X-ray Diffraction Studies of Low-Energy Ion-Irradiation Defects in Model Targets

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Outline

- Surface X-ray Diffraction
- Silicon as “ideal” target
- Oxygen dosing results
- High energy Ar^+ irradiation
- CTR method
- Ion Damage as Vacancy or Relaxation
- Ex-situ samples from AO source
- Future plans

Goals of Project

- Materials modifications due to 5eV oxygen present in Low Earth Orbit
- Focus on Silicon as “ideal” target
- Develop X-ray diffraction methods
- Utilize X-ray resources at
  - Brookhaven National Lab (X16A NSLS)
  - Argonne National Lab (sector 34 APS)

Why are 5eV oxygen ions interesting?

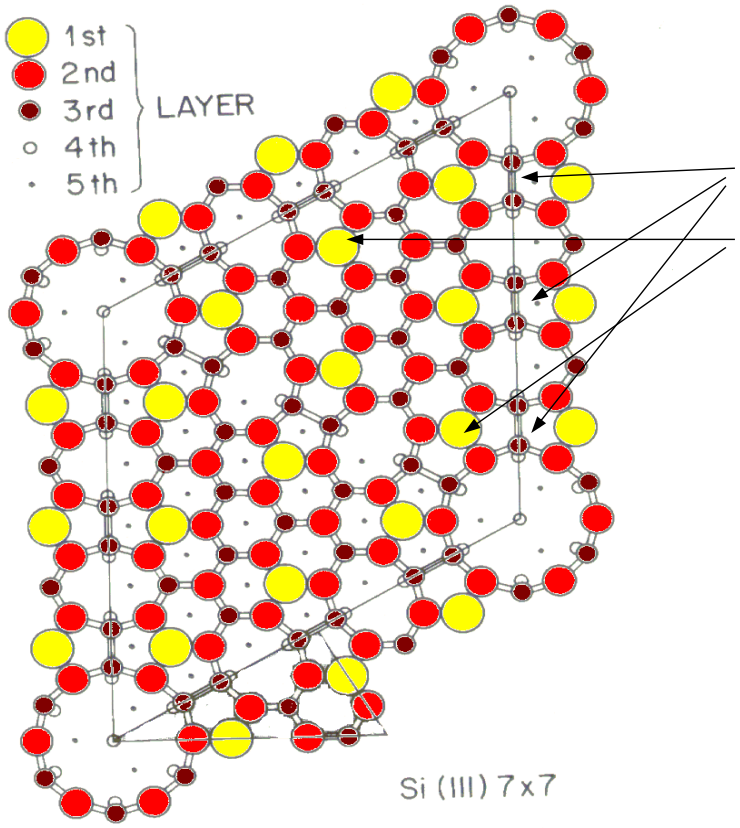
- Chemical interaction
  - 5eV O is reactive
  - Breaks bonds
  - Forms new bonds
  - Adsorbed species
- Physical interaction
  - 5eV O is a projectile
  - Causes collisions
  - Results in point defects
  - Defects seen as strain

- Crossover energy = "Sputtering threshold"
- Around 15eV for Silicon
  - Orientation dependence?
  - Site-specific dependence?

