

Combining MEIS with TRIDYN Modelling to Characterise a Plasma Doping Process

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Overview

- Description of plasma doping (PLAD)
- Observations to be explained
- Use of dynamic bca model TRIDYN to describe PLAD
- TRIDYN PLAD Model 1 - Simple
- Metrology to measure PLAD - why MEIS
- Use of TRIDYN to guide analysis of MEIS
- Use of MEIS to guide inputs to TRIDYN
- TRIDYN PLAD Model 2 – Calibrated by MEIS
- Summary

PLAD Process Integration

0. Lithography

Patterned photoresist
selects implant areas

1. Implant

Introduce dopant

2. Wet Cleans

Remove photoresist

3. Anneal

1000°C spike
Activate dopant
Repair damage

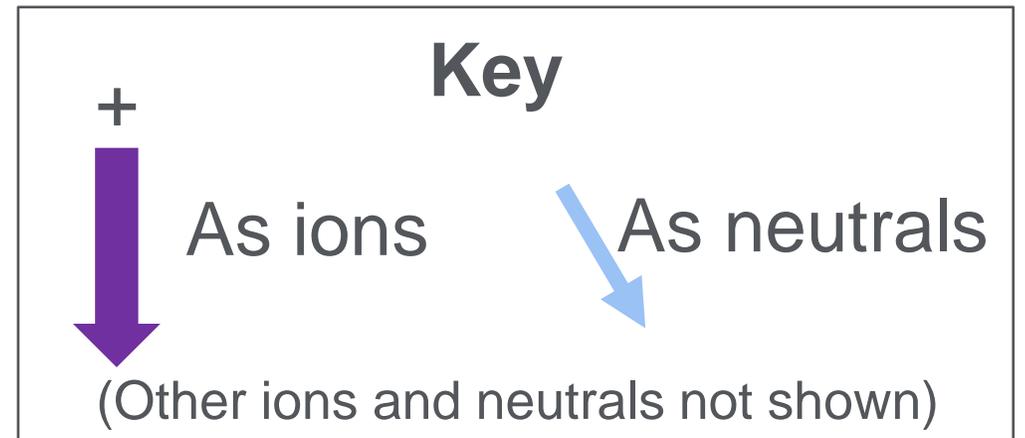
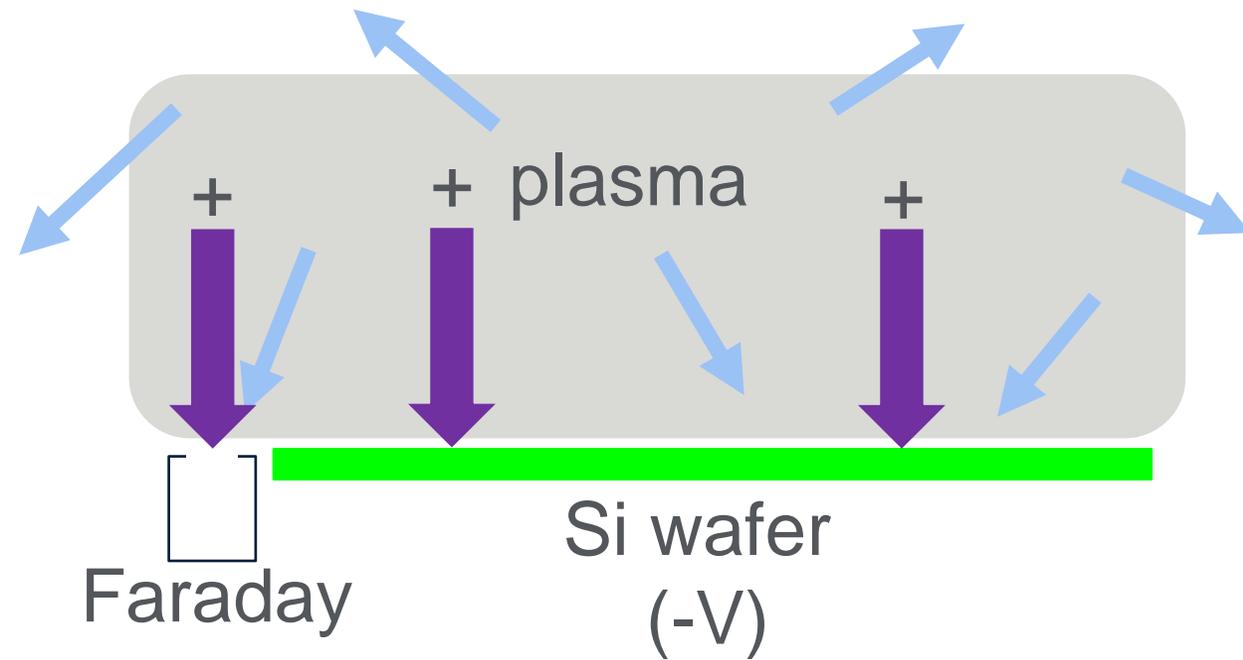
4. DHF

Remove surface oxide

- Substrates in this study are un-patterned wafers
- No photoresist, but follow steps 1-4 to mimic production process

PLAD Process

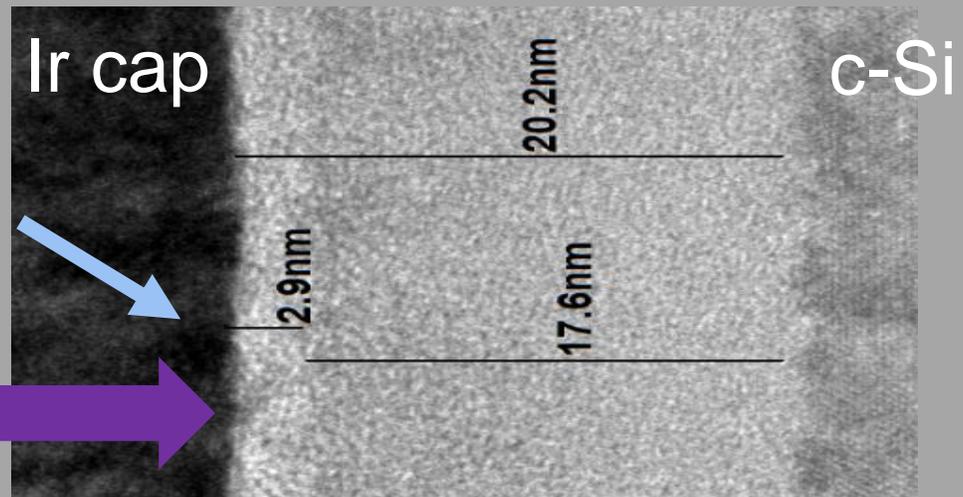
- Wafer biased (pulsed) in AsH_3/H_2 plasma
- Wafer irradiated with:
 - Ions
 - ▶ Total flux measured in Faraday
 - ▶ Composition unknown
 - ▶ Direction normal to substrate - ions accelerated across the sheath
 - Neutrals
 - ▶ Flux unknown
 - ▶ Composition unknown
 - ▶ Direction unknown
 - ▶ Sticking coefficients unknown



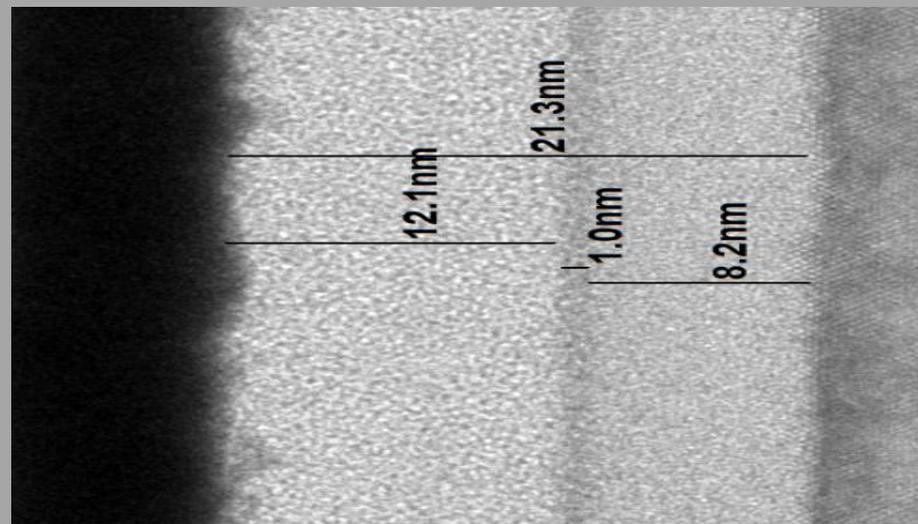
TEM

Post Implant

Implant direction



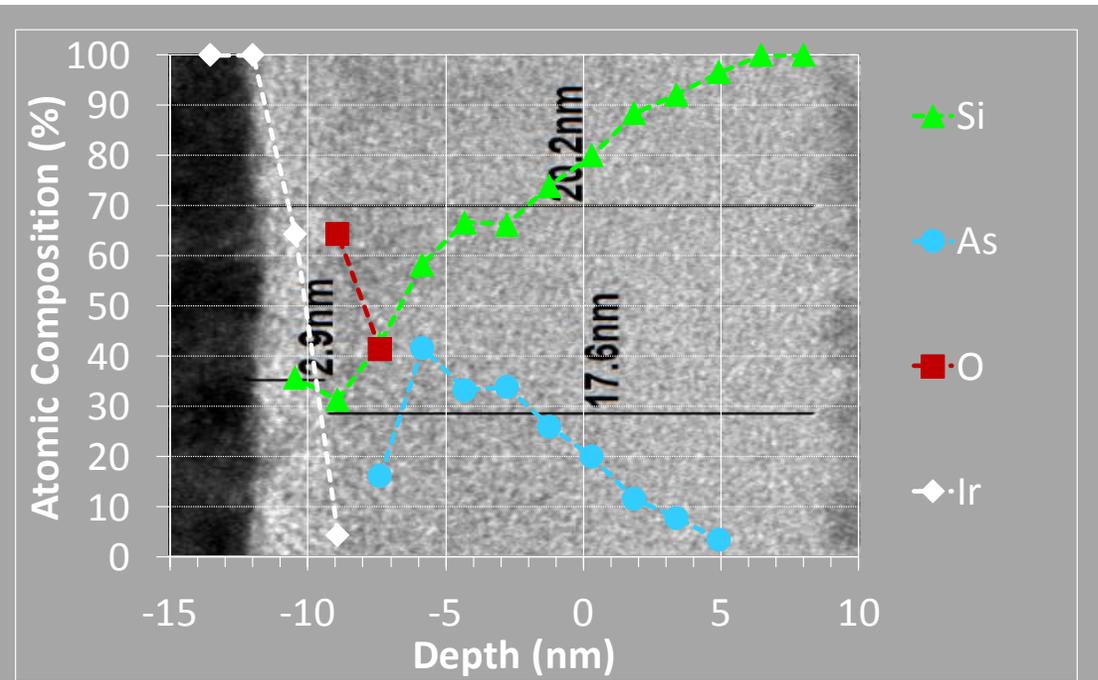
Post Clean



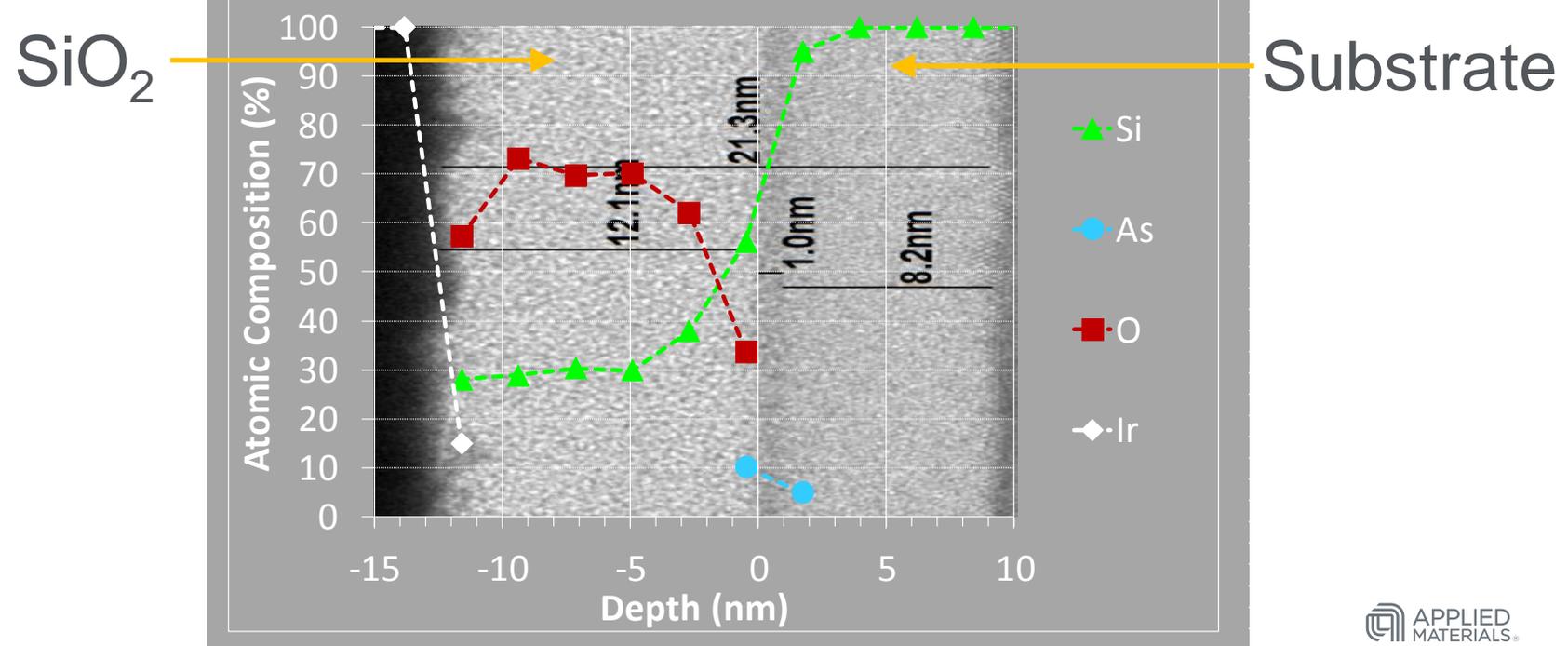
$\text{AsH}_3/\text{H}_2/7\text{keV}/1\text{E}16\text{cm}^{-2}$

TEM / EDS

Post Implant



Post Clean

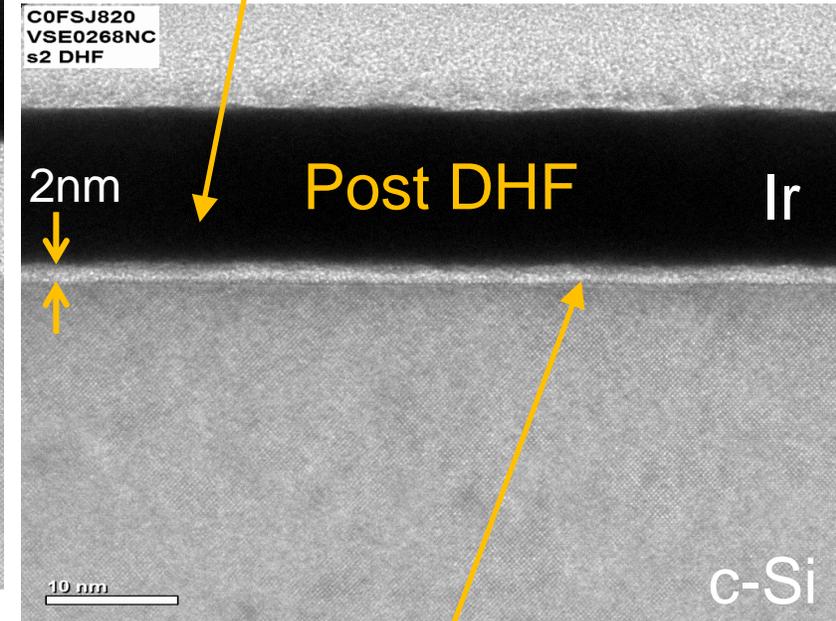
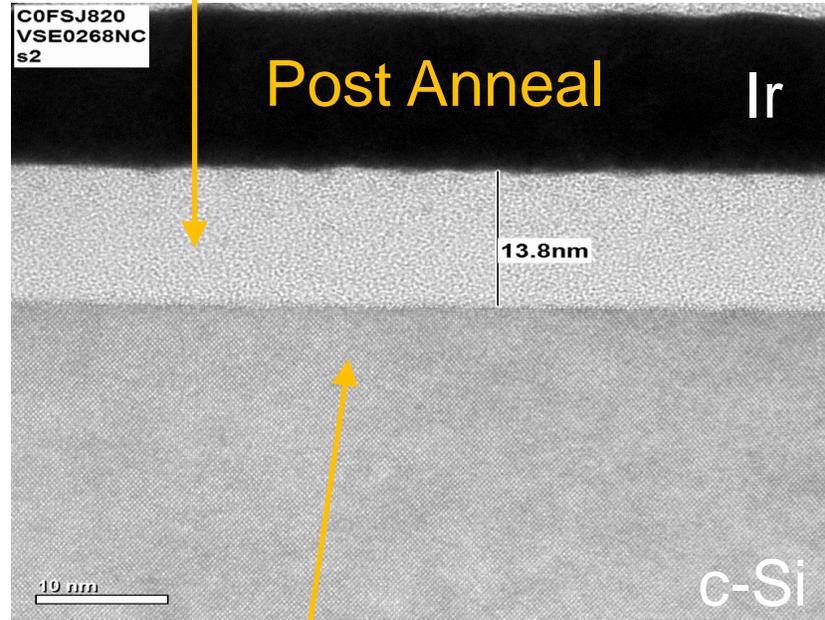
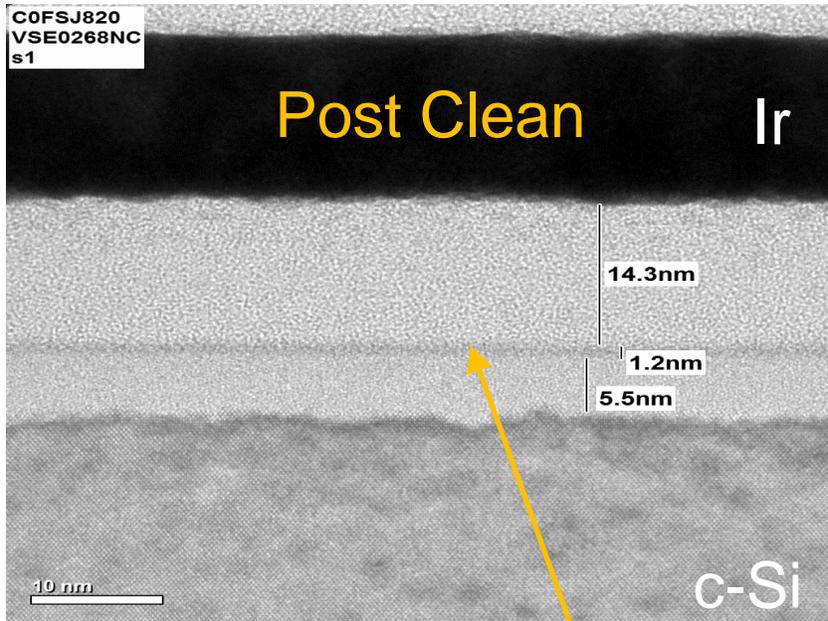


AsH₃/H₂/7keV/1E16cm⁻²

TEM - Clean, Anneal, DHF

(Most) oxide survives anneal

(Most) oxide removed



Dark line associated with wafer "surface"

