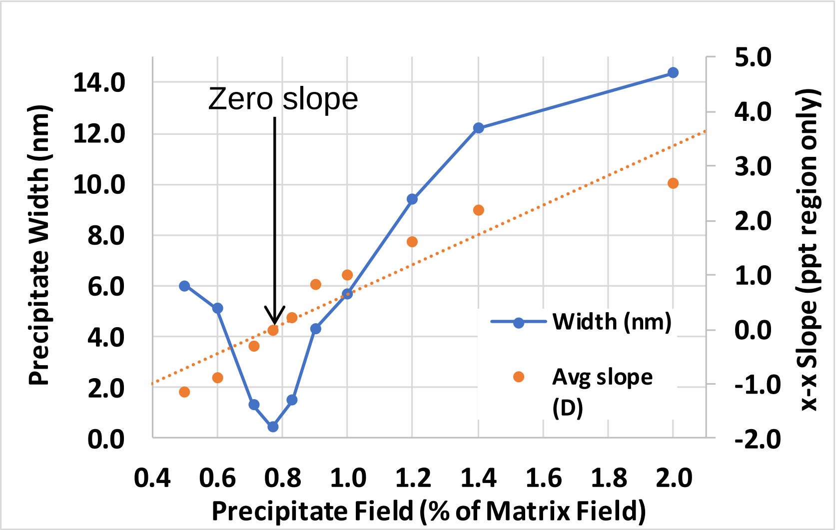
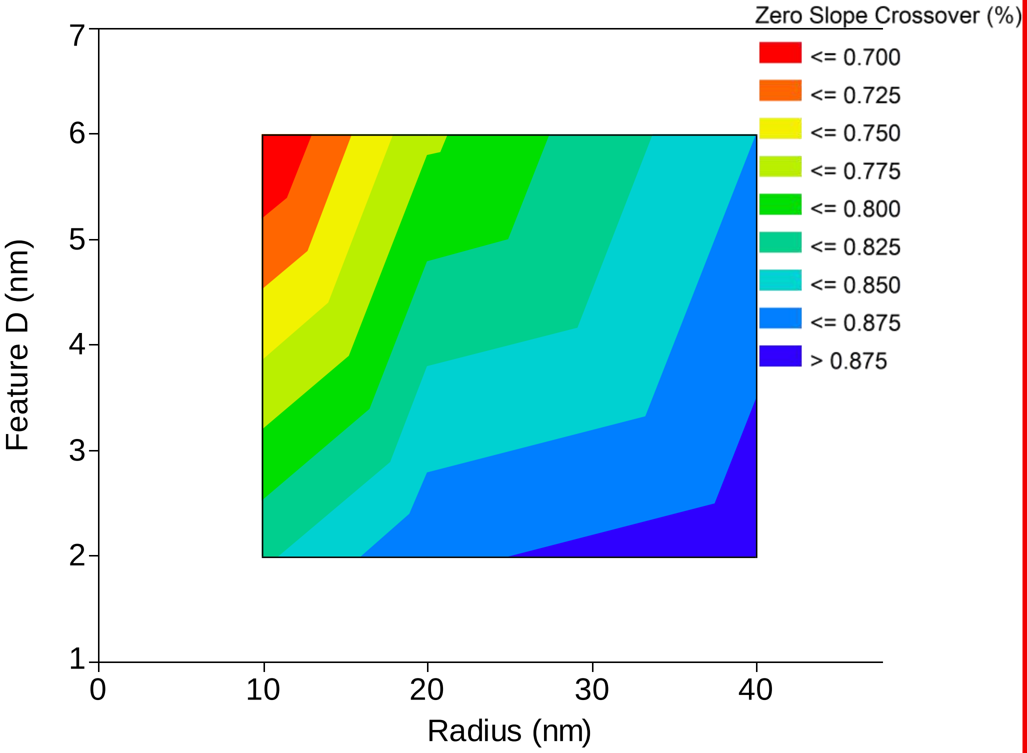
Zero Slope Points