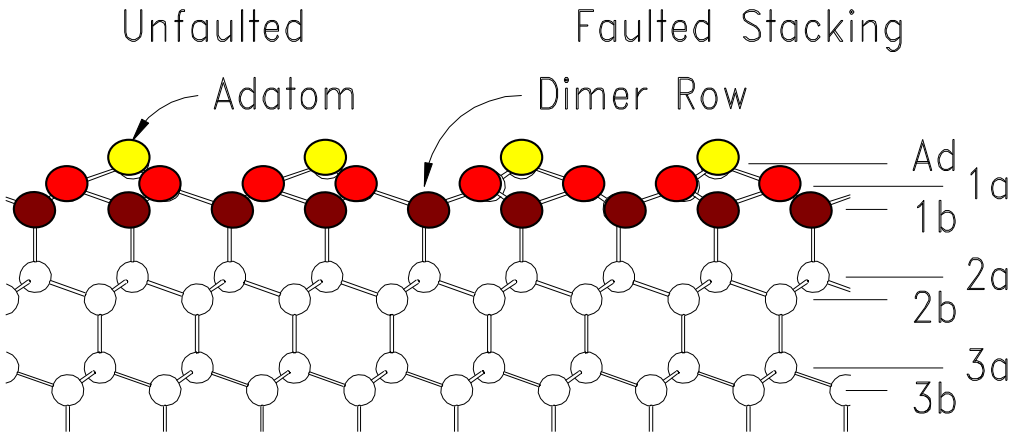
Surface X-ray Diffraction

- Surface sensitivity comes from symmetry
- Buried interfaces equally accessible
- Kinematical diffraction is quantitative
- Ordered superstructure or “1×1”
- Direct methods under development