Re-crystallised layer

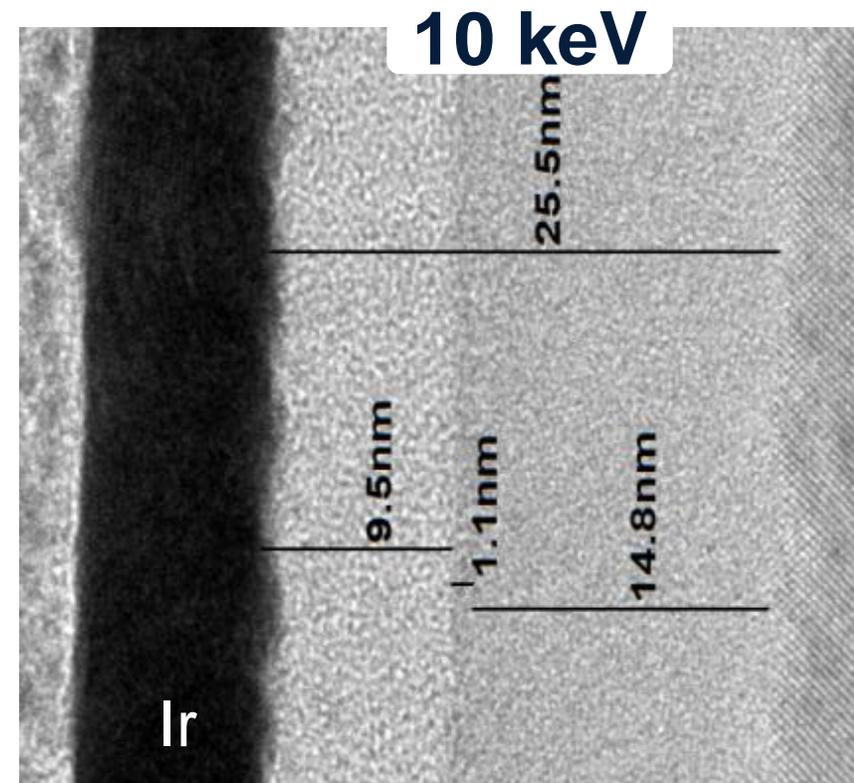
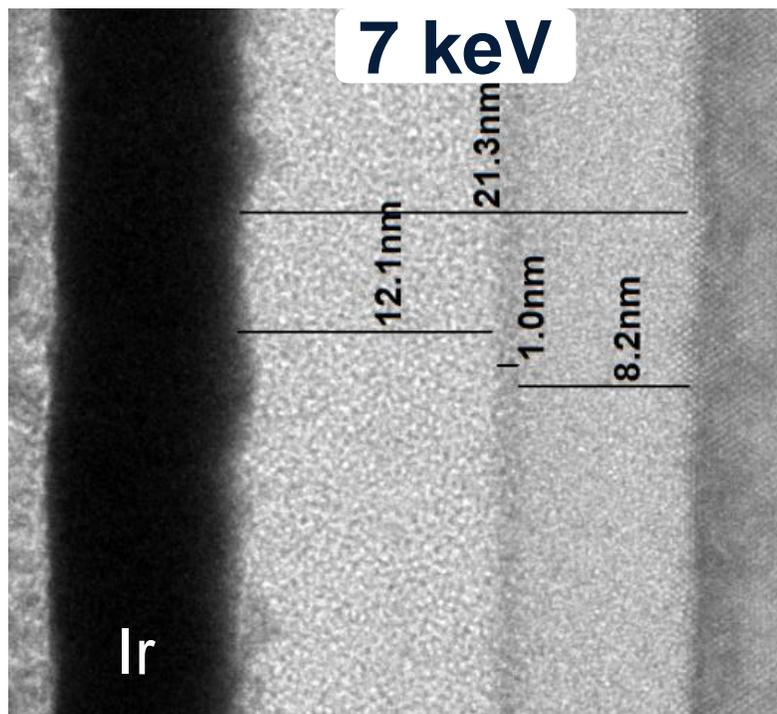
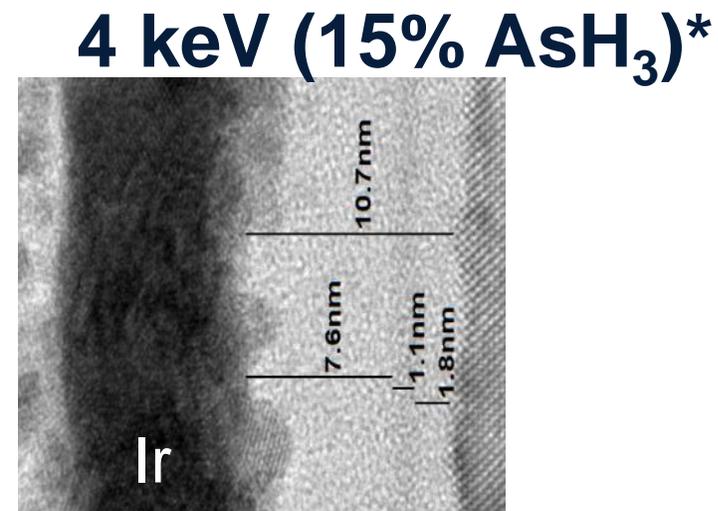
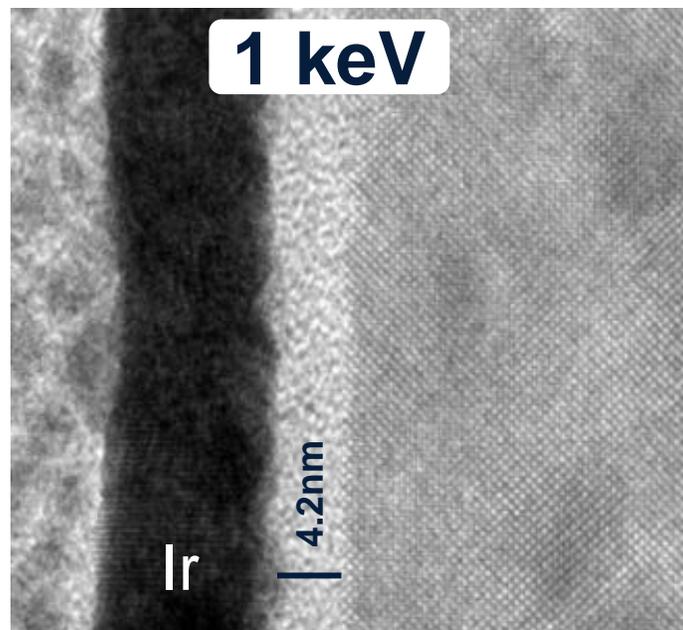
Re-grown native oxide (?)

$\text{AsH}_3/\text{H}_2/7\text{keV}/1\text{E}16\text{cm}^{-2}$

Post Clean TEM vs Energy

AsH₃/H₂/1E16cm⁻²

*5% AsH₃ except 4keV case



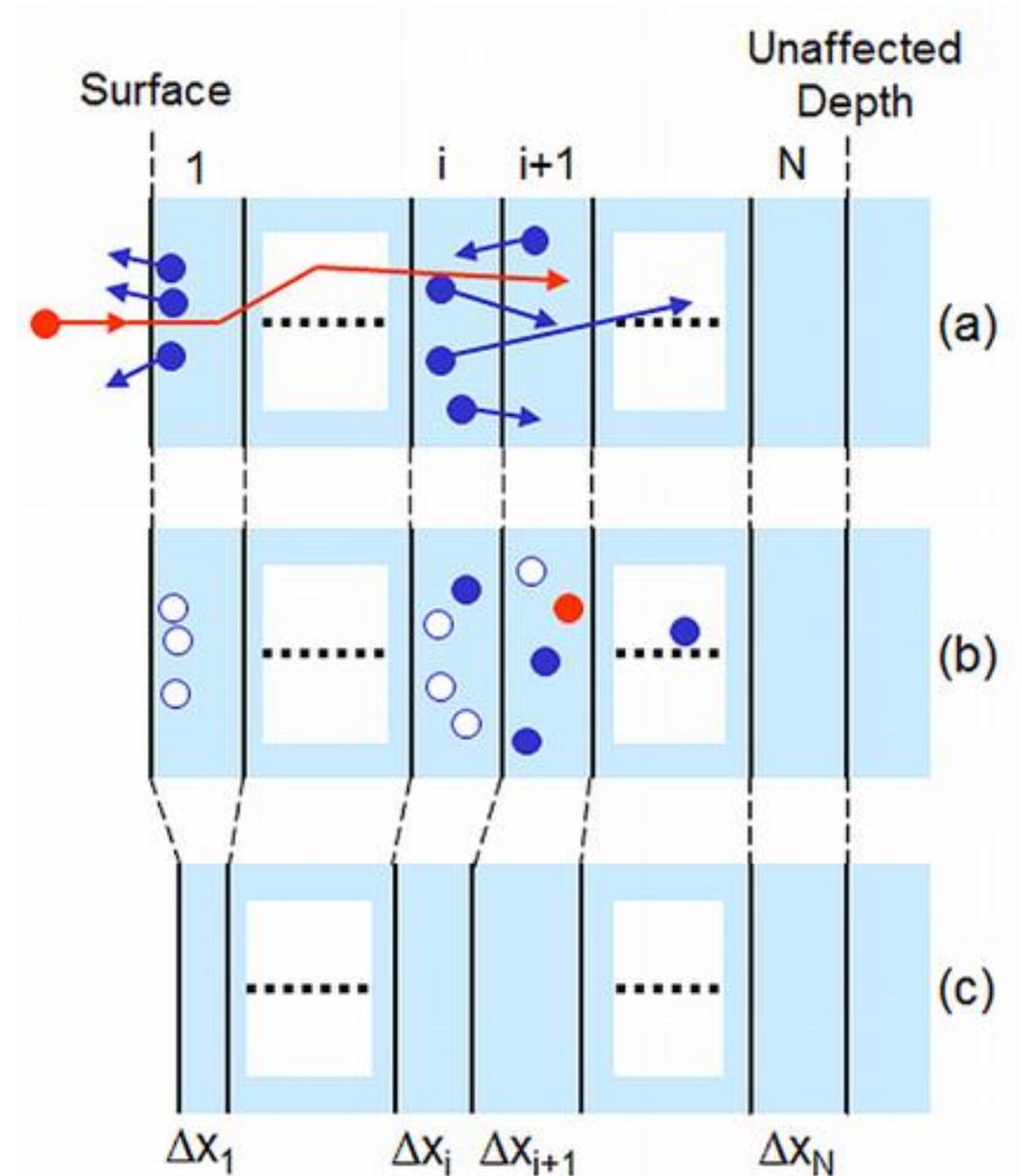
Planar Particle Beam Models

“TRIM”:

- Developed by Biersack & Ziegler in 1983
- Define target by elemental composition of layers
- Layers are STATIC - do not change during implant
- Particle collisions - binary collision approximation
- www.srim.org

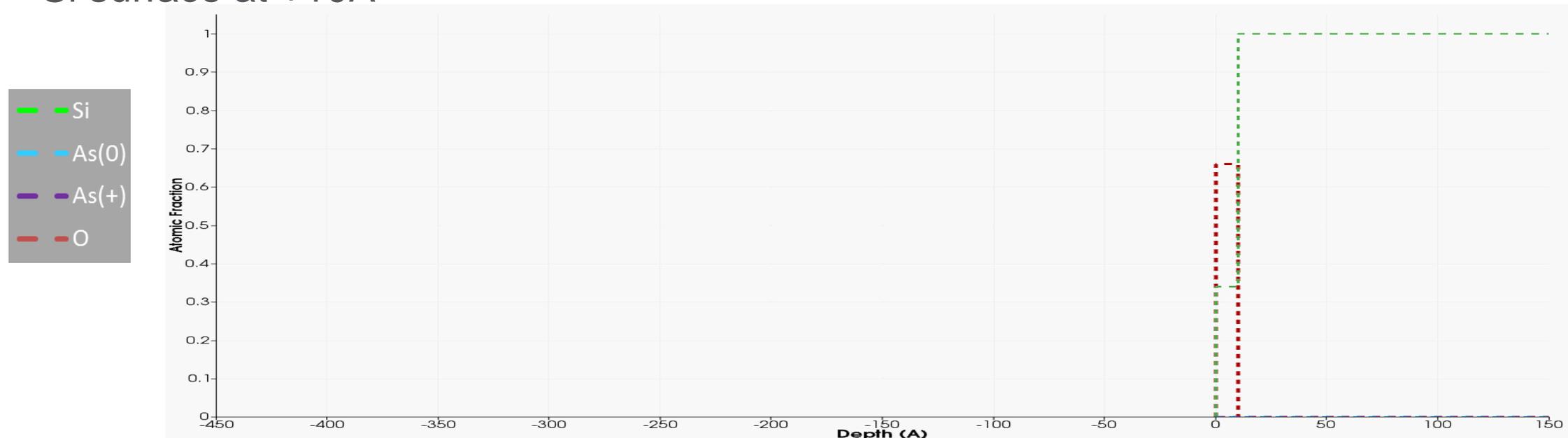
TRIDYN:

- Developed by Moeller and Eckstein in 1984
- Uses “TRIM” core of binary collision approximation
- Define target by elemental composition of its layers
- Layers are DYNAMIC - account for atoms entering/leaving substrate and moving between layers
- W. Moeller and W. Eckstein, NIM **B2** (1984) 814
- TRIDYN page via <https://www.hzdr.de>



TRIDYN Model 1 - Simple

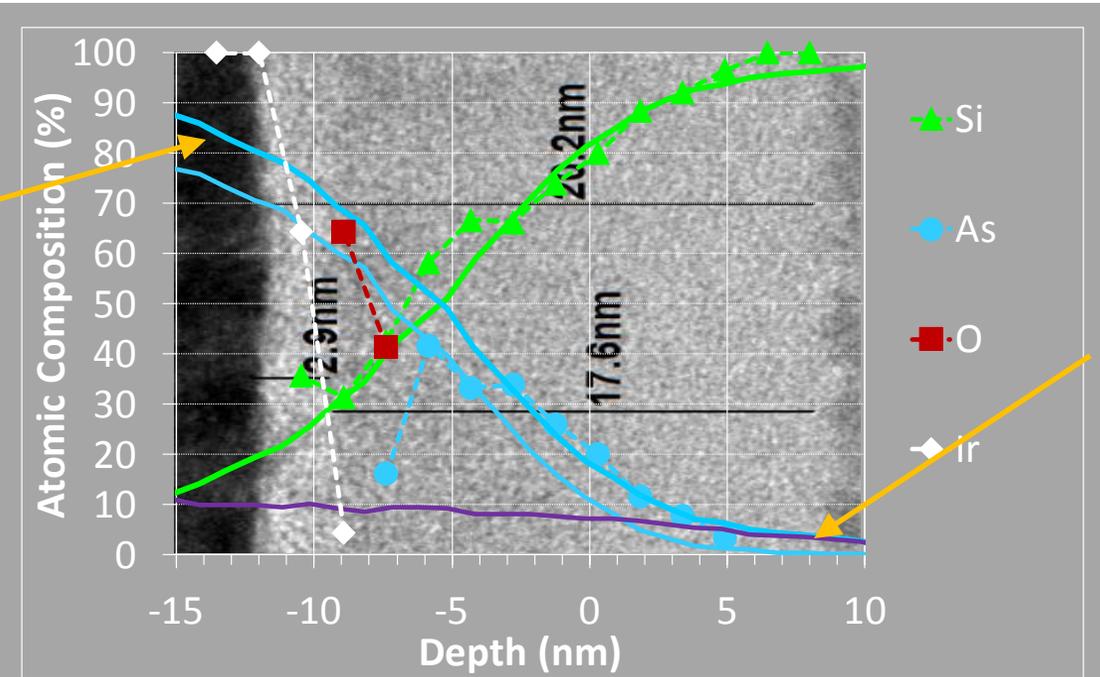
- Ions
 - ▶ Total ion flux ($1E16/cm^2$) assumed to be As^+ with normal density of elemental As
- Neutral Deposition
 - ▶ All neutrals assumed to be AsH_x° atoms deposited simultaneously with ions
 - ▶ AsH_x° neutral flux of 10x As^+ ion flux gives reasonable fit to data
 - ▶ AsH_x° represented by elemental As with density 35% of “normal” As
- Si surface at +10Å



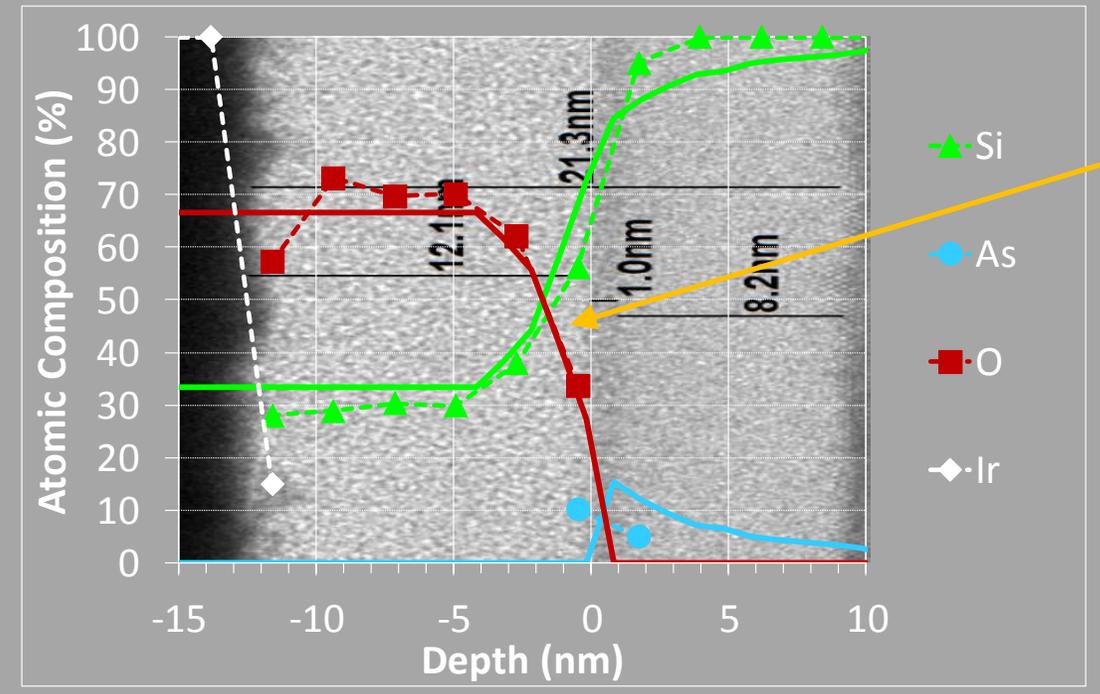
TEM / EDS

What happened to the extra deposition?