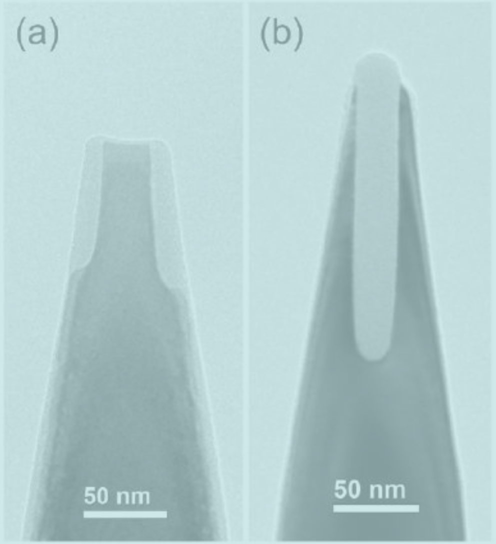


B. P. Geiser, D. A. Reinhard and D. J. Larson, Mat. Characterization (2018) in press.

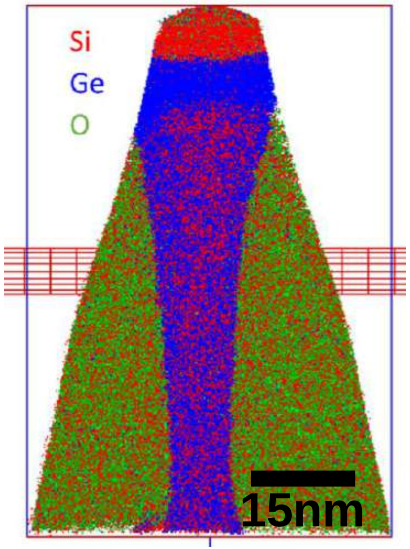


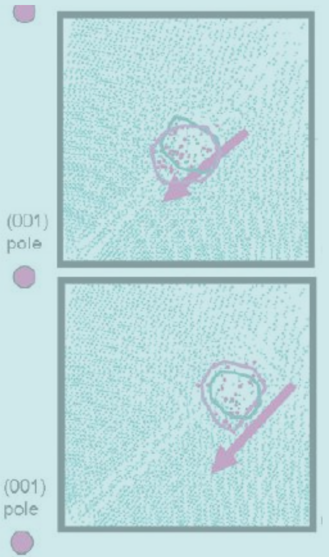
- Nothing too surprising here
- Conclusion: you want small radii and large feature size in order to minimise issues – make your tips sharp!