Si(111) 7x7

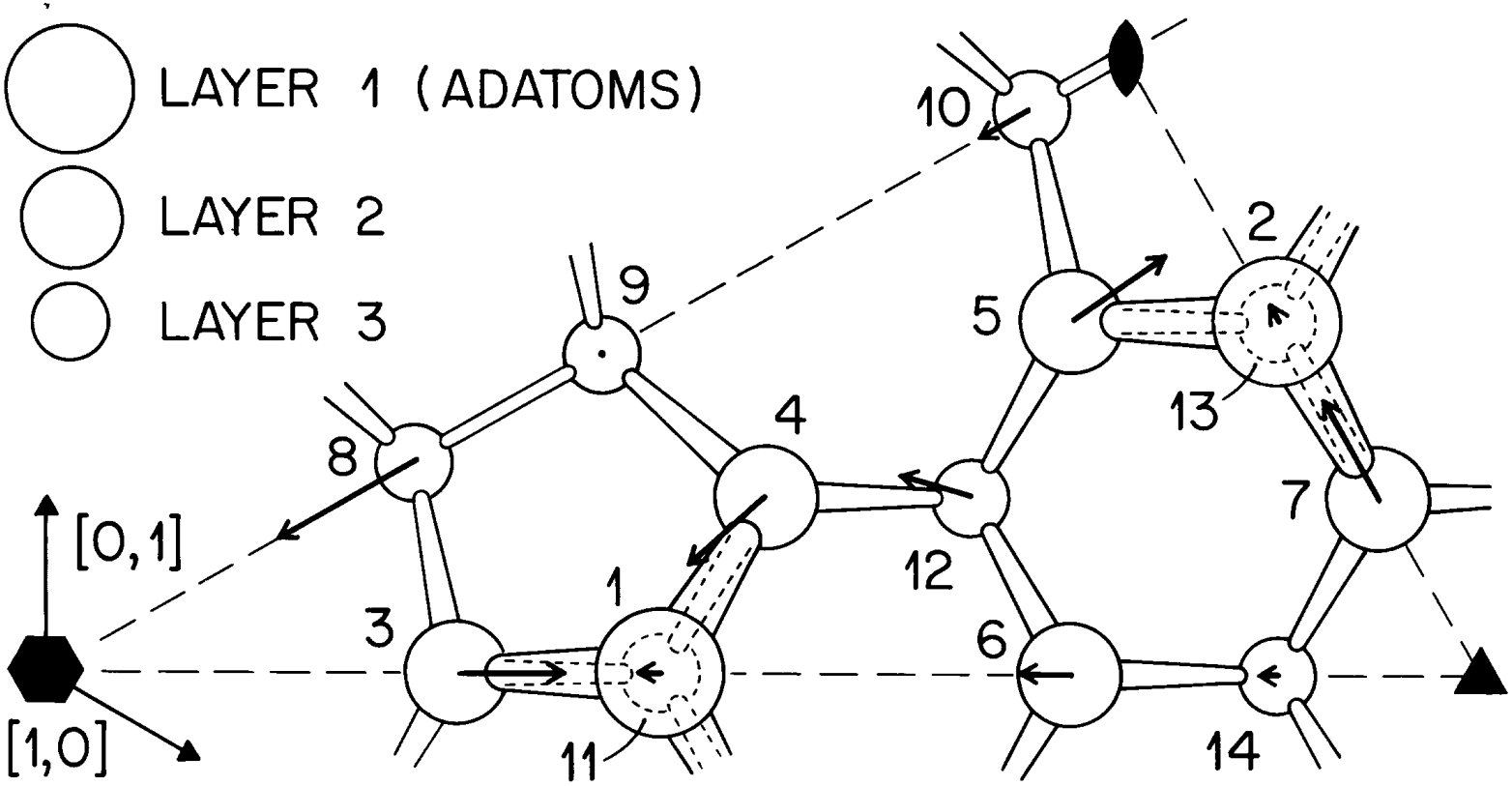


Dimers +
Adatoms +
Stacking Fault
= DAS model



Asymmetric Triangle

Contains all unique atoms in the P6mm structure