- 35% dense As has same Z contrast as Si
- Modelled clean by:
- Removing all As down to Depth (0)
- Assuming $[O] = 2x[Si]$...
- ... but reducing $[O]$ when $[Si] > 2.3E22 \text{ cm}^{-3}$



Deep As ions not measured

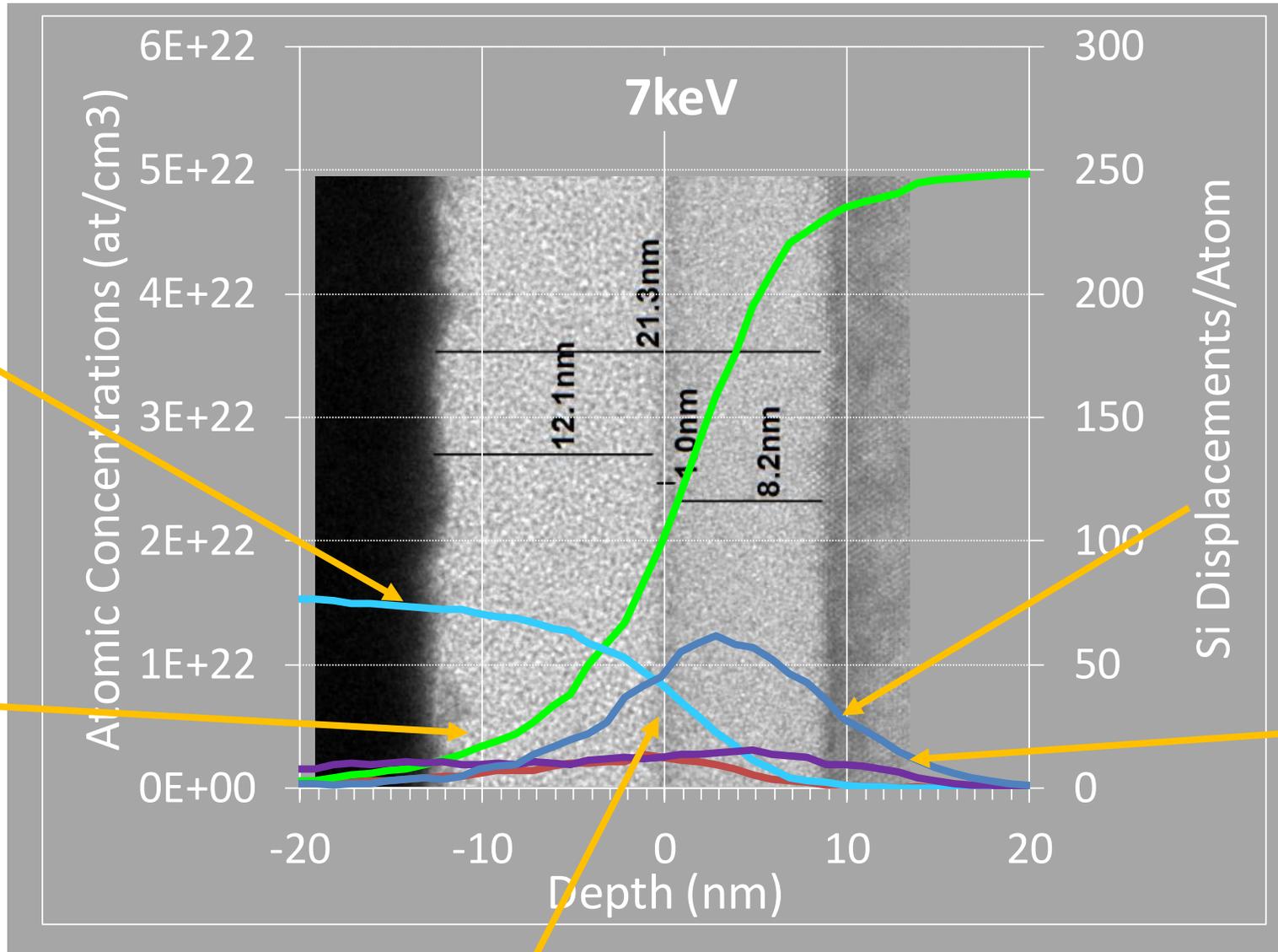


[O] reduced in this region

TRIDYN Model 1 – Profile Features

Thicker deposition than observed

Range of intermixed Si defines layer that survives clean

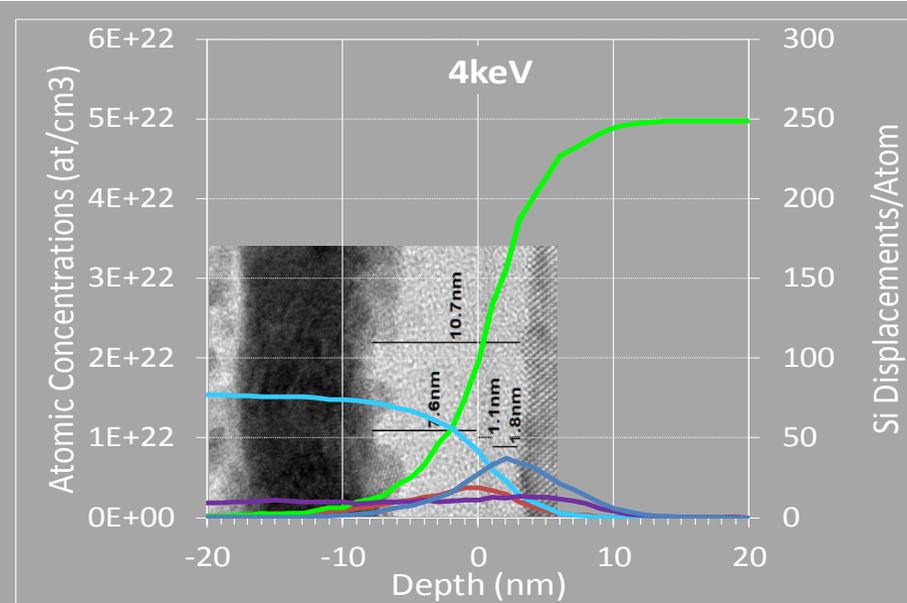
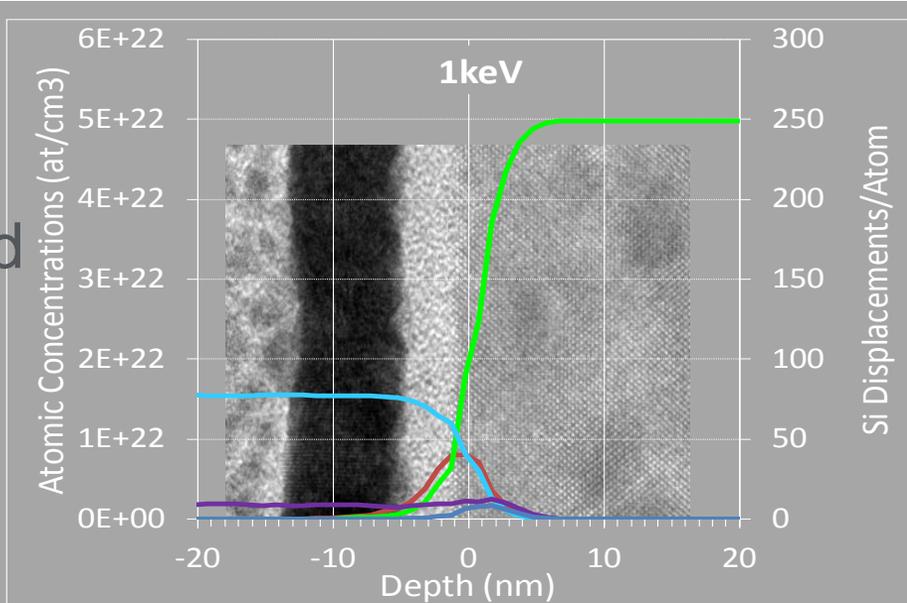


Damage beyond a/c interface seen by MEIS

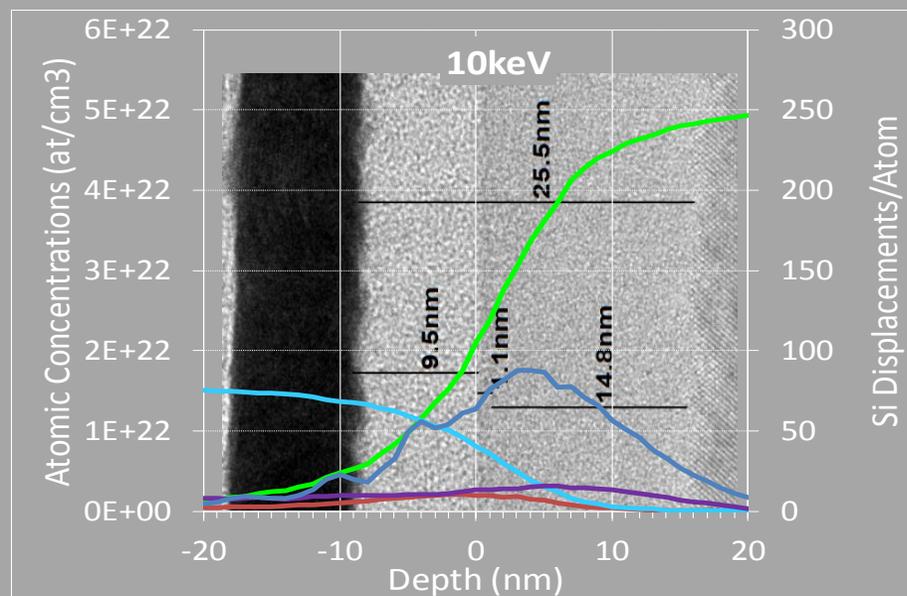
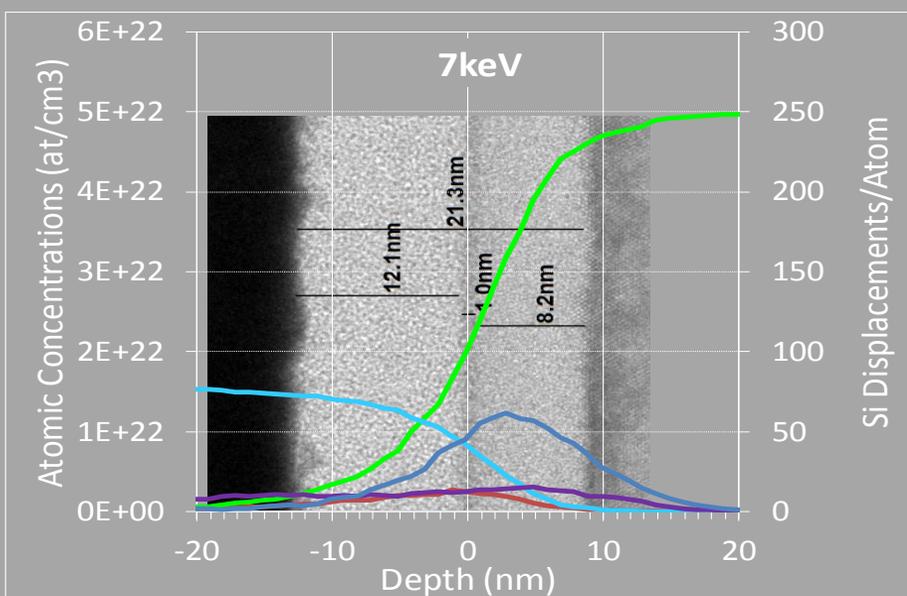
TRIDYN profiles aligned to dark line

TRIDYN Model 1 – Profiles vs Energy

1keV case
not
amorphised

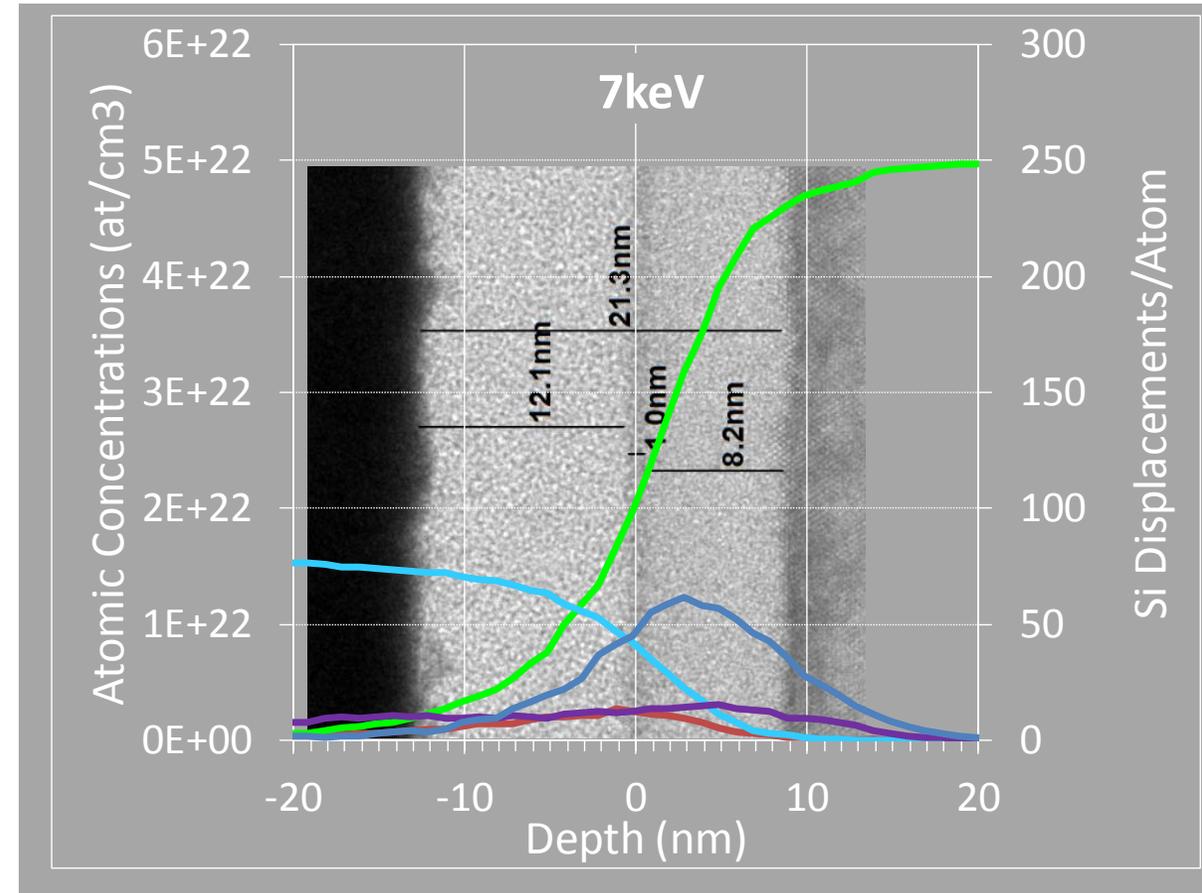


a/c
interfaces
at
different
Si dpa



Comments -1

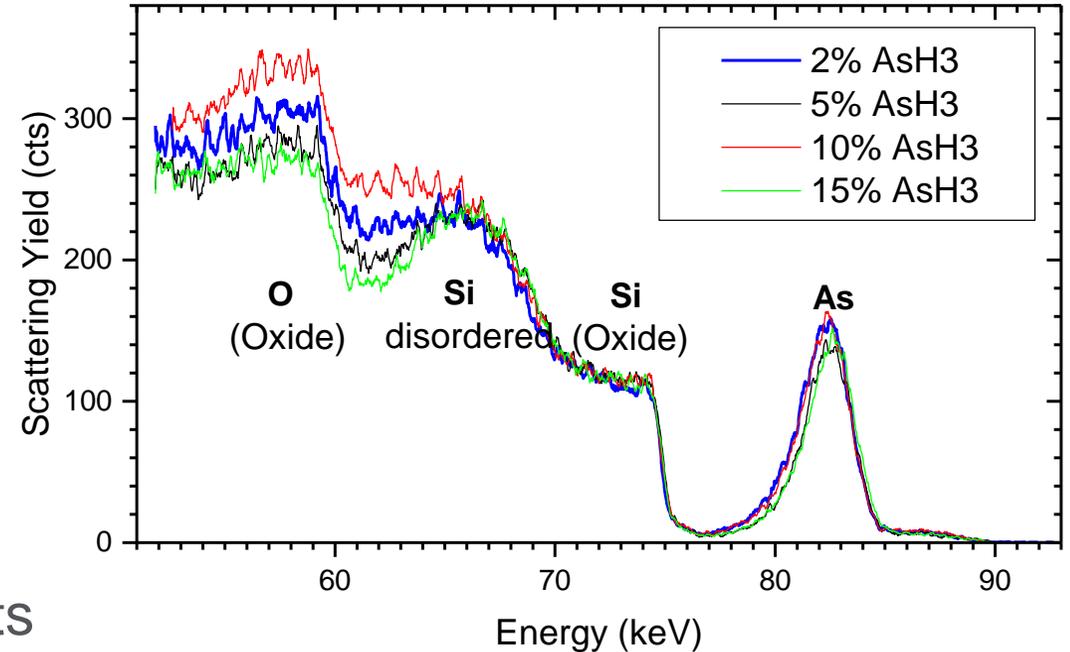
- TRIDYN PLAD Model 1 qualitatively explains features observed in PLAD implants
- Only invoked binary collision approximation physics (e.g no RED)
- Chemistry can happen (surface decoration, snow ploughing, segregation)
- Graded density oxide predicted – can we measure this*?
- Thicker deposition than observed – explain
- Can improved TRIDYN model show the a/c interface occurring at same Si dpa?
- How quantitative can an improved TRIDYN model be?



* Igor Alencar - this session
Joshua Rideout poster – PAS of these samples

Metrology – Why MEIS

- Avoided dynamic SIMS and dynamic XPS
 - ▶ Ion beam mixing / variable sputter rate effects
 - ▶ Matrix effect for secondary ionisation in SIMS
- TEM / EDS
 - ▶ “Curse of the TEM” – what does a grey layer represent?
 - ▶ EDS reports atomic fractions only
- MEIS
 - ▶ No ion beam mixing or variable sputter rate effects
 - ▶ No matrix effects
 - ▶ Absolute atoms / cm² (→ atoms/cm³ with independent thickness measurement)
 - ▶ Understand spectrum fitting
 - ▶ Control sample orientation



MEIS spectra showing samples not significantly different for % AsH3

Medium Energy Ion Scattering Methodology

Apparatus

- He/100keV 54.7° scattering angle 90° for double aligned (47.7° tilt, 7° twist for random) at Huddersfield¹
- Report atomic fraction profiles using IGOR

MEIS Spectral Analysis

- I require atomic concentrations to compare to TRIDYN
- Atomic fraction (without density) often implies standard densities - not the case in these samples?
- I used POWERMEIS² with small number of input layers
- Did I do it right?
- TRIDYN informed POWERMEIS layer densities / compositions
- TEM oxide thicknesses (not always same samples)