Different Phases Cause Problems…

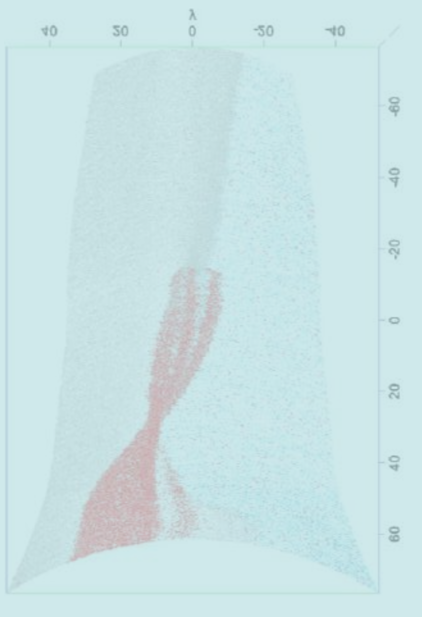


J.H. Lee et al., Micron 58 (2014) 32





E. Marquis and F. Vurpillot,
Micro. Microanal 14 (2008) 561



A. Franquet et al., Appl. Surf. Sci. 365 (2016) 143
D. Melkonyan et al., Ultramicroscopy 179 (2017) 100

Lets go back to one of the examples previously shown

Comparison to Real Data

Current Simulation

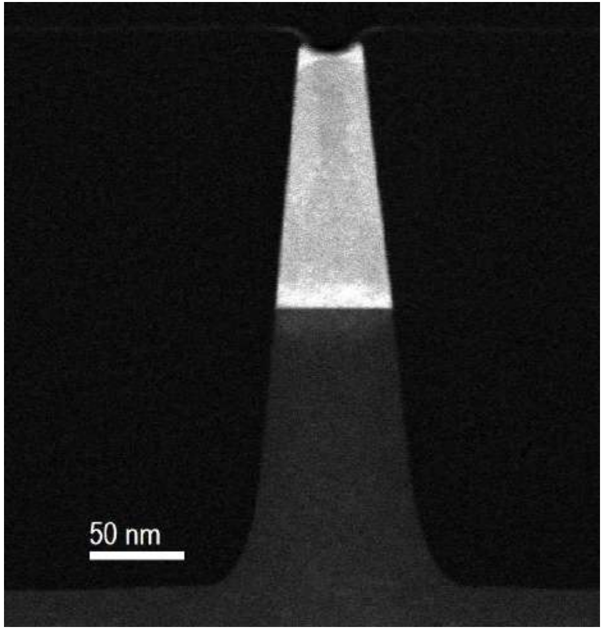
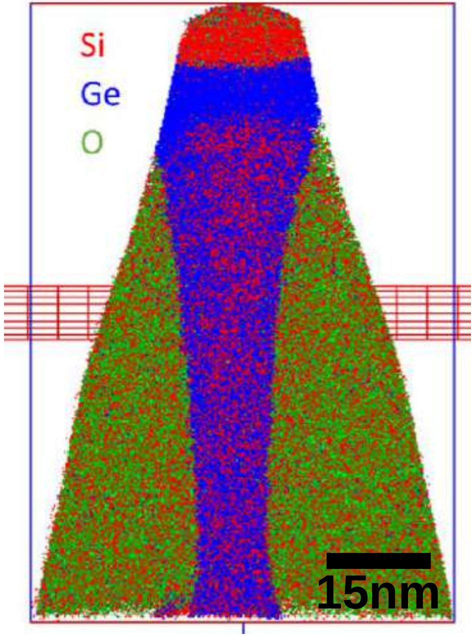
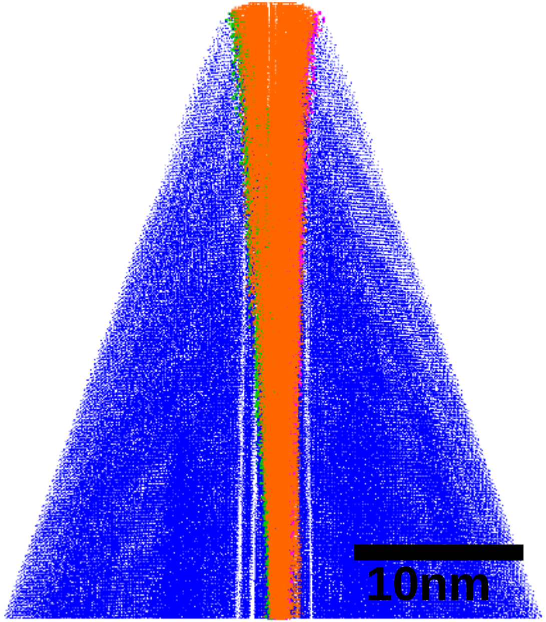


Image courtesy W. Vandervorst (IMEC)