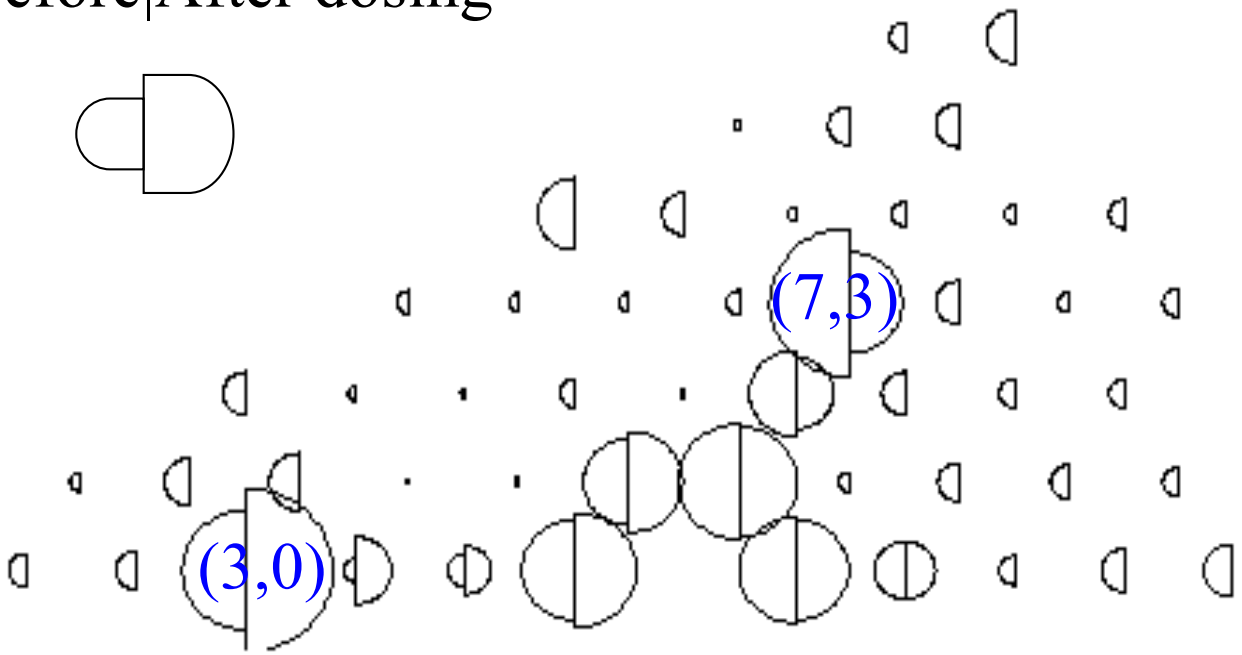


Structure factor Measurements

After averaging over p6mm symmetry

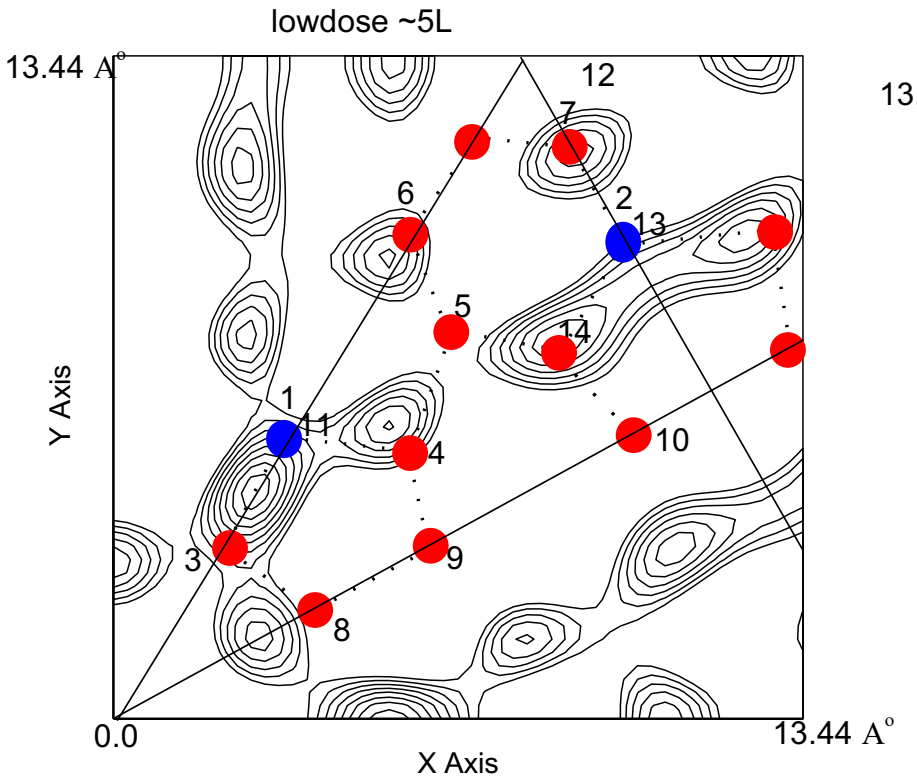
Two most sensitive reflections indicated