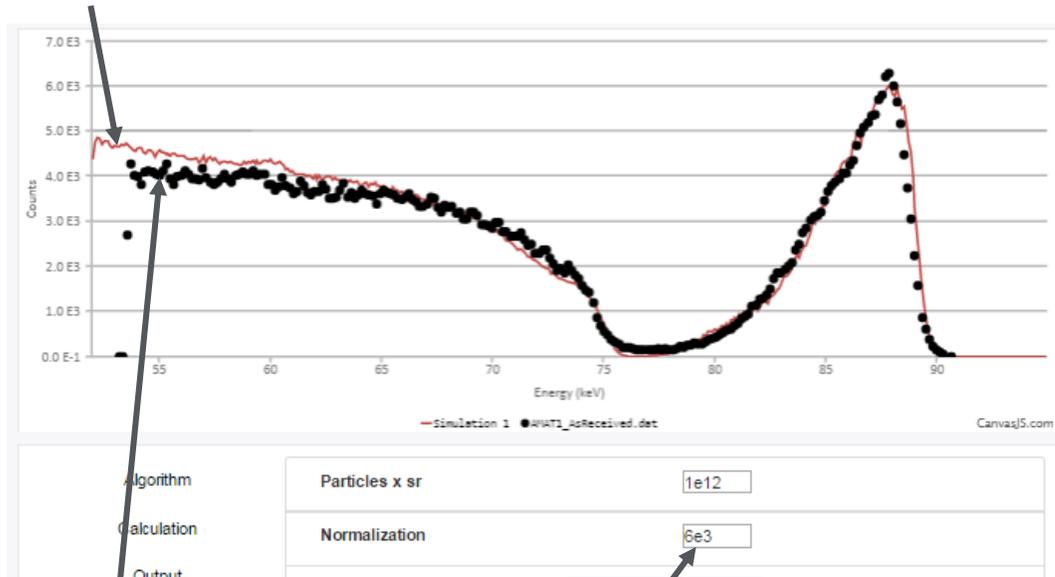


1. Jaap van den Berg / Andrew Rossall talks
2. Gabriel Marmitt poster - POWERMEIS

Spectrum Fitting

MEIS Spectrum

Red line = POWERMEIS fit



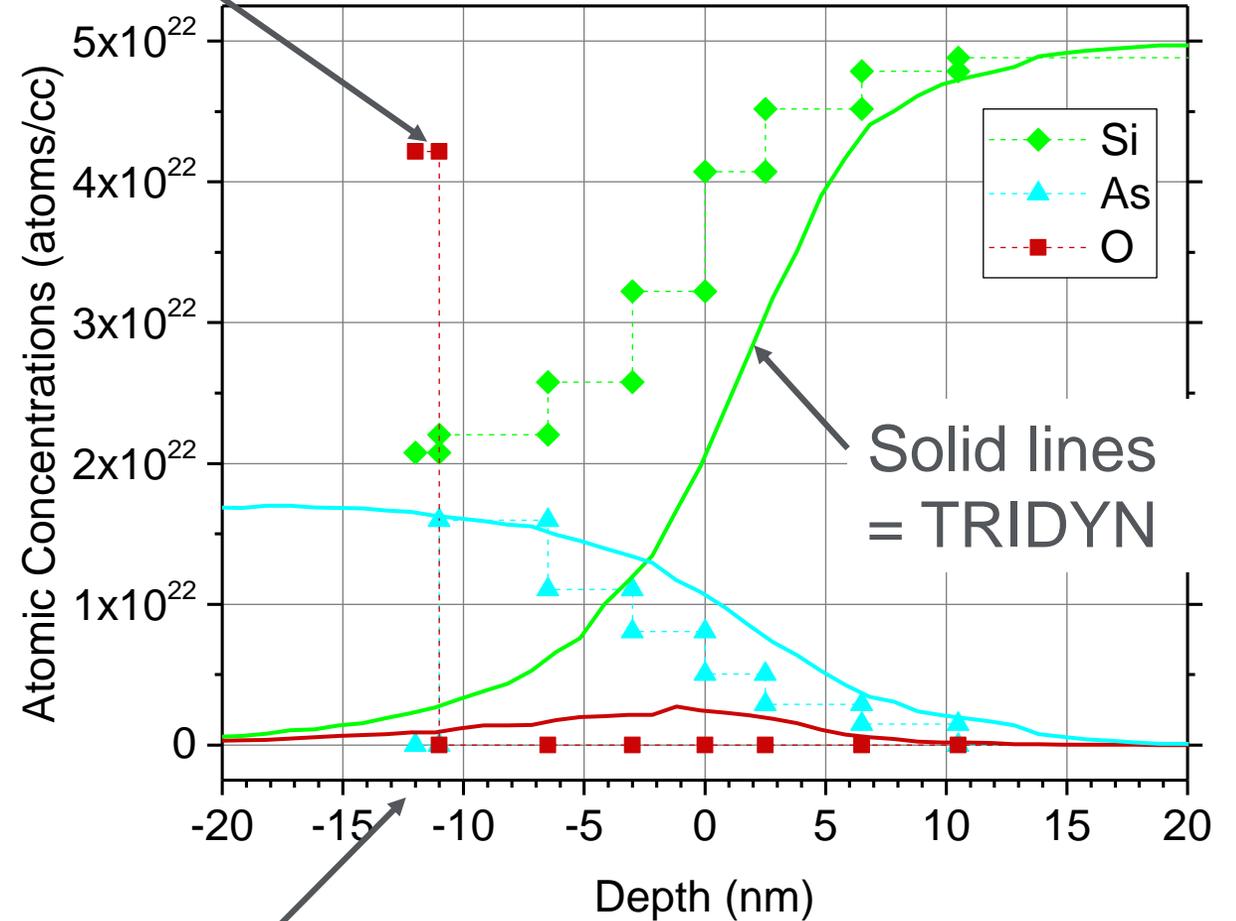
■ = Data

Normalisation factor between data and fit

Symbols/dotted = POWERMEIS

Concentration Profiles

As Received

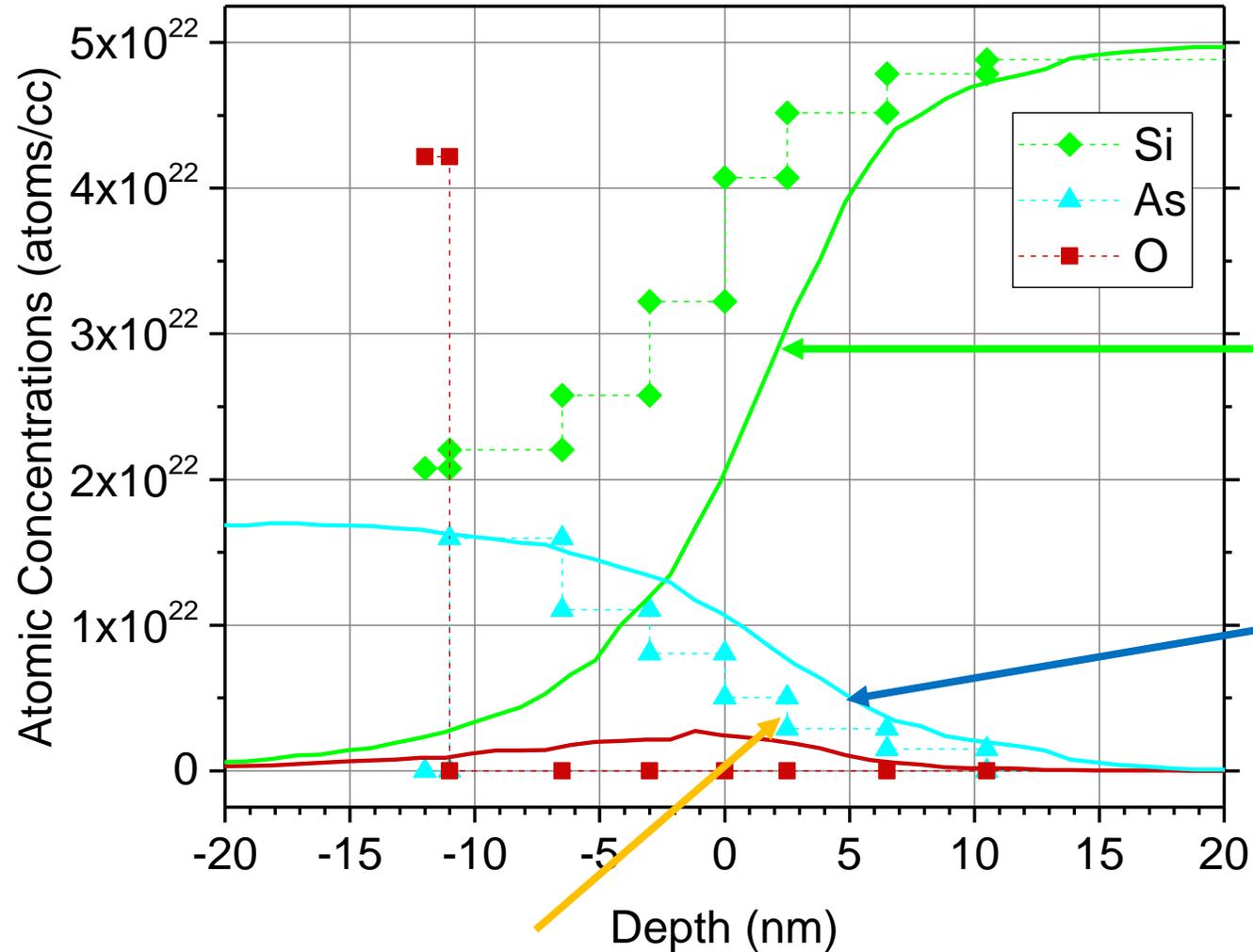


Thickness of deposition from TEM

Depth (0) = original Si surface in TRIDYN Models

As Implanted

As Received



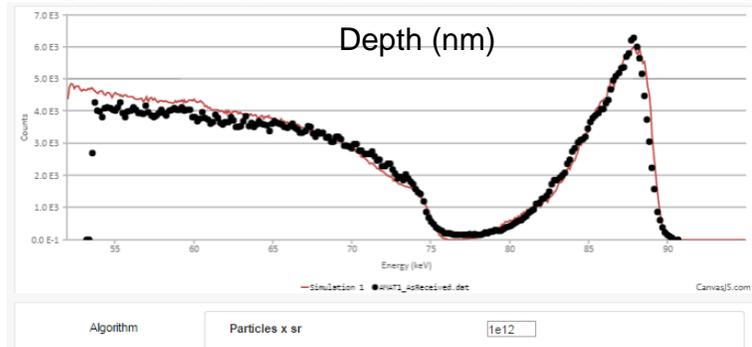
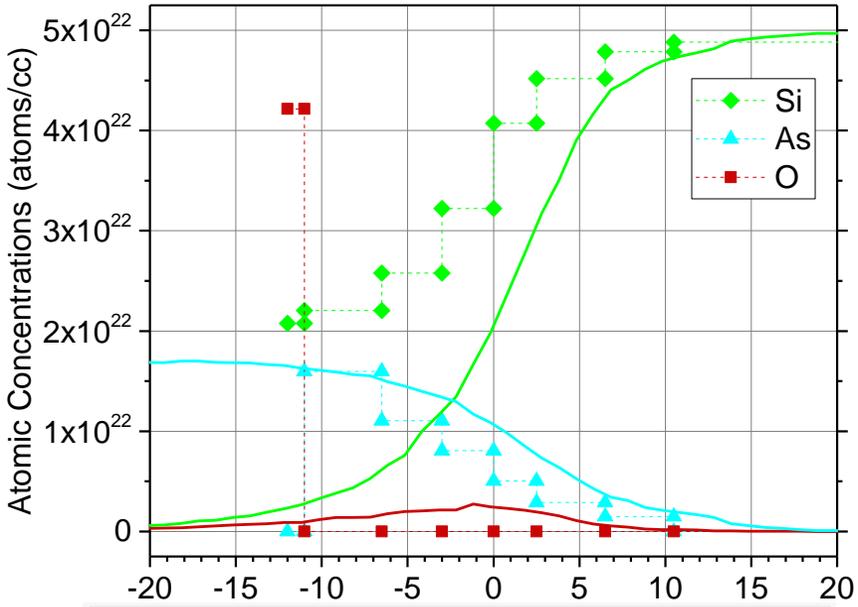
TRIDYN Model 1
under-estimated
[Si]

TRIDYN Model 1
over-estimated
[As]

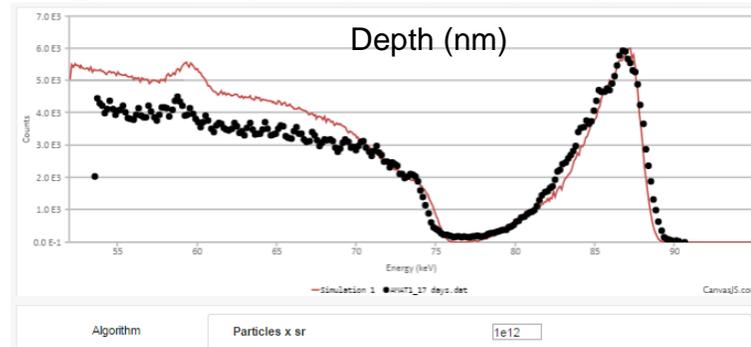
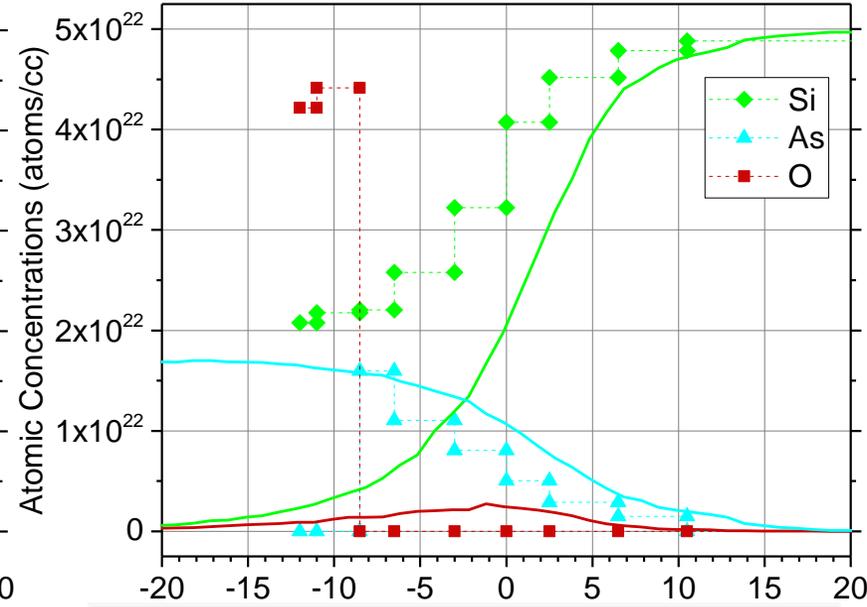
Profile within substrate will be used to explain post clean and anneal

As Implanted – As Effusion

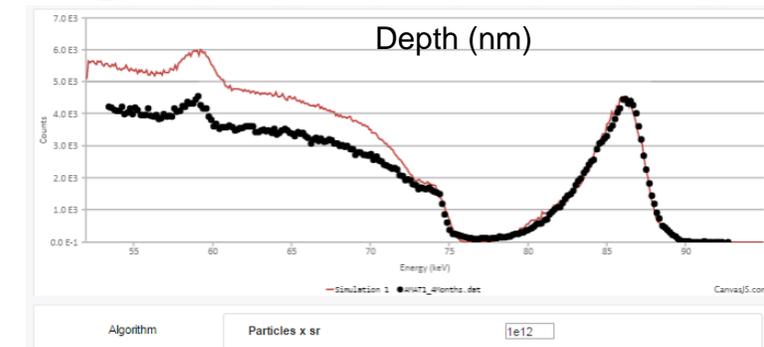
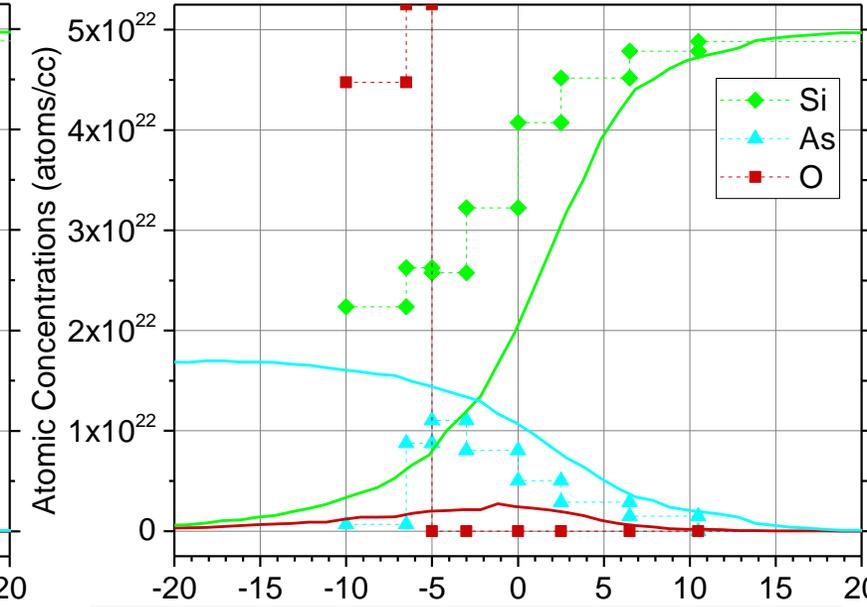
As Received



After 17 Days in Atmosphere

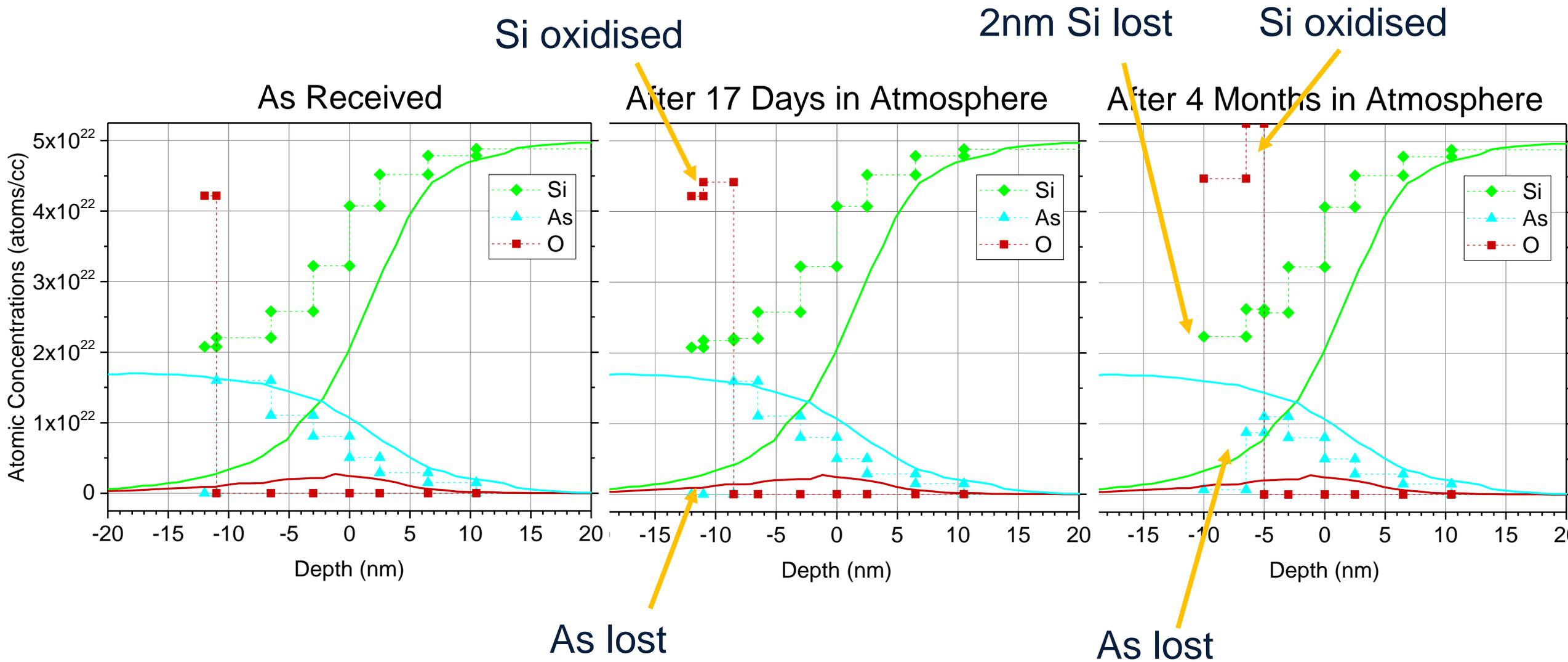


After 4 Months in Atmosphere



- Normalisation factor kept constant
- Sample left *in vacuo* for 17 days did not change (not shown)
- Clearly sample has lost As, gained O over 4 months

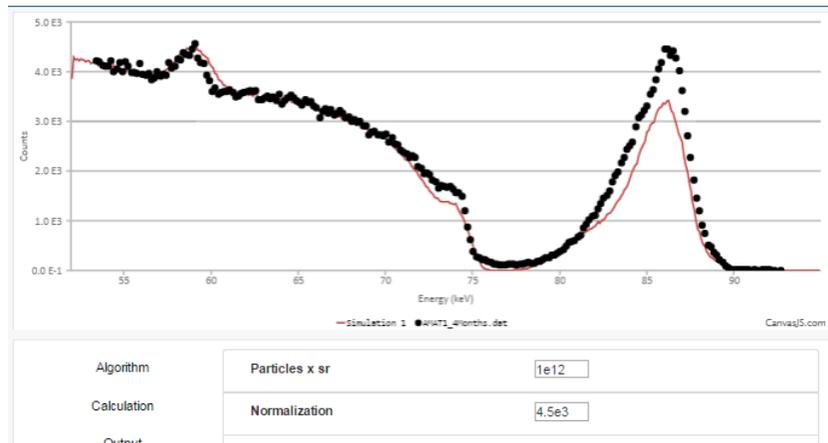
As Implanted – As Effusion



- MEIS analysis guided by TRIDYN suggests sample has also lost Si !