A. Franquet et al., Appl. Surf. Sci. 365 (2016) 143

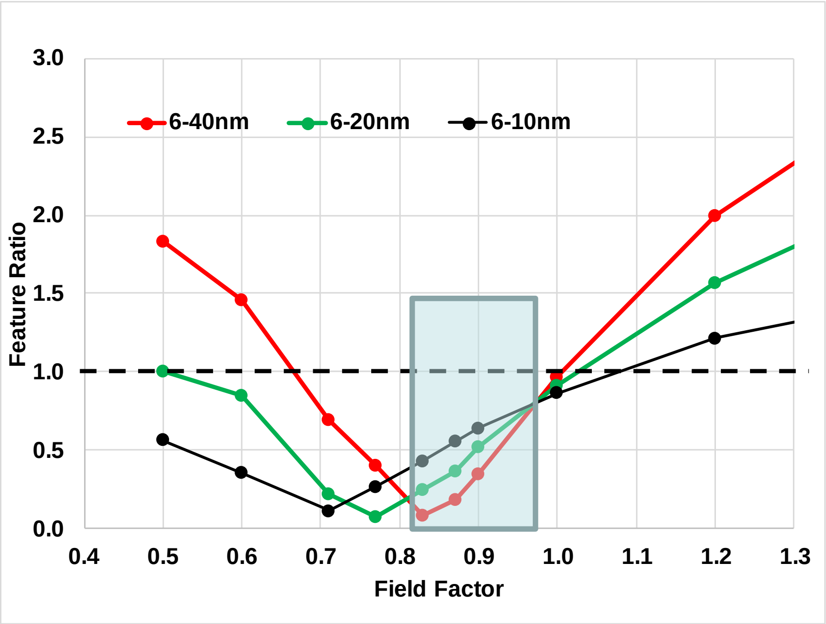


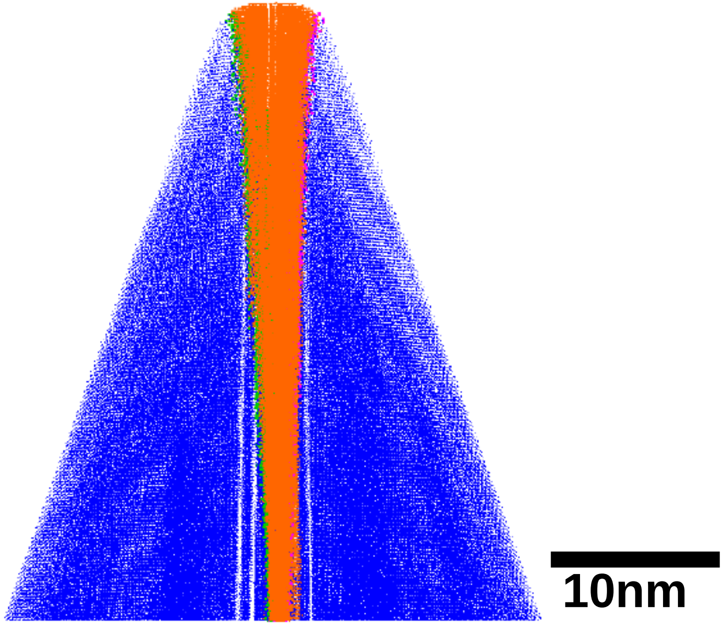
Feature 6nm width, F_{BA}=0.8

- Example of a 40nm width Si-70Ge trench in silicon
- Scales not exactly the same, but the trend is consistent: decreasing feature size with depth into the sample

Consider Effect of Increasing Radius During Experiment

Feature Size 6nm



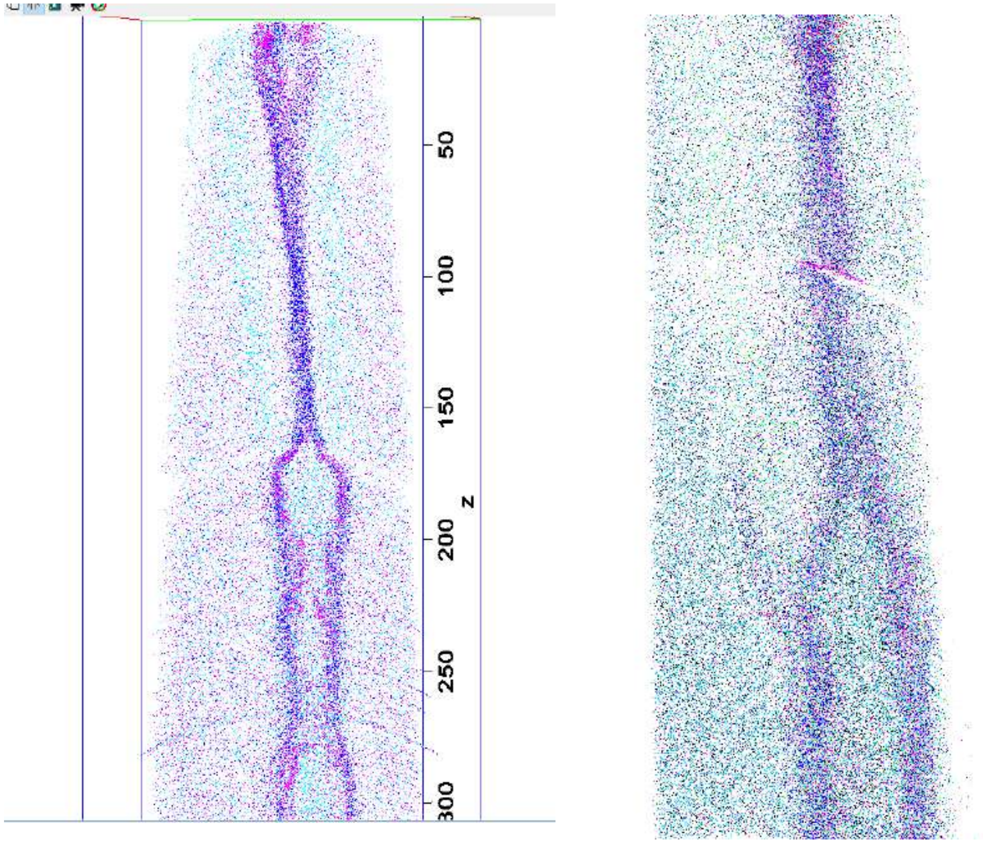


- This is our previously shown normalized data for a feature size of 6nm
- Increasing radius in the region between field factor ~0.8 and 0.95 leads to a thinner and thinner region being detected (black to green to red)

What Is Happening Here?