Before|After dosing

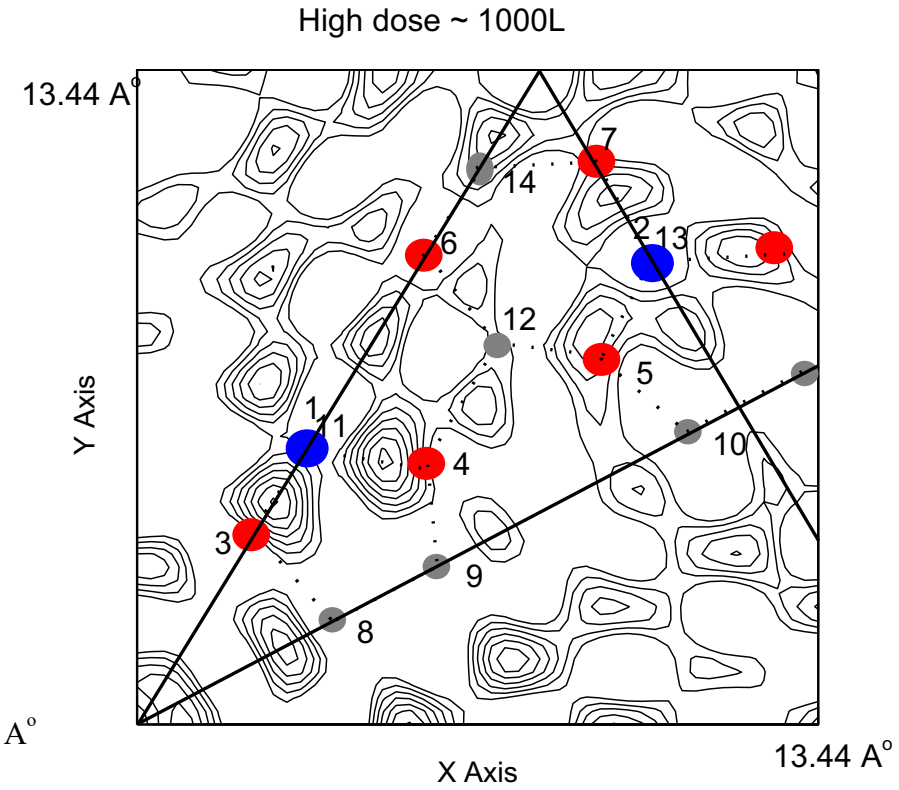


Difference Maps: effect of dose

Low dose, ~5L

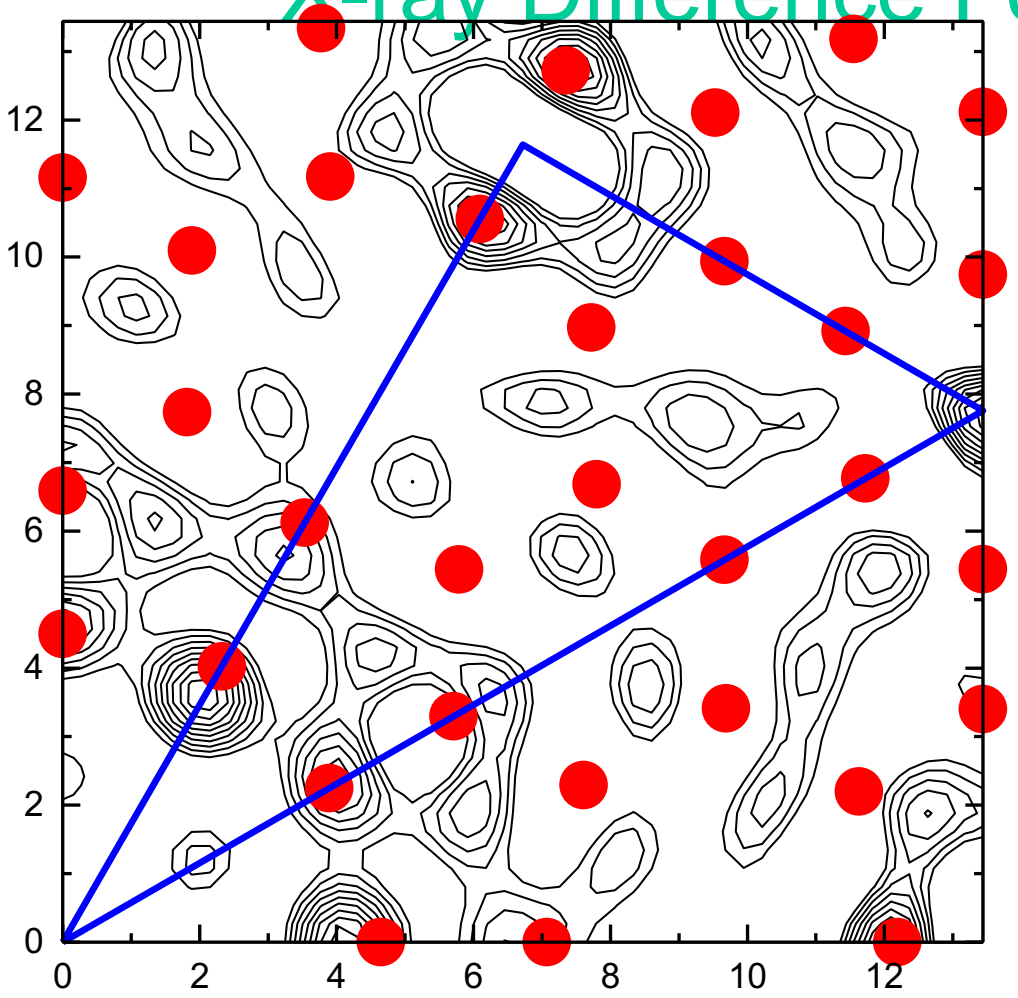


High dose, 1000L

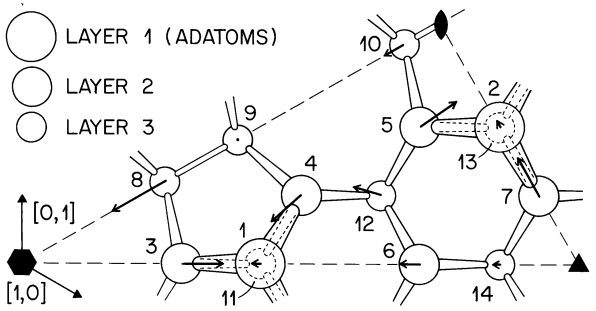


Oxygen Gas Modification of Silicon