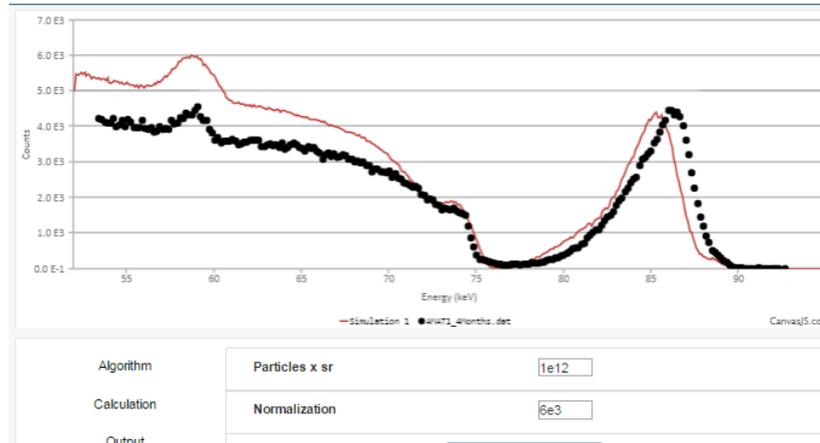
Alternative Fitting – Post Implant after 4 Months

Change Normalisation



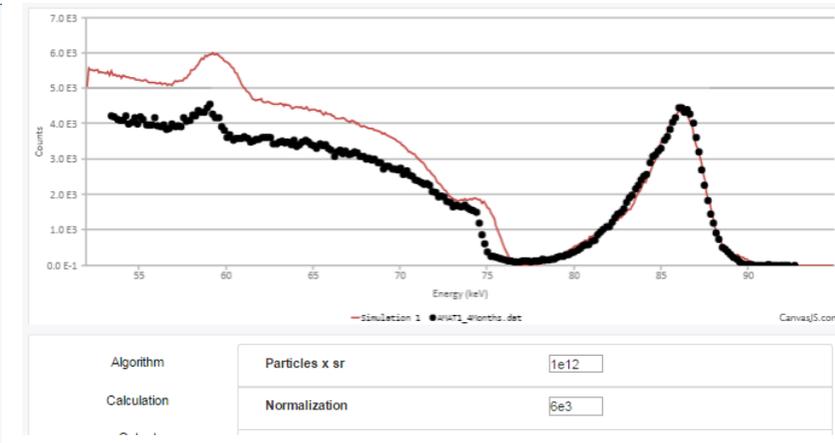
- Would have to increase As in sample

Only As Effuses



- ... leaving Si behind
- Would need to adjust As profile at all depths

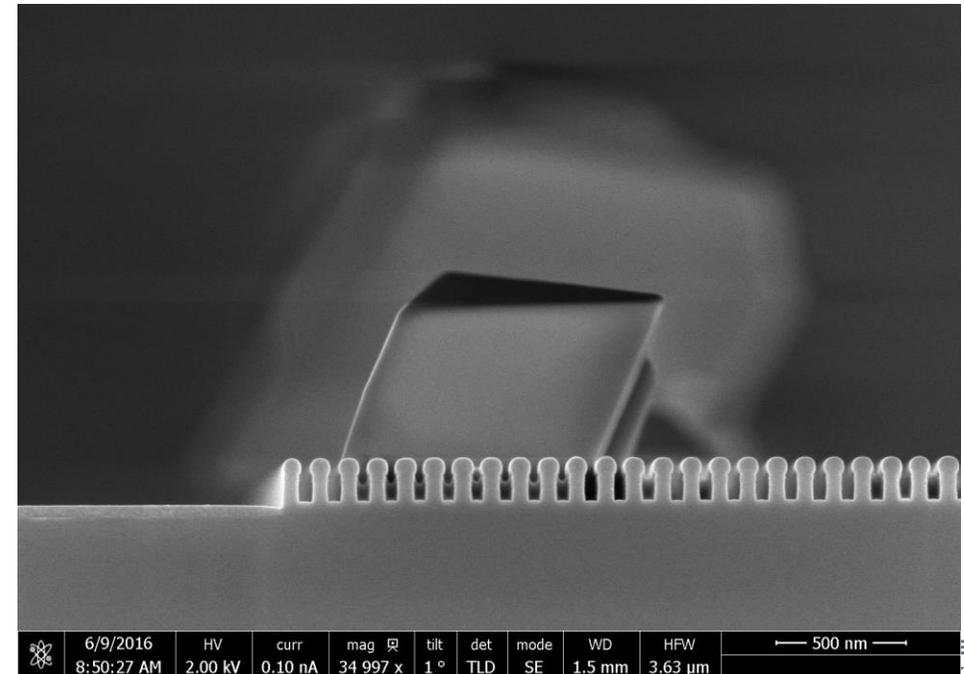
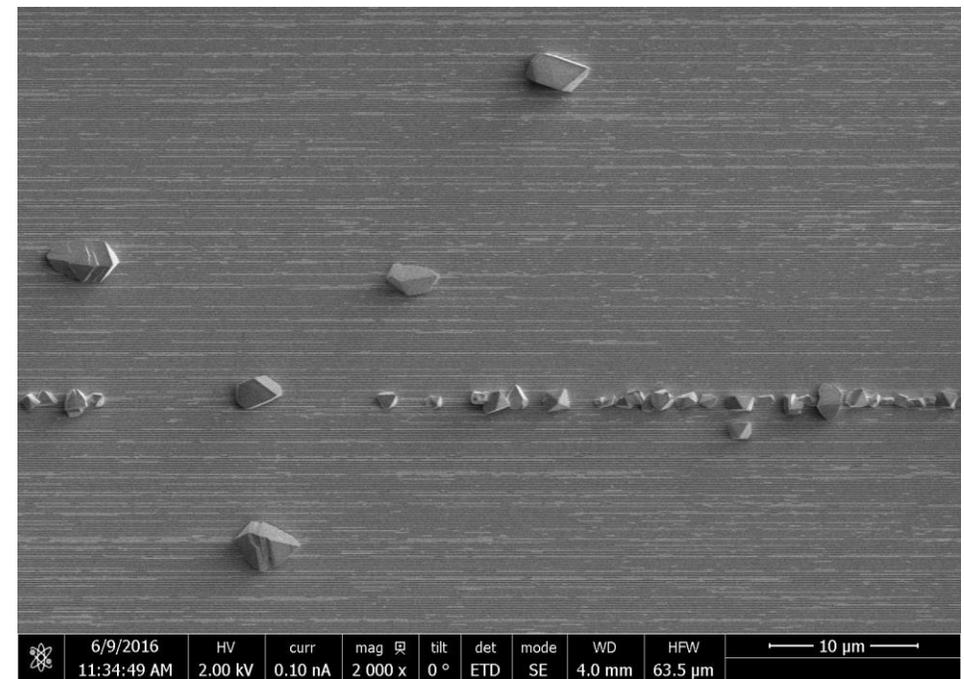
Change Beam Energy



- Increase 99.5 to 100.5 keV fits As peak - how fit Si edge?
- Variations with incident angle weak

Arsenolite Formation

- As effuses from surface in atmosphere – not in vacuo – over a time scale of months
- Consistent with report of Meirer et al, Applied Physics Letters 101 (2012) 232107
- Si cap forms and oxidises (– forming a barrier to slow down As effusion?)
- Si also lost?
- As profile in substrate unchanged

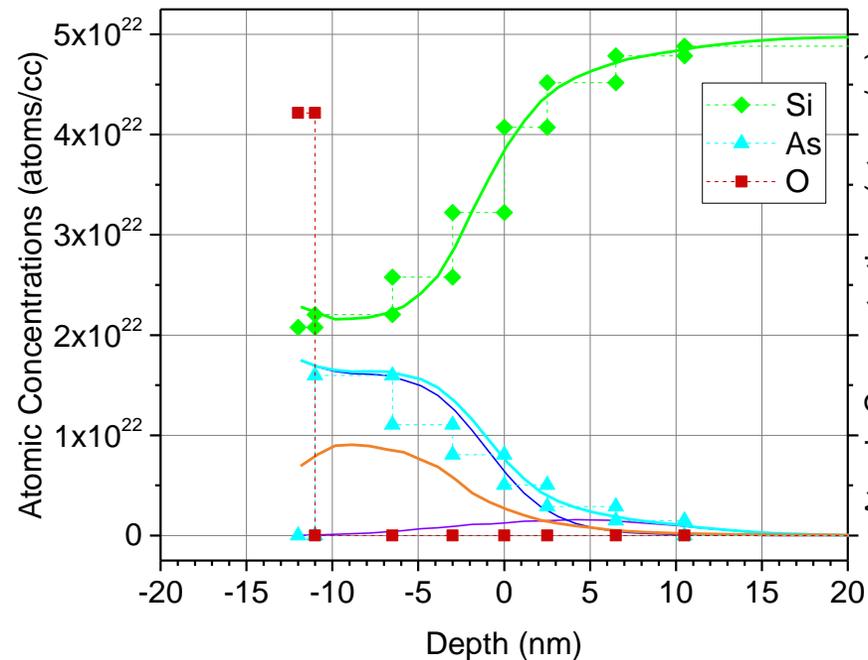


TRIDYN Model 2

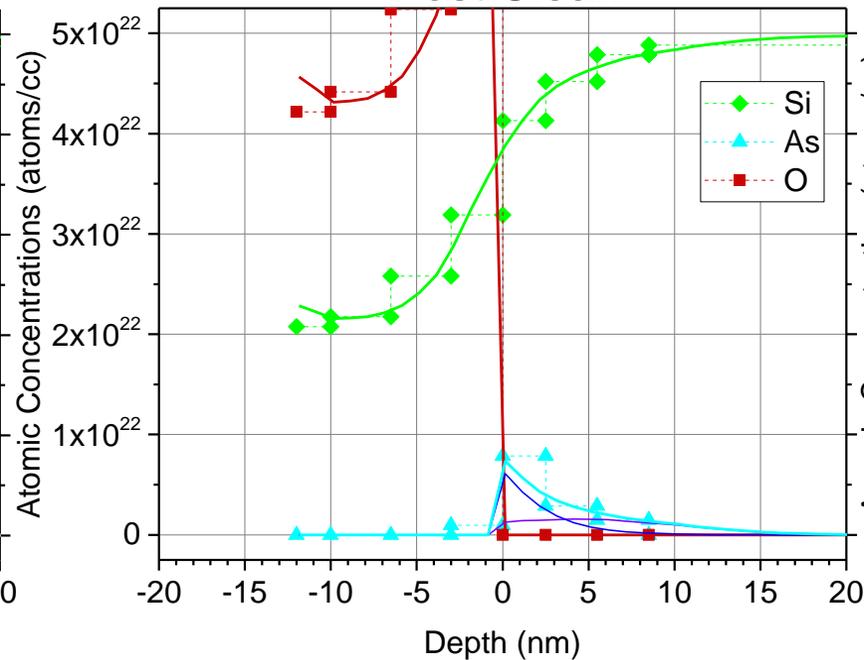
- MEIS shows need to improve TRIDYN model inputs
- Reduced “heavy” ion fluence to half measured ion fluence
- Remainder are H ions (not included)
- Decreased neutral : heavy ion ratio vs energy using a linear relationship to be consistent with other observations (not shown)
- As neutrals assumed to have elemental density
- H neutrals included to account for under-dense deposition
- Add Si neutral flux to give $\sim 1\text{E}22\text{cm}^{-3}$ Si observed in deposited layer at 7keV
 - ▶ Assumed constant through implant – simplest assumption
- Si ions included - if there are neutrals – should be ions
 - ▶ Reduces deep As to better fits TEM/EDS
- No native oxide on substrate – assumed to be immediately etched away by H plasma

TRIDYN Model 2 – Post Implant, Clean, Anneal

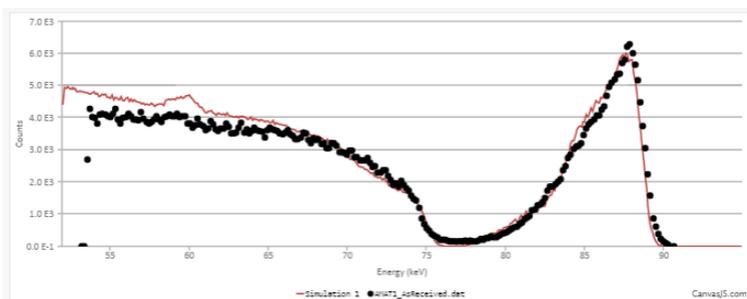
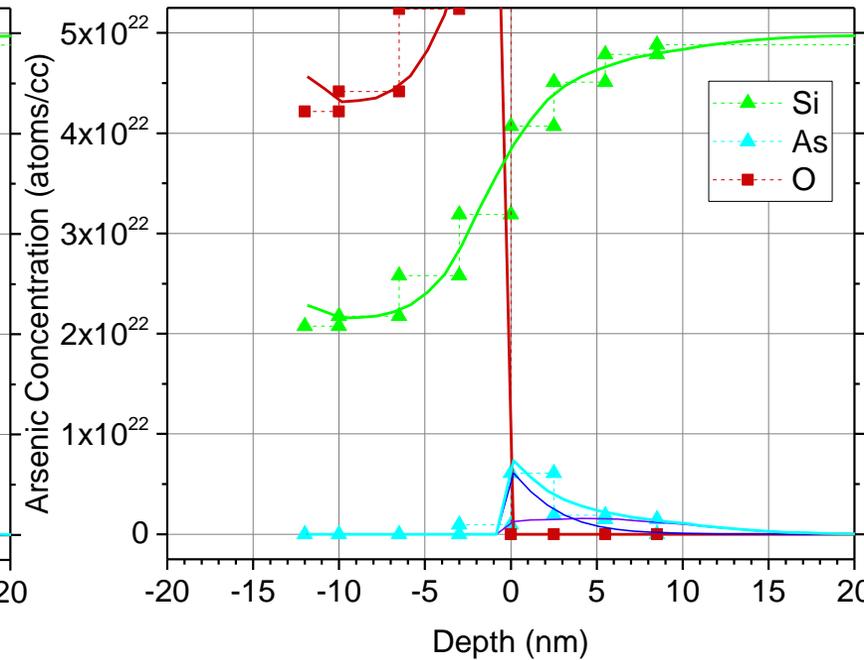
As Received



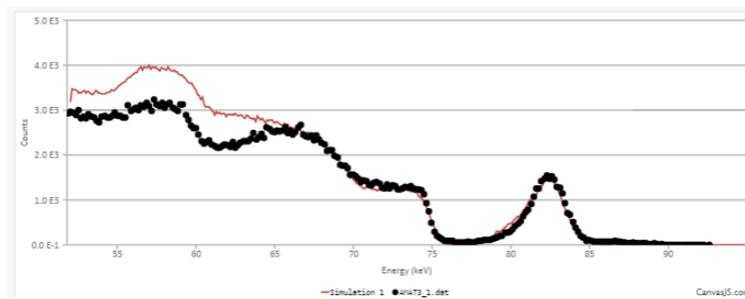
Post Clean



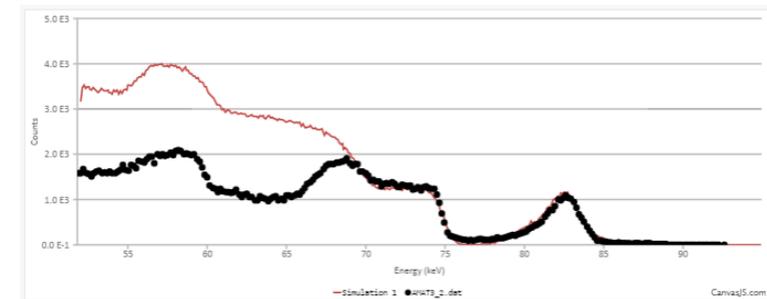
Post Anneal



Algorithm	Particles x sr	<input type="text" value="1e12"/>
Calculation	Normalization	<input type="text" value="1e3"/>
Output	Download simulation	
Beam		
Detector	File name	AMAT1_AsReceived.dat

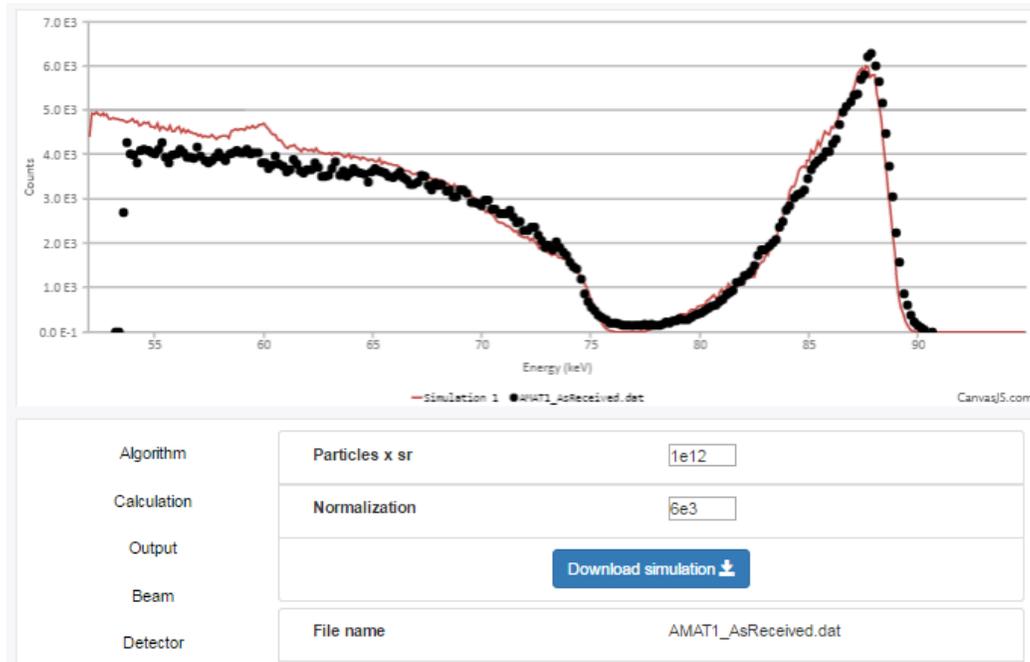


Algorithm	Particles x sr	<input type="text" value="1e12"/>
Calculation	Normalization	<input type="text" value="1e3"/>
Output	Download simulation	
Beam		
Detector	File name	AMAT3_1.dat

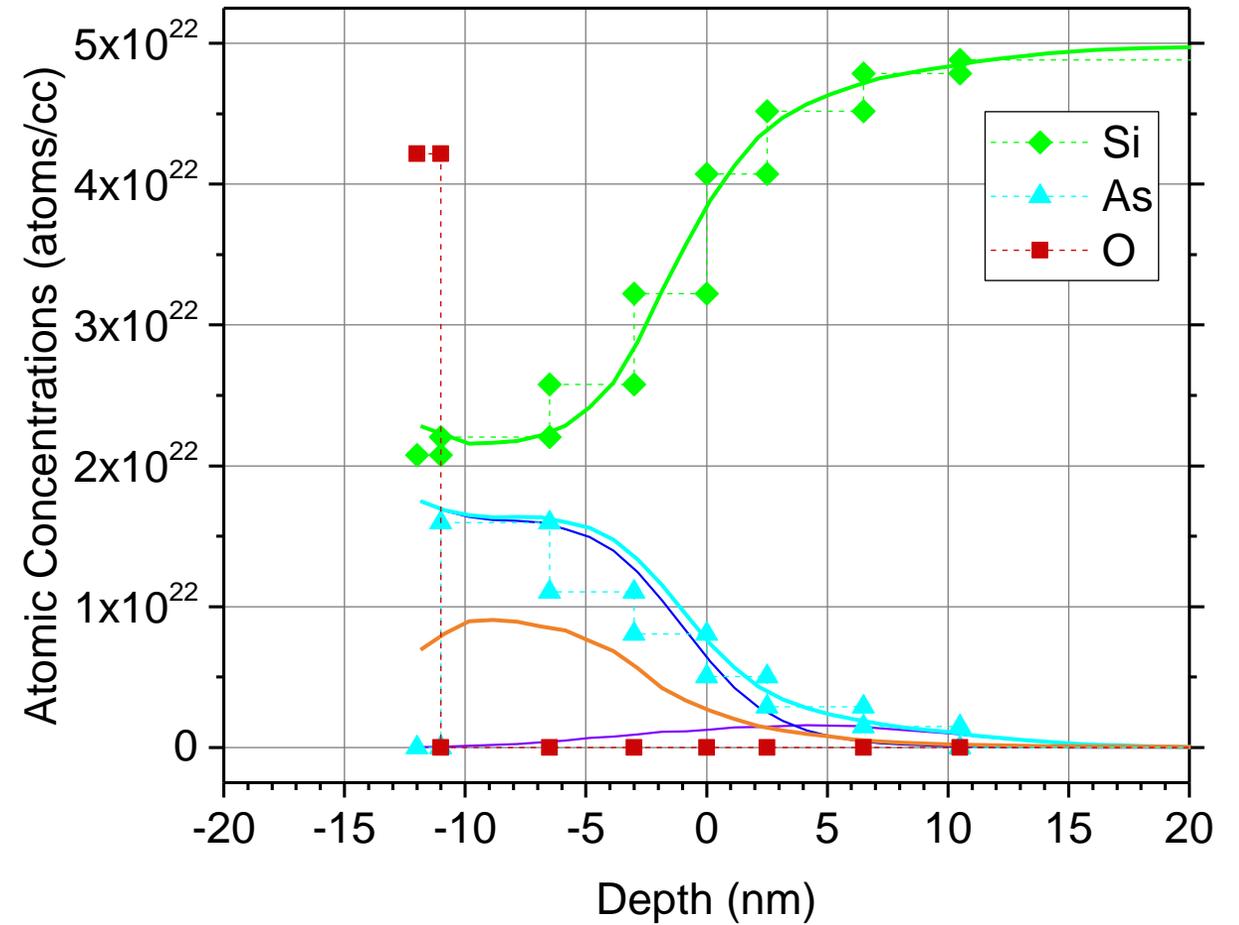


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Output	Download simulation	
Beam		
Detector	File name	AMAT3_2.dat