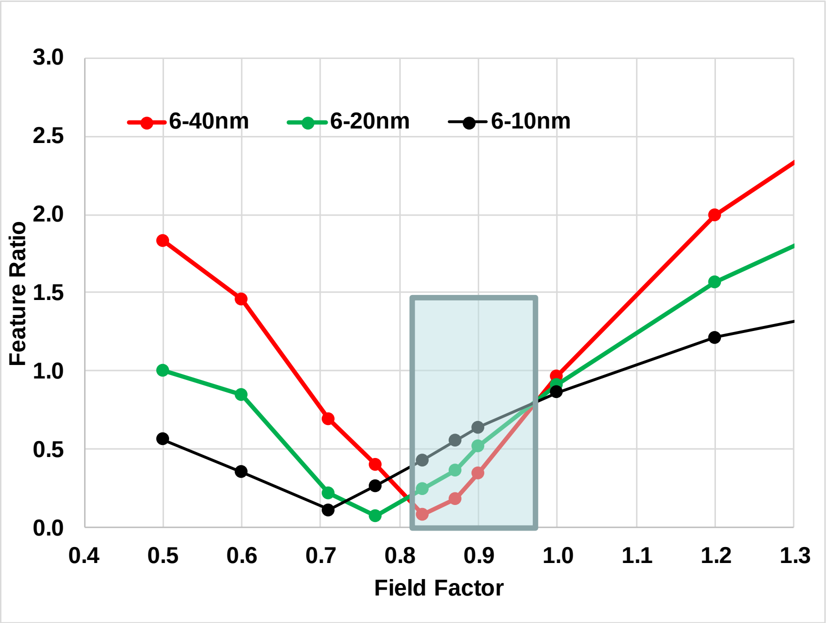
- These are two different runs – this is a reproducible effect
- Structure is complex ABCBA type sample analysed in cross section
- Lets consider another section of our F_{AB} vs Feature Ratio plot…