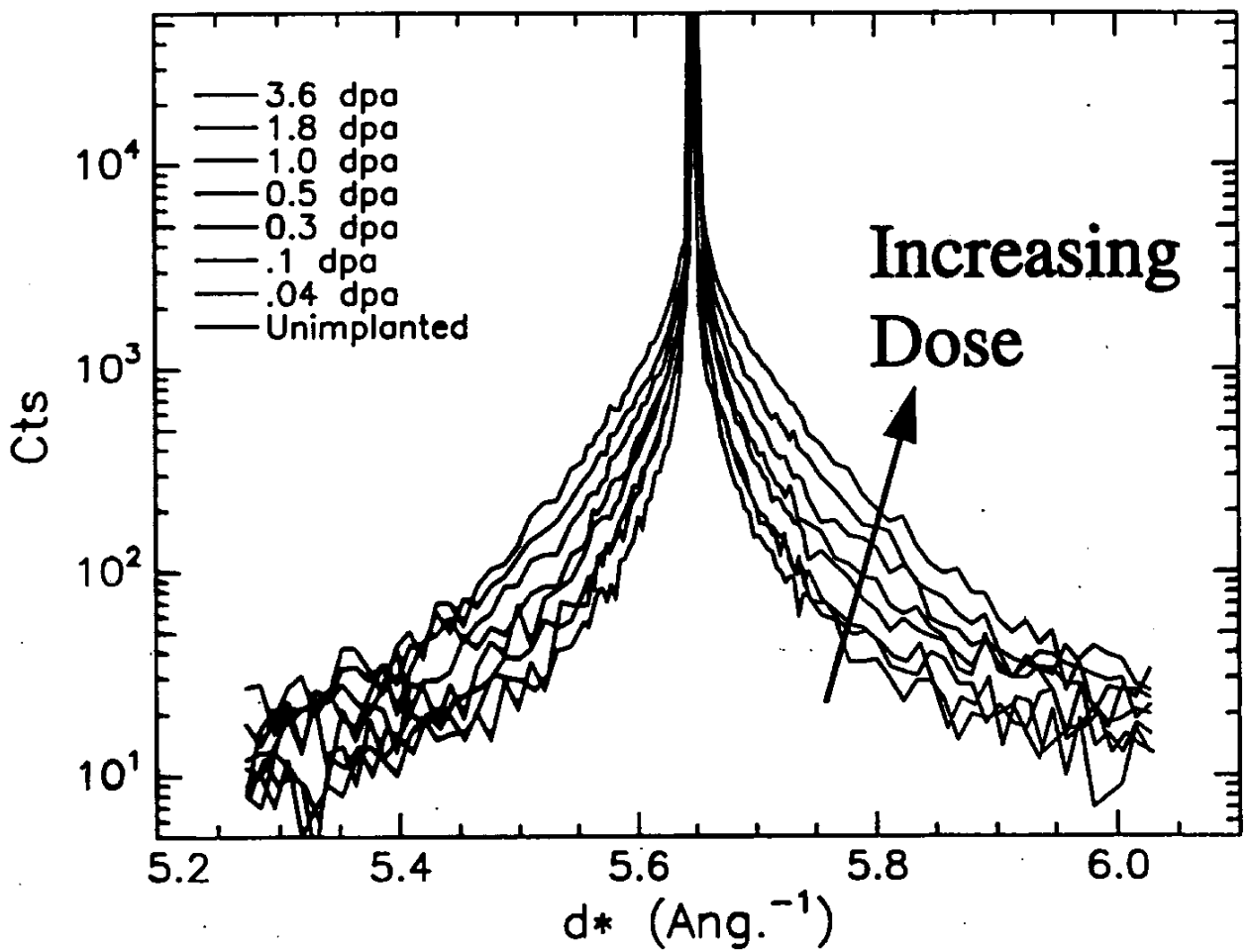
X-ray Difference Fourier Map



- X-ray Diffraction Measurement #1
- Oxygen Gas dose of Si(111) Surface
- X-ray Diffraction Measurement #2
- Difference Map of Negative Changes