TRIDYN Model 2 – Post Implant

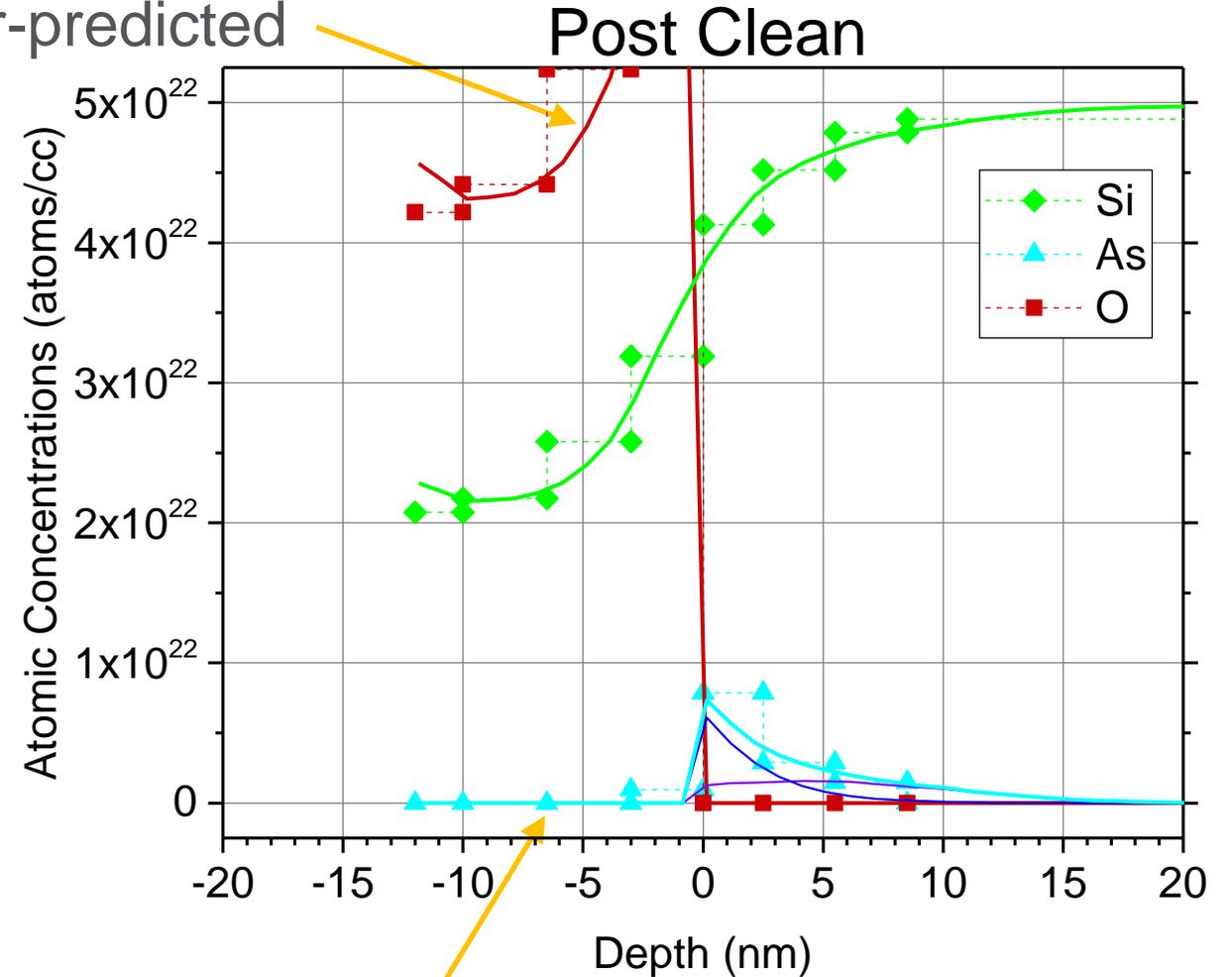
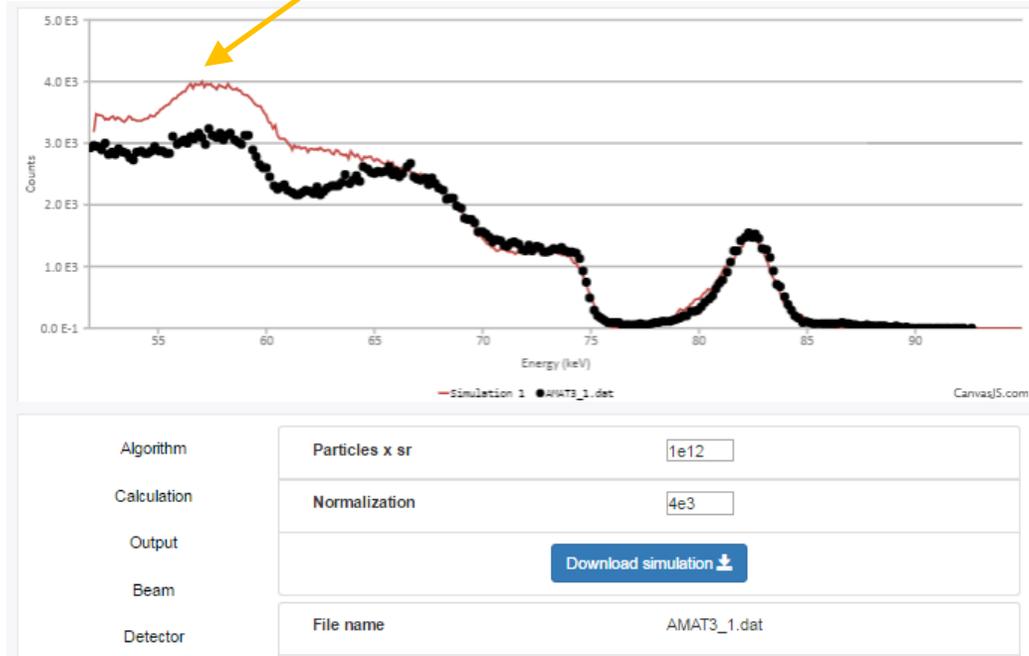


As Received



TRIDYN Model 2 – Post Clean

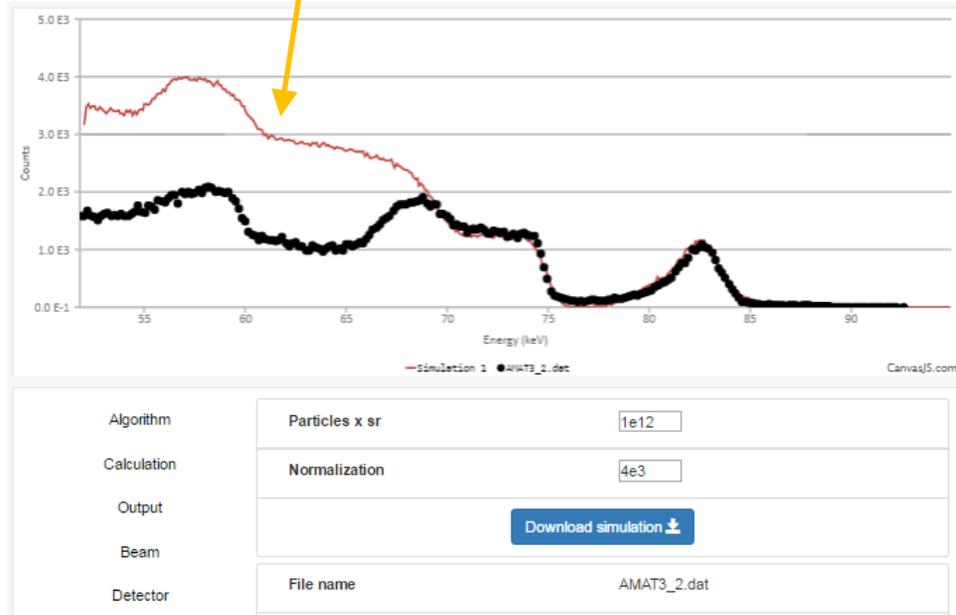
Cannot have this much [O] in this layer as [Si]>2.3E22 cm⁻³ – hence O peak over-predicted



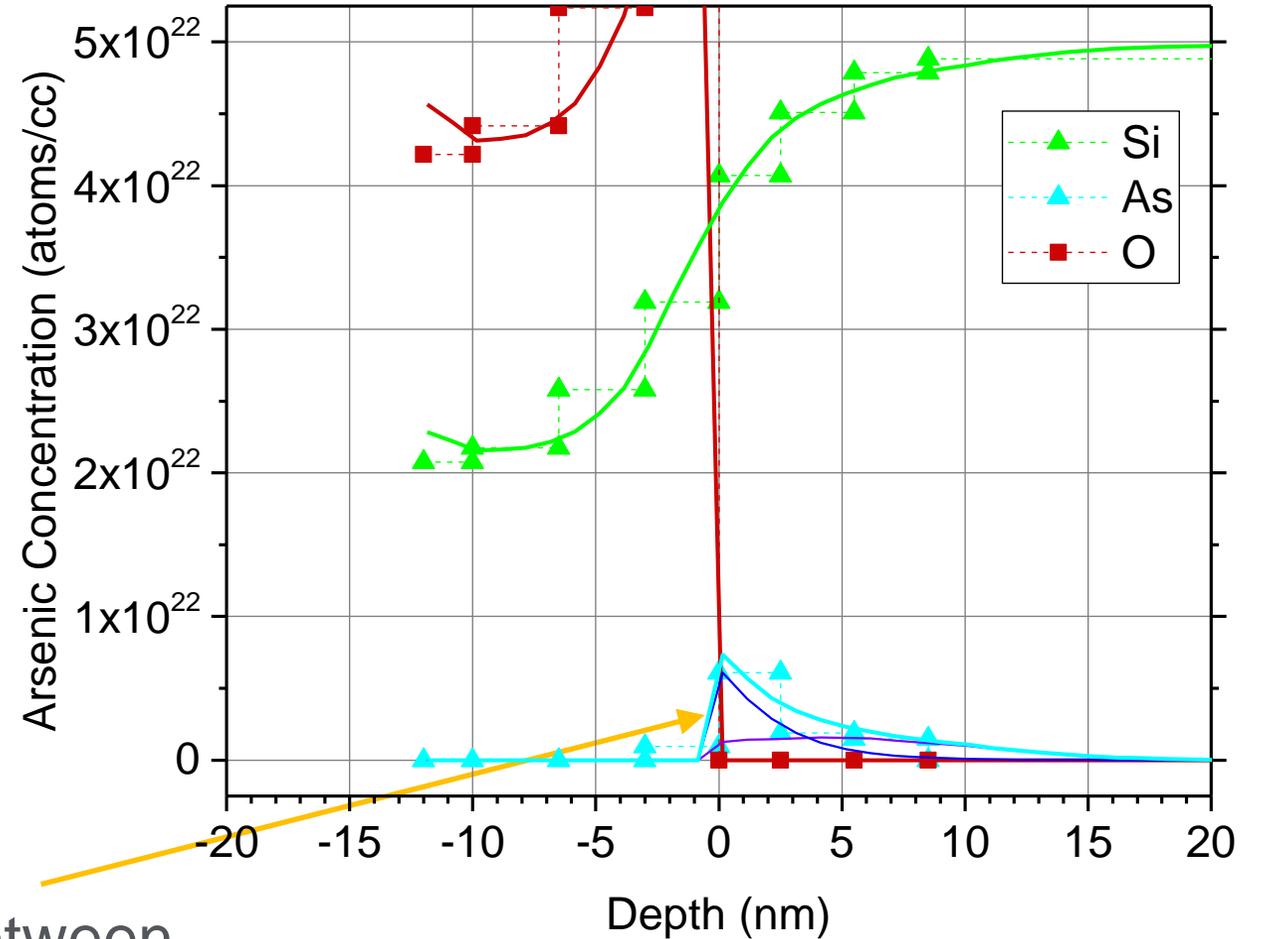
Removed As down to Depth(0)

TRIDYN Model 2 – Post Anneal

Aligned data – POWERMEIS
calculates random



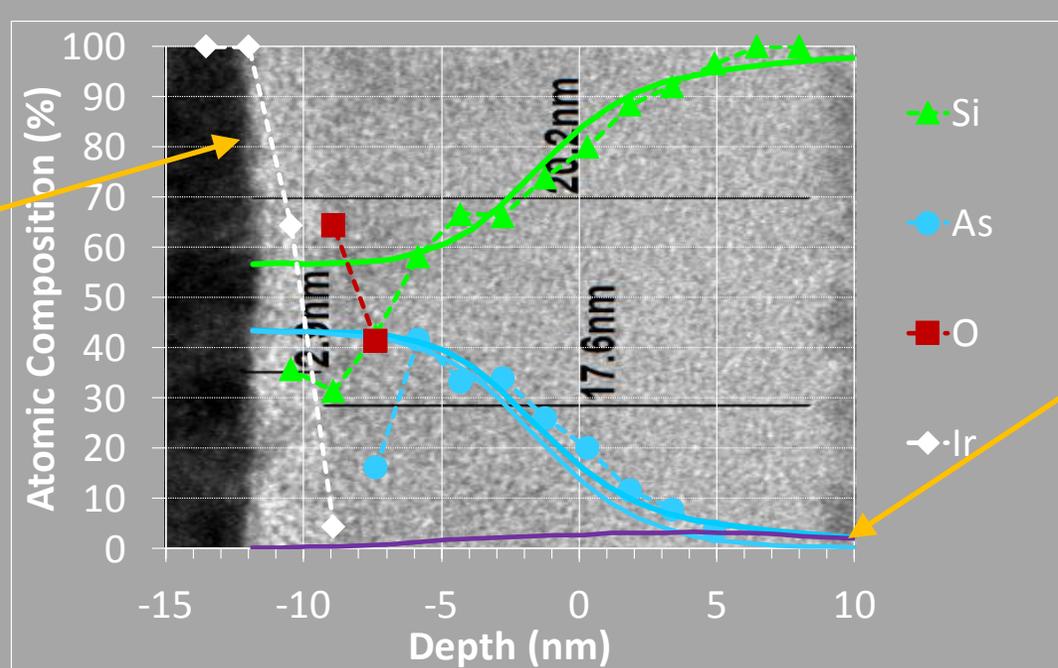
Post Anneal



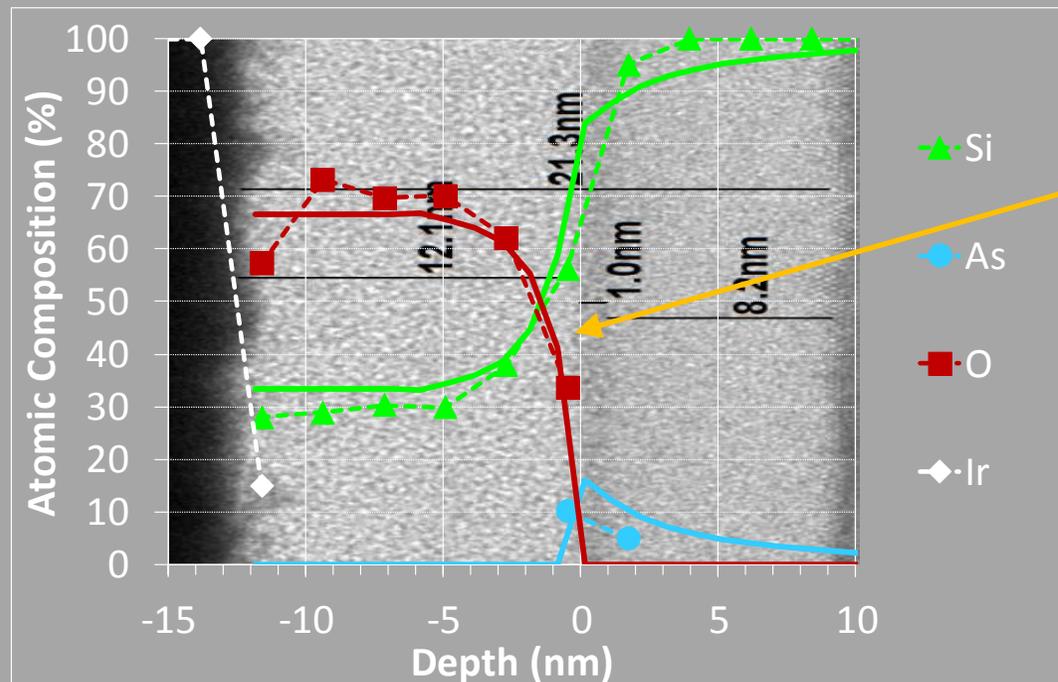
Major difference between
anneal and clean is less As in
surface bin