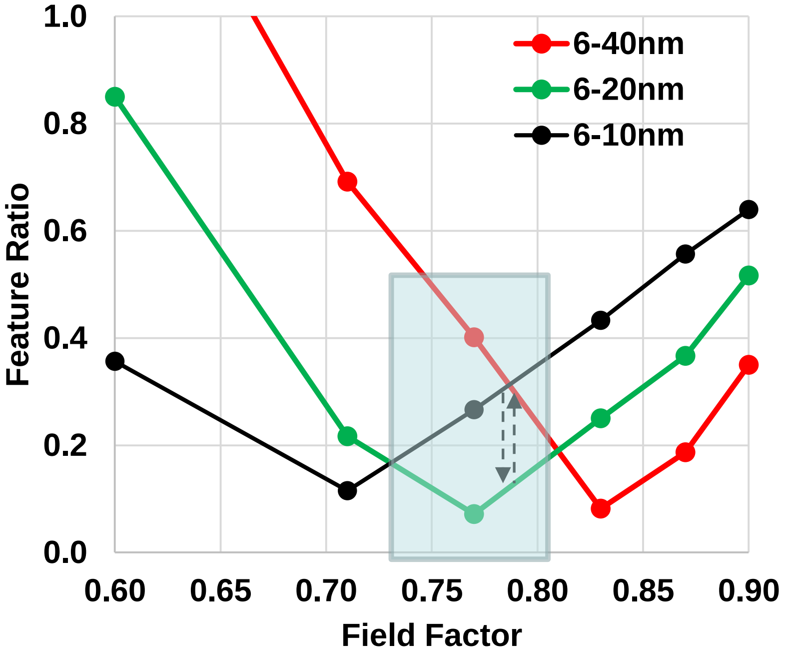
Oxide/nitride/silicon/nitride/oxide



Consider Increasing Radius Effect

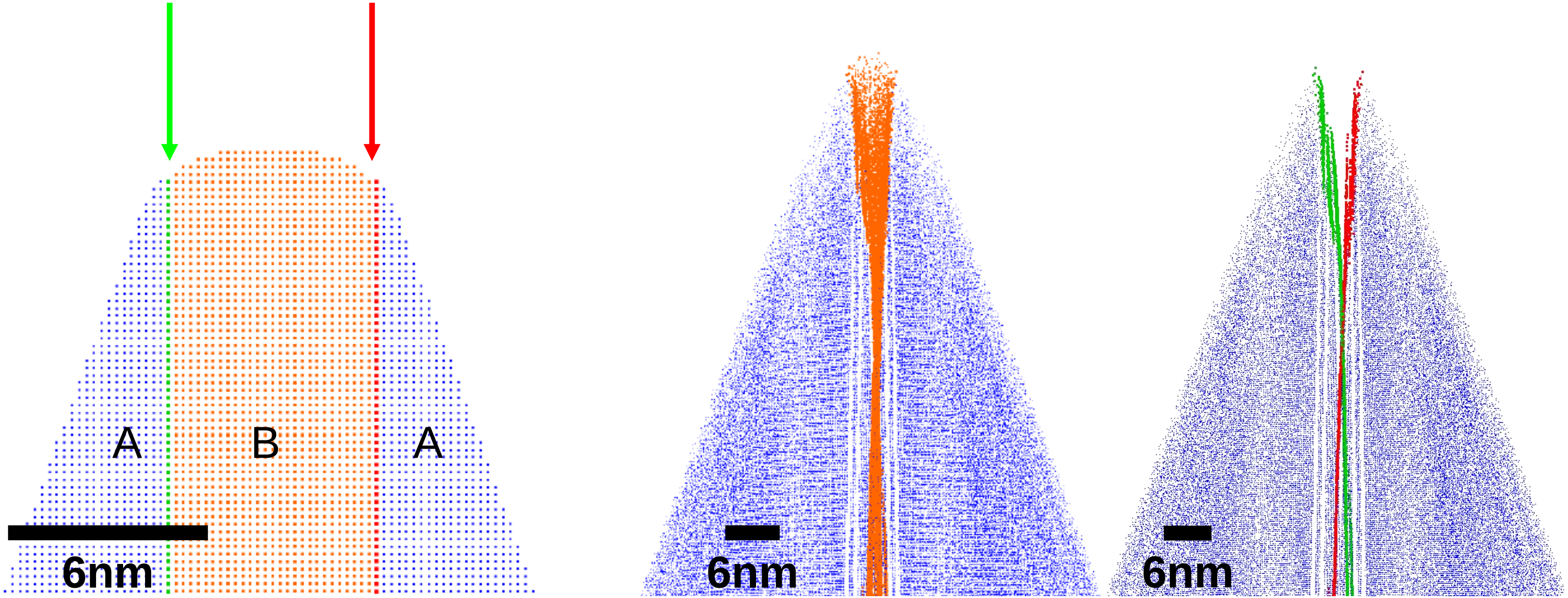
Feature Size 6nm





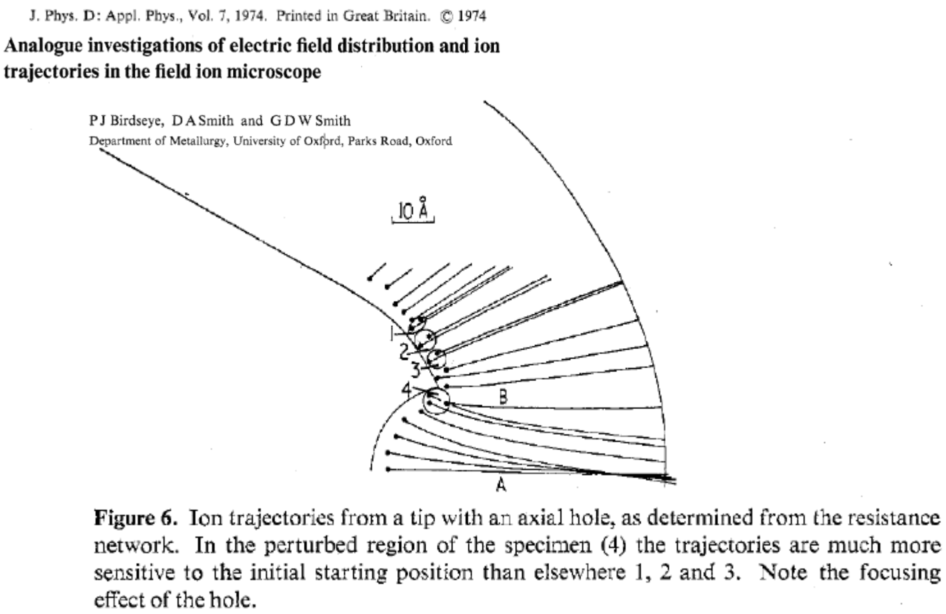
- This is our previously shown normalized data for a feature size of 6nm
- What is going to happen for the region shown above right as radius increases (black to green to red)?