Diffuse Scattering During Irradiation



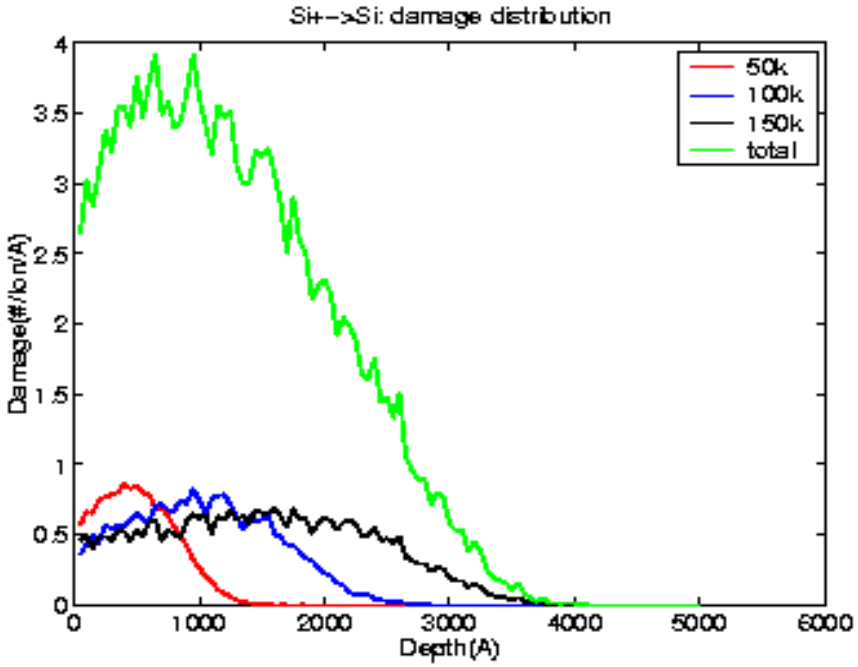
Si(111) substrate

In-plane (422) reflection

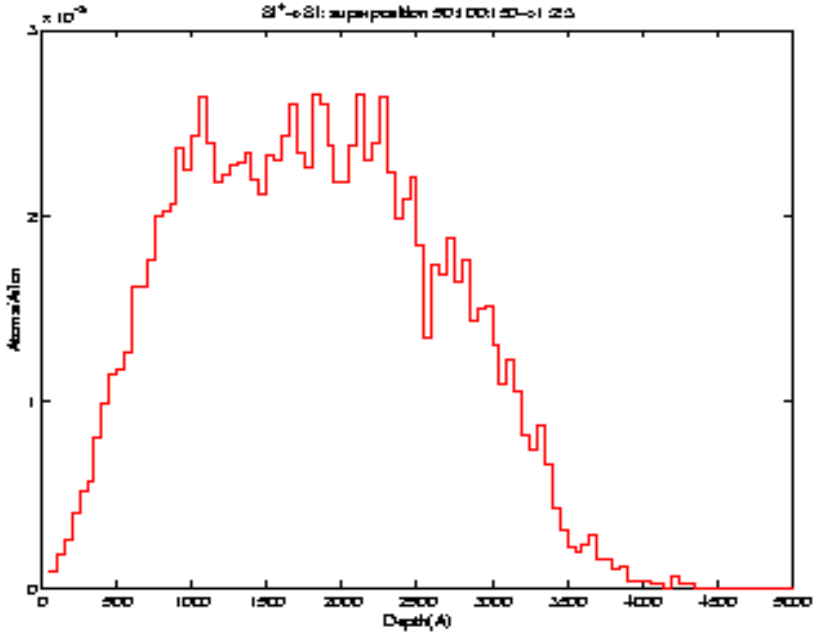
4.5keV He^+ at 210K

TRIM Calculation of Irradiation