Model2 - AsH₃/H₂/7keV

No extra deposition predicted at 7keV



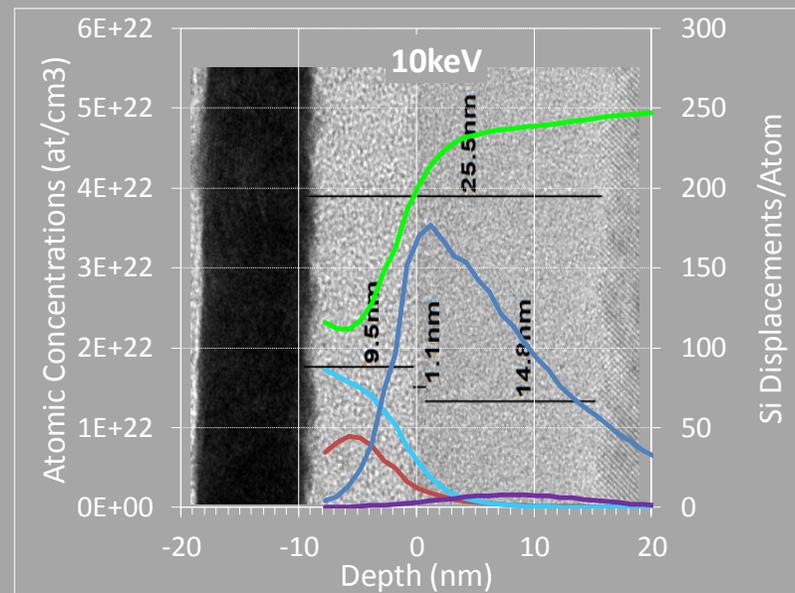
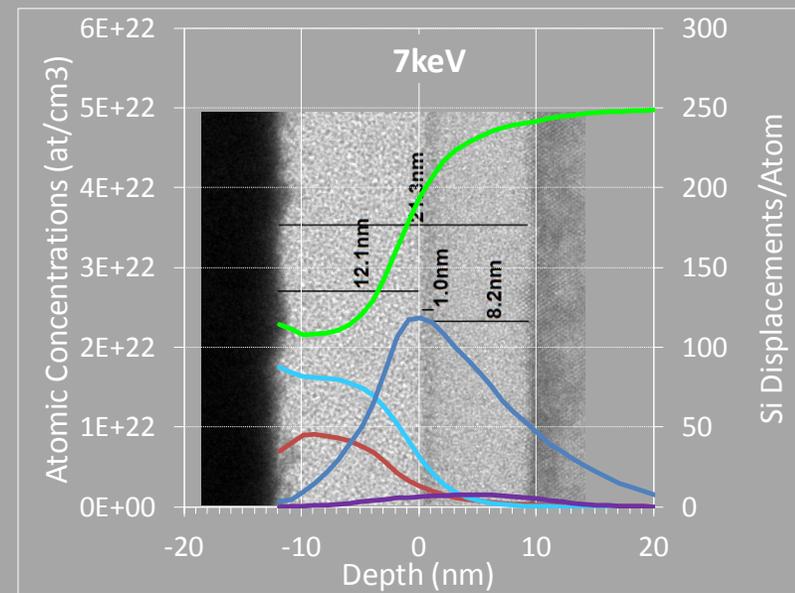
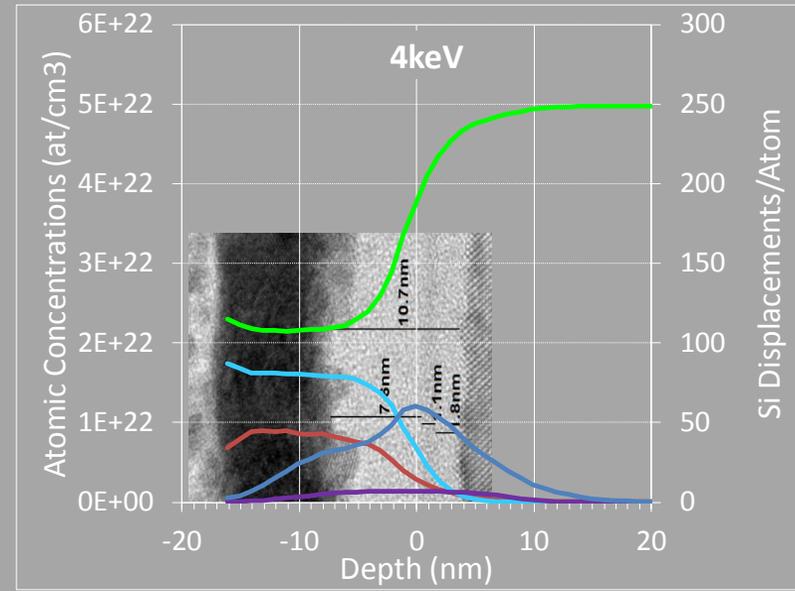
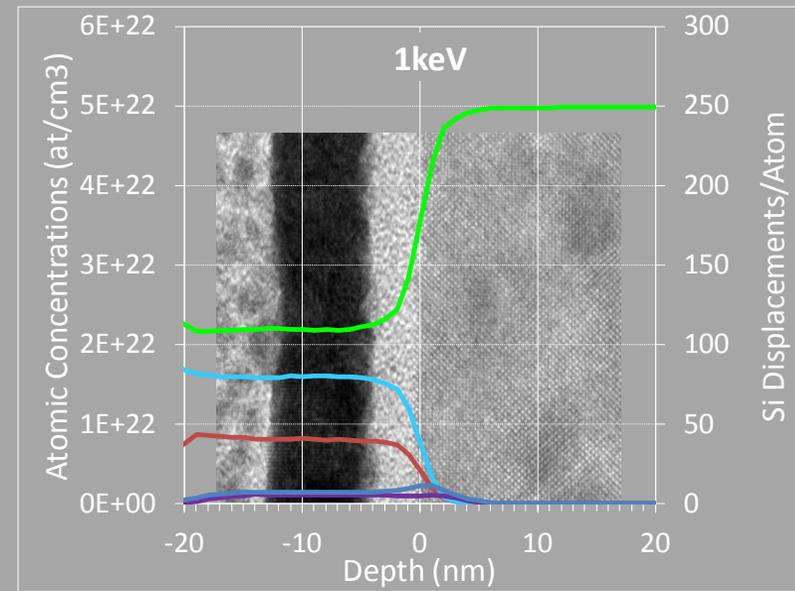
Less deep As ions



[O] reduced in this region

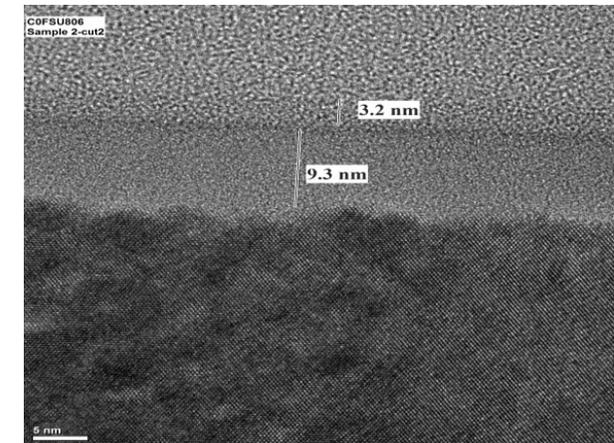
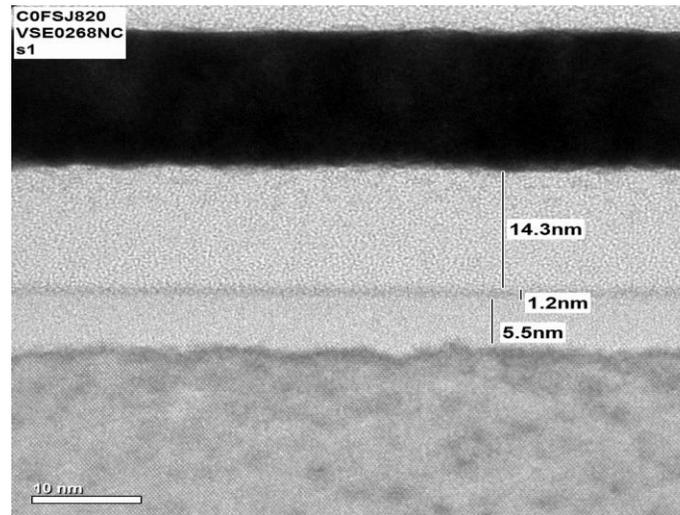
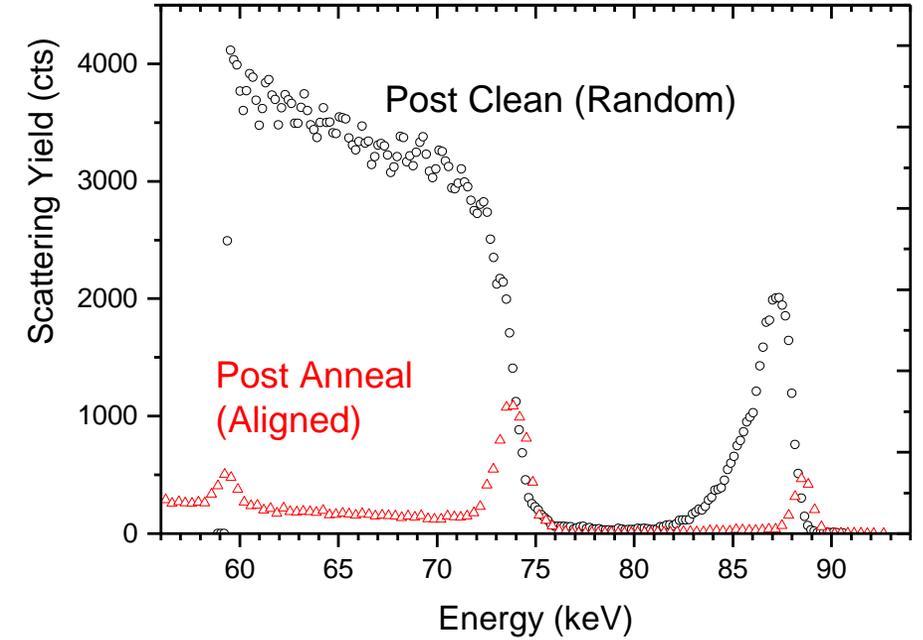
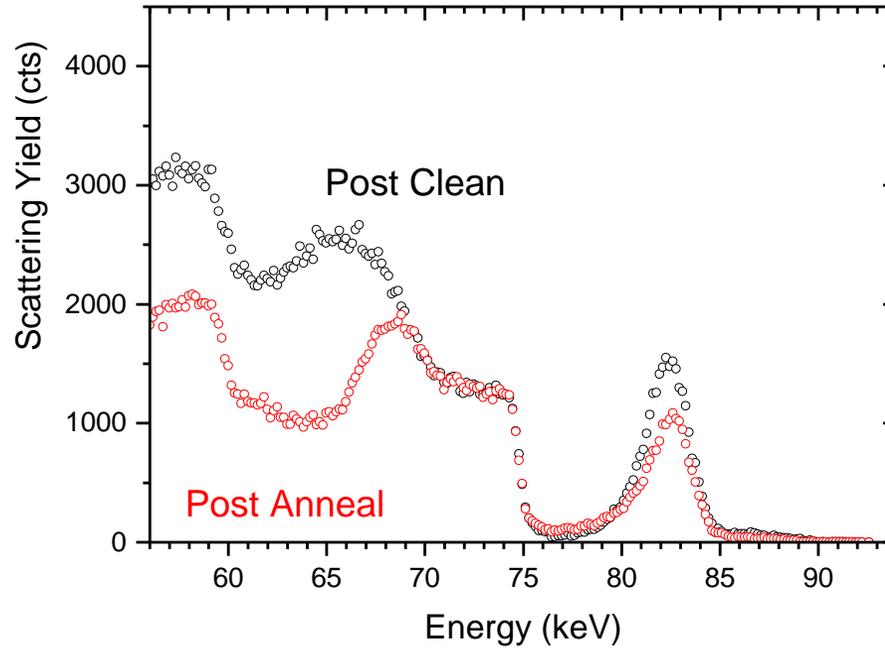
Model 2 vs Energy

- a/c interface at same Si dpa (50) for all energies
- Depth of As ions consistent with displaced Si measured by MEIS
- At 7keV, as-implanted thickness same as post clean thickness

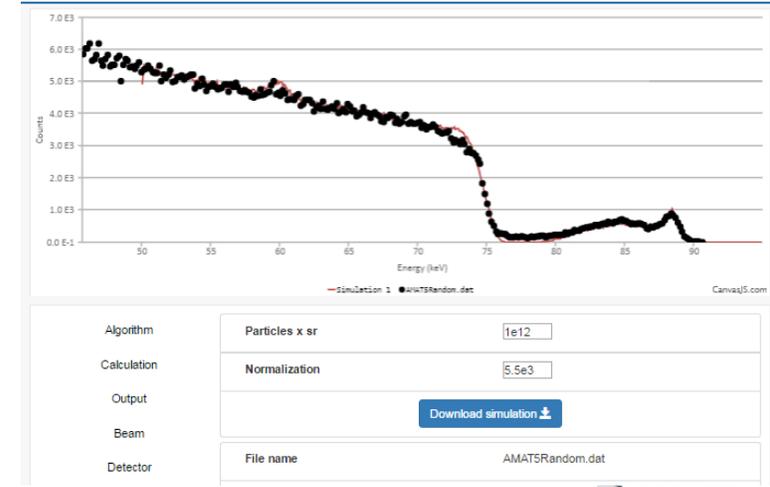
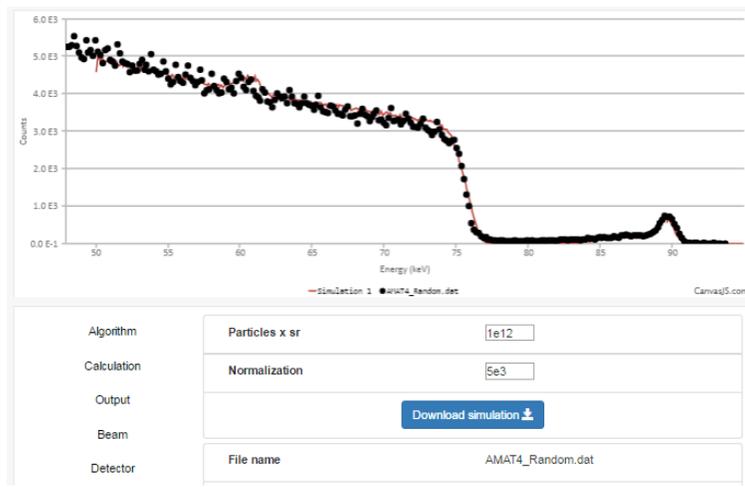
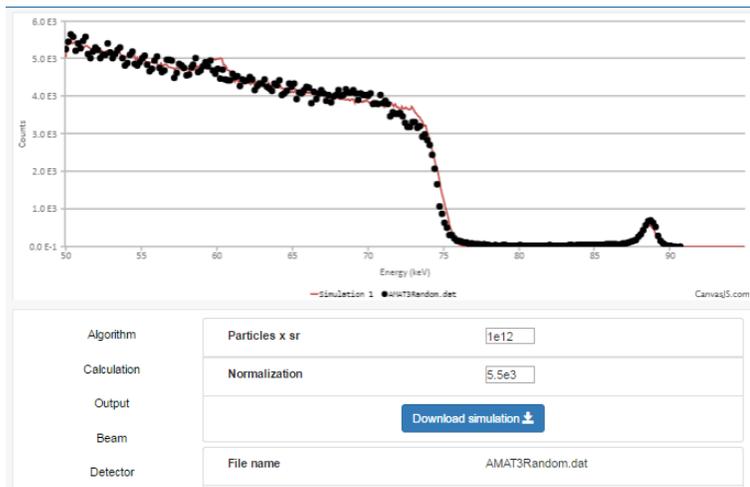
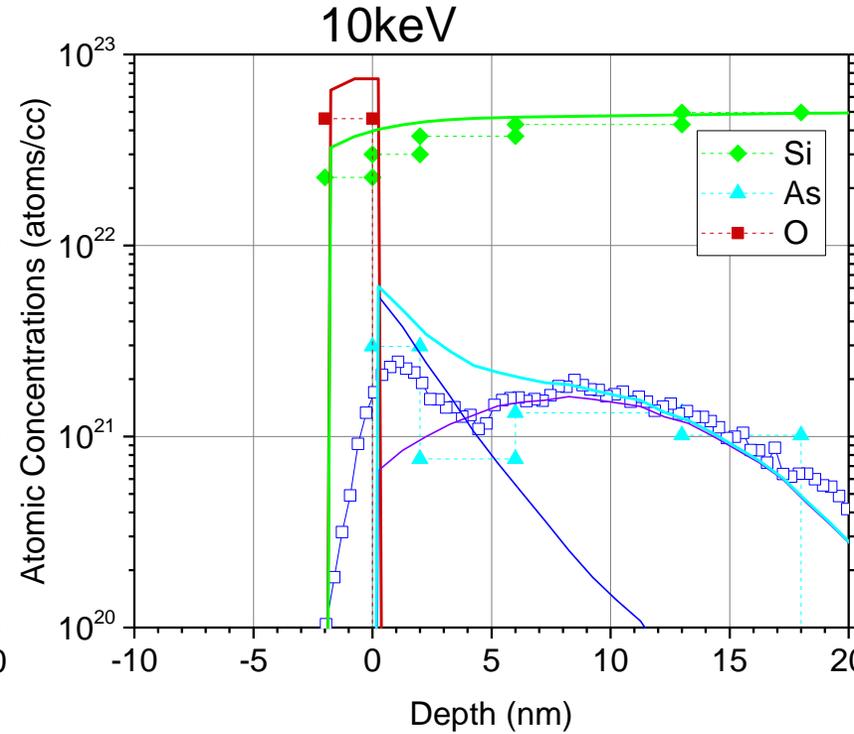
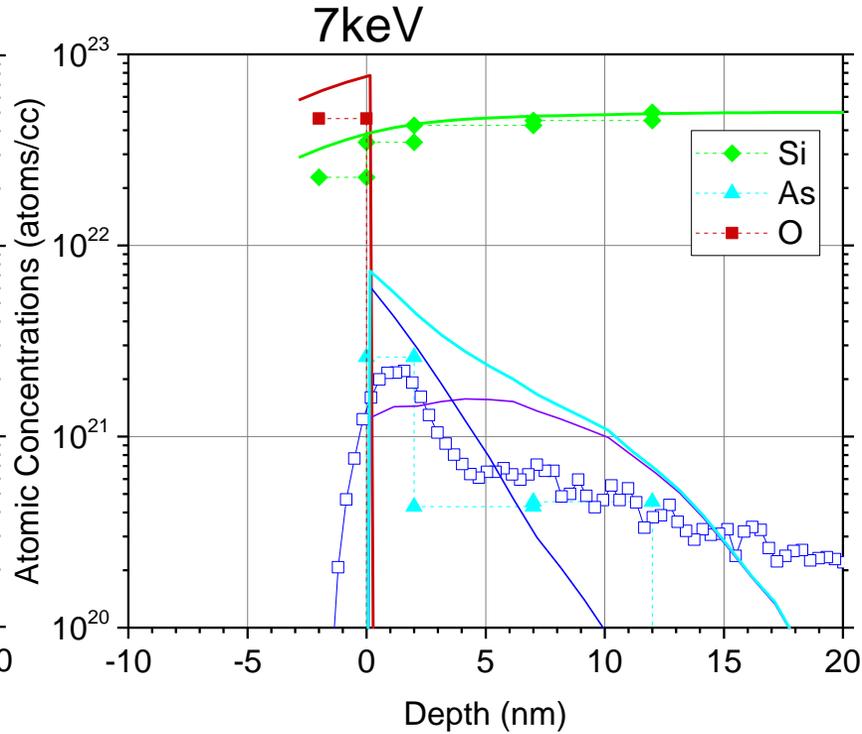
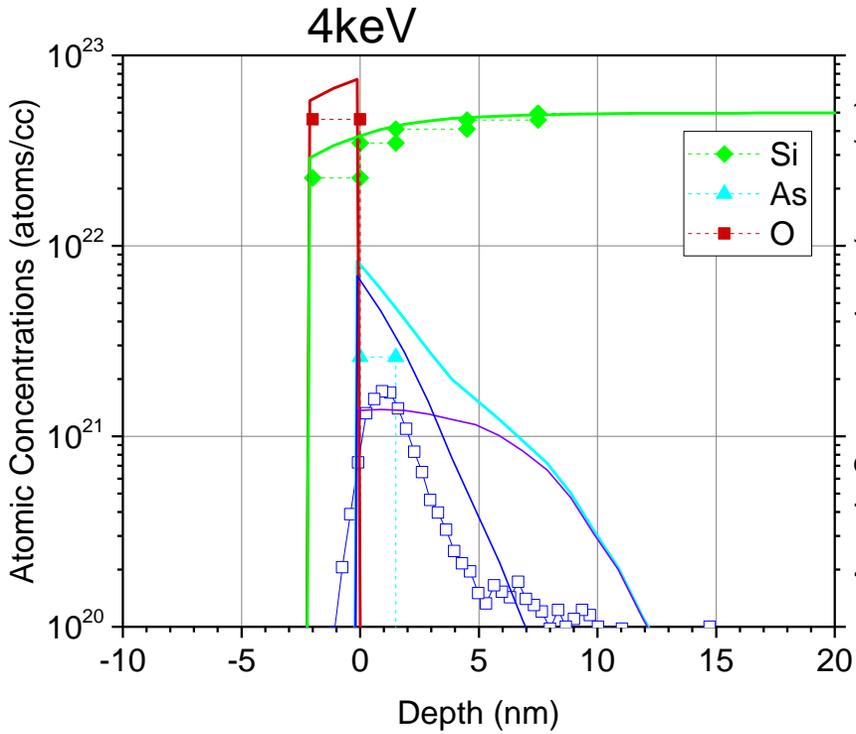


Dose Retention vs Oxide Thickness

- Energy variation samples are post anneal – would have preferred post clean!
- Samples are thin oxide case