Let’s Track the Feature Edges



- Simulation starts of 6nm feature with F_{AB}=0.8, initial R=5nm and shank=10deg
- Features gets thinner and thinner with increasing radius but then starts to get larger again as radius increases further…

Who’s Familiar With This Paper?



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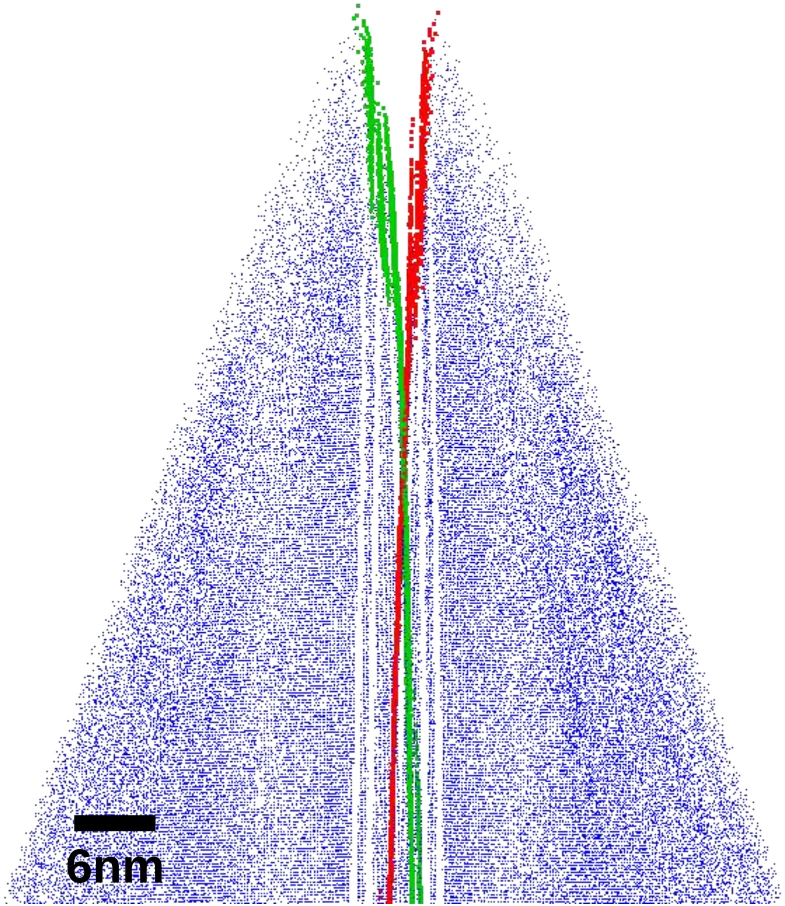
Analogue investigations of electric field distribution and ion trajectories in the field ion microscope

P J Birdseye, D A Smith and G D W Smith
Department of Metallurgy, University of Oxford, Parks Road, Oxford

Figure 6. Ion trajectories from a tip with an axial hole, as determined from the resistance network. In the perturbed region of the specimen (4) the trajectories are much more sensitive to the initial starting position than elsewhere 1, 2 and 3. Note the focusing effect of the hole.

- Proposed nearly 45 years…
- We need to understand the details/limitations of our methods in order to deal with them and to better interpret our data



Summary

- Simulation of a simple steady-state ABA structure was done with variables:
  - Specimen radius
  - Feature size
  - Evaporation field difference
- Analysed metrics were:
  - Reconstructed feature width
  - Magnification (slope of X_{orig} vs X_{recon} plot)
- Simulations showed changing feature width with different specimen radius, F_{AB} values, and feature widths
- For further details of this work see: B. P. Geiser, D. A. Reinhard and D. J. Larson, *Materials Characterization* (2018) in press.