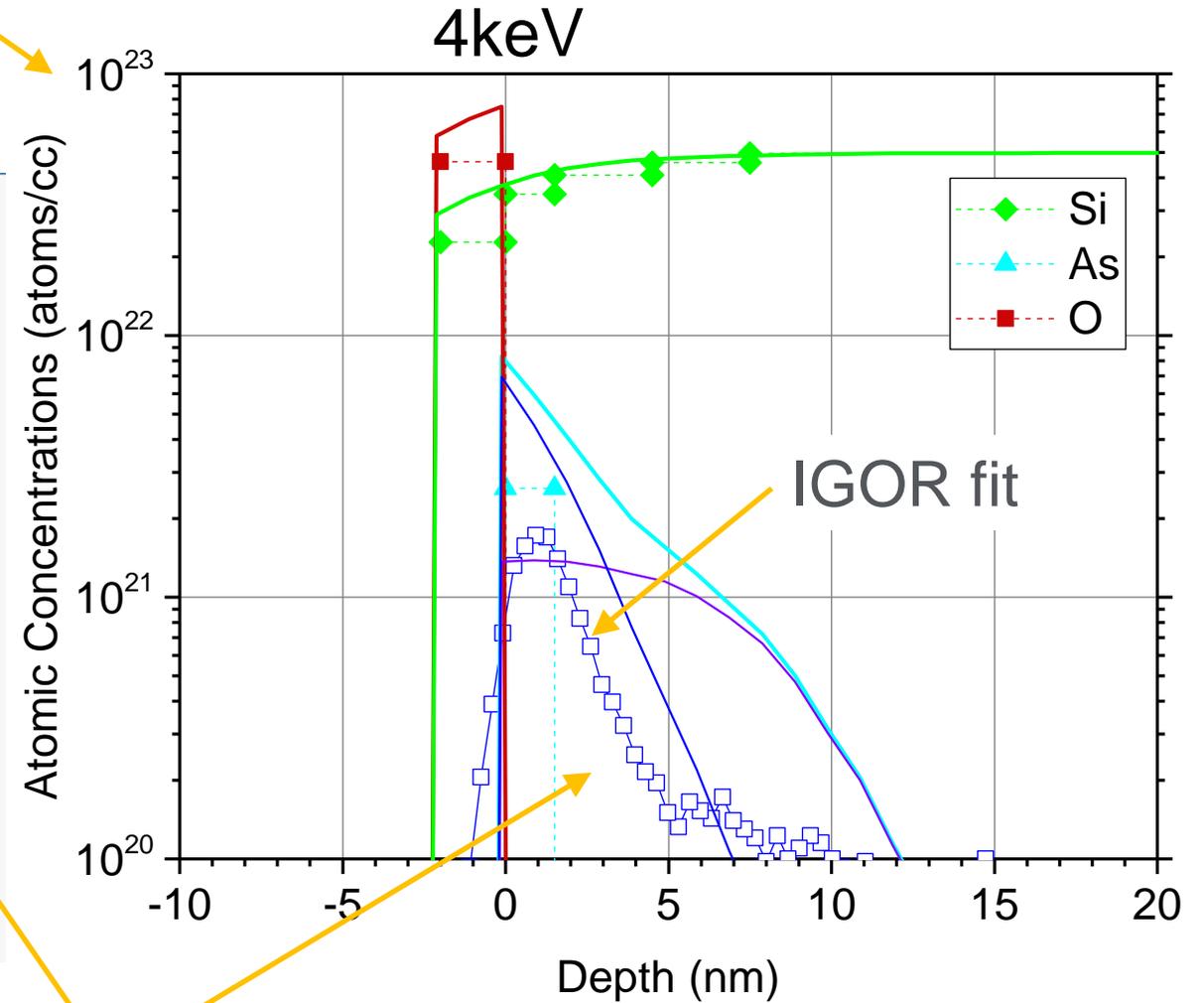
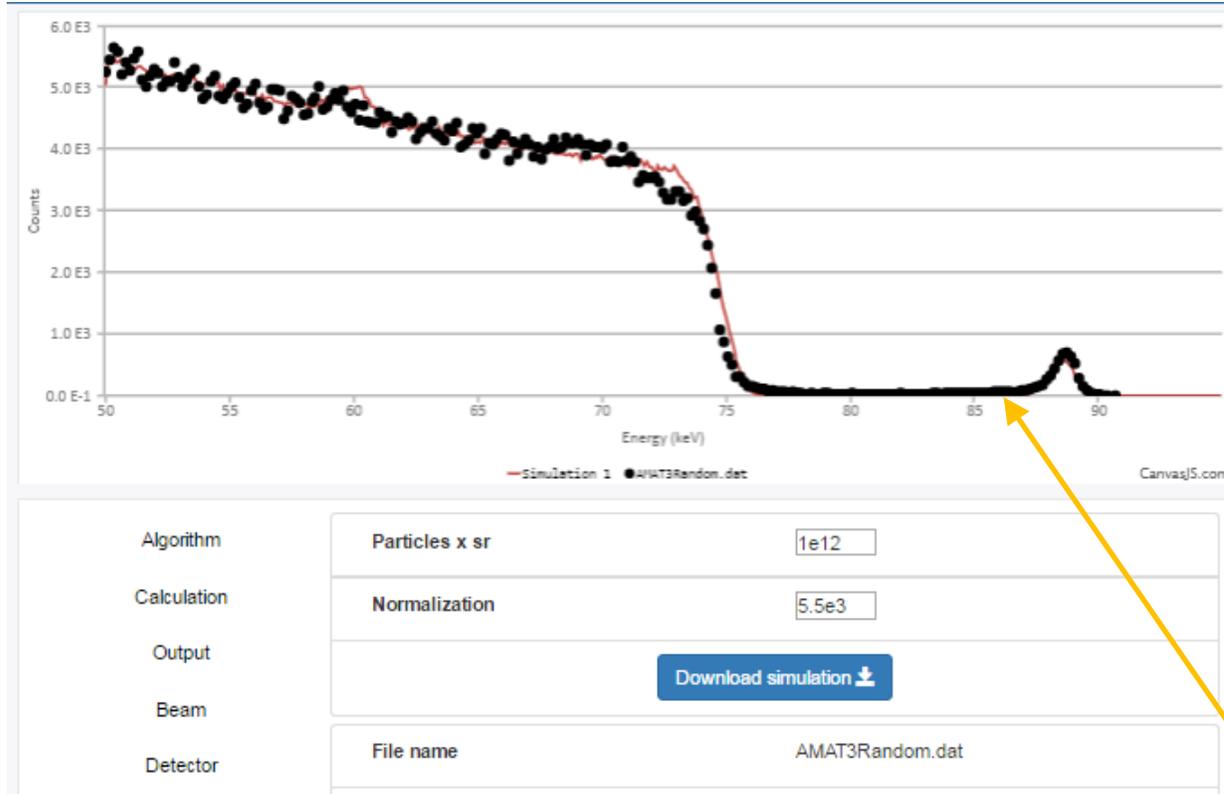


MEIS (Post Anneal) vs TRIDYN (Post Clean)



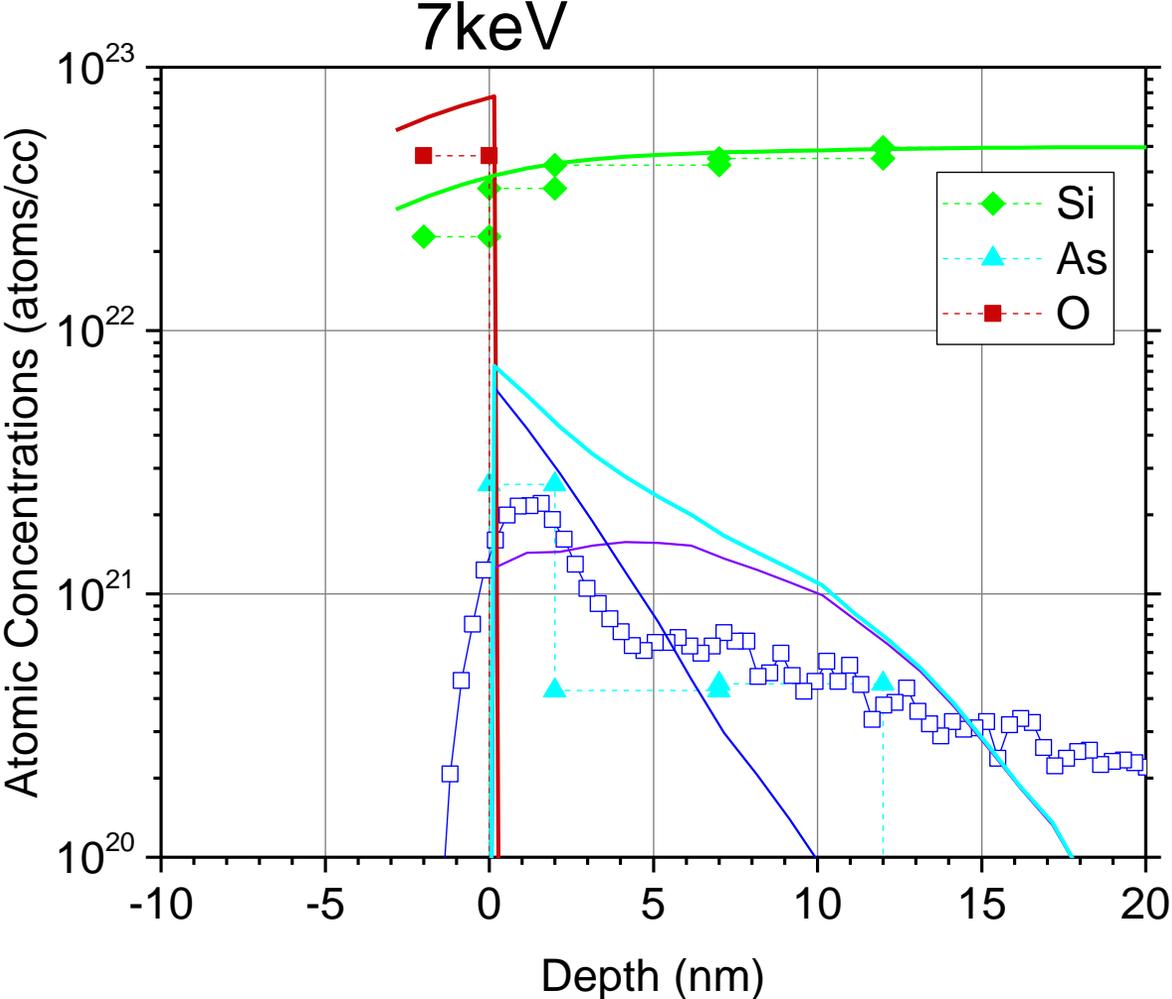
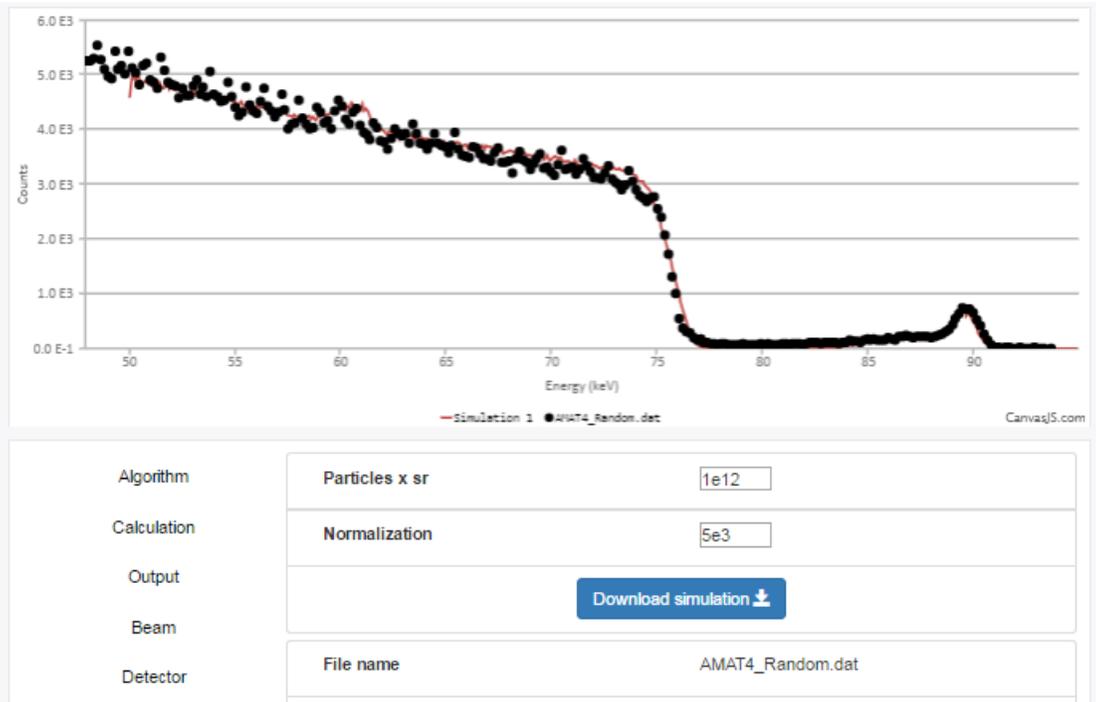
MEIS (Post Anneal) vs TRIDYN (Post Clean)

Note log scale



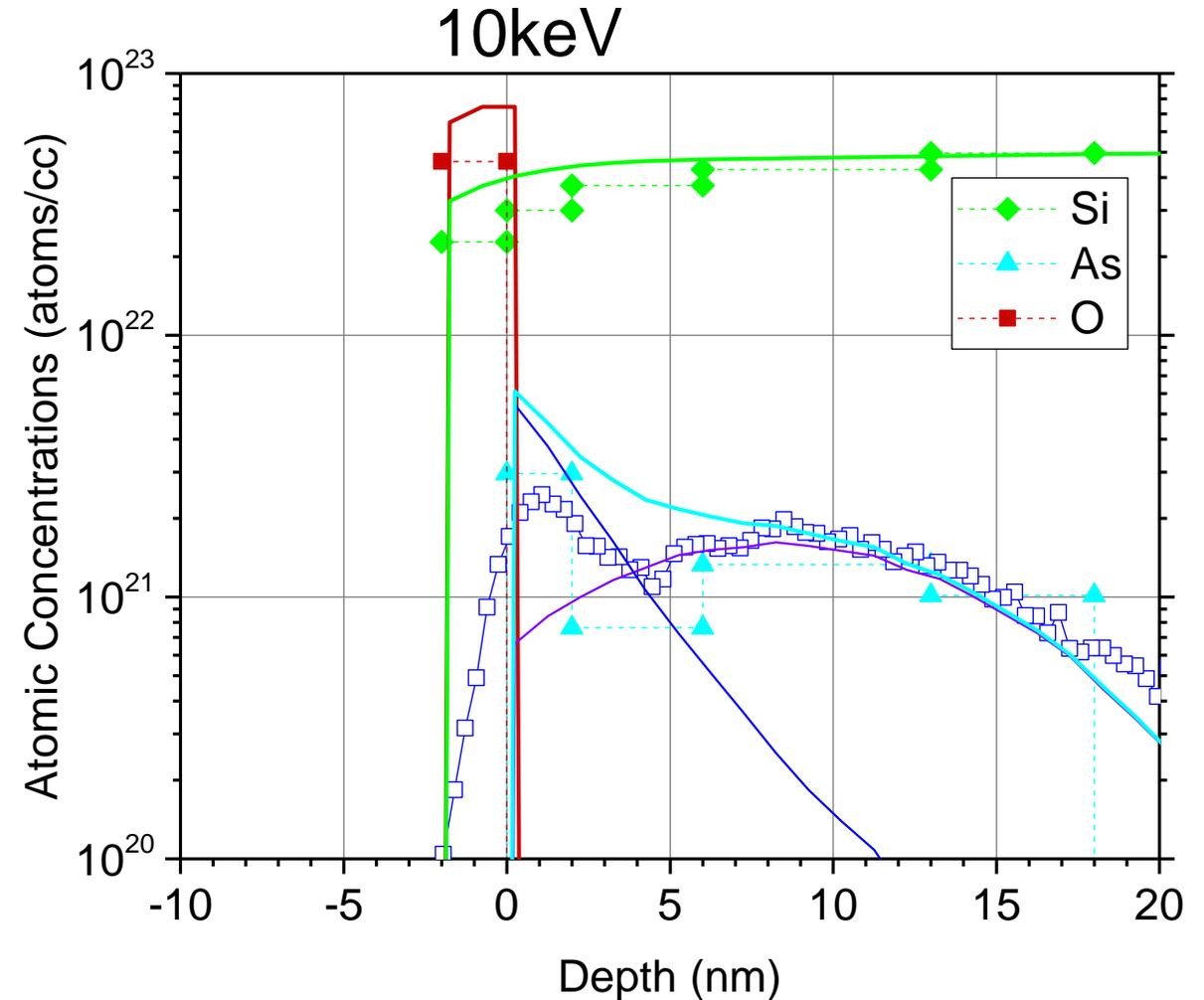
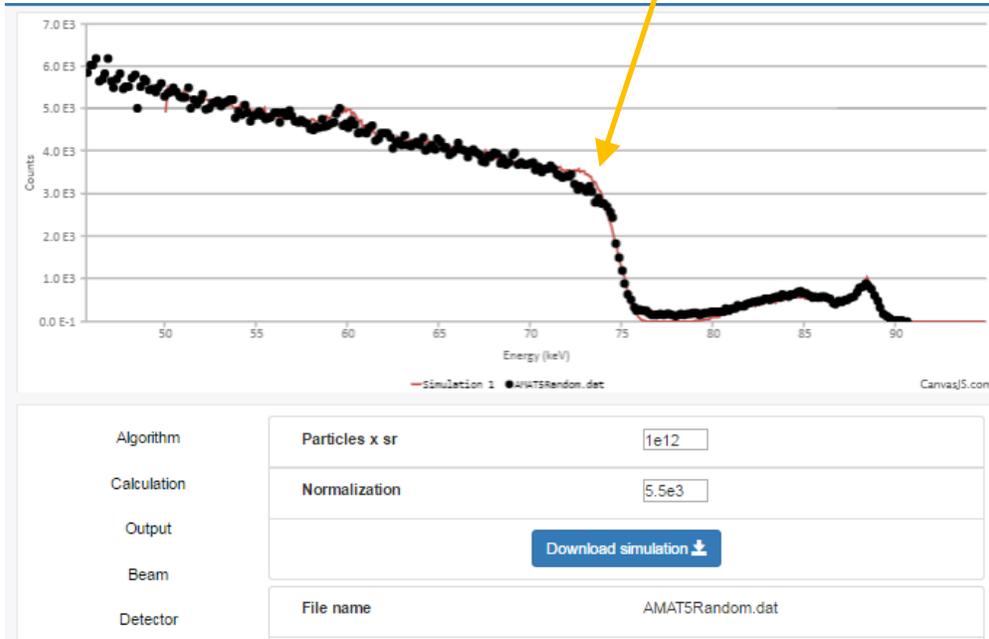
Deep As not included

MEIS (Post Anneal) vs TRIDYN (Post Clean)



MEIS (Post Anneal) vs TRIDYN (Post Clean)

Surface contamination?



- Contributions from ions and knock-ins to As profile more evident with energy
- As retention increases with energy

Summary

- Many features of planar PLAD can be described using TRIDYN
- MEIS allows TRIDYN input species and fluxes to be measured
- Based on MEIS feedback a simple TRIDYN model was improved by
 - ▶ Including Si neutrals and ions
 - ▶ Reducing flux of As and Si ions
- TRIDYN can aid analysis of MEIS spectra
- Small details can give deep insights into PLAD process
- Choices of process and metrology conditions important
- Did a good job of fitting spectra with POWERMEIS?
- This work is being applied to 3D fins using TRI3DYN and TOF-MEIS with PowerMEIS analysis*

*Henrique Trombini – 3D Structures at UFRGS
Daewon Moon – KMAC TOF-MEIS
My talks at IBMM and ANU Workshop

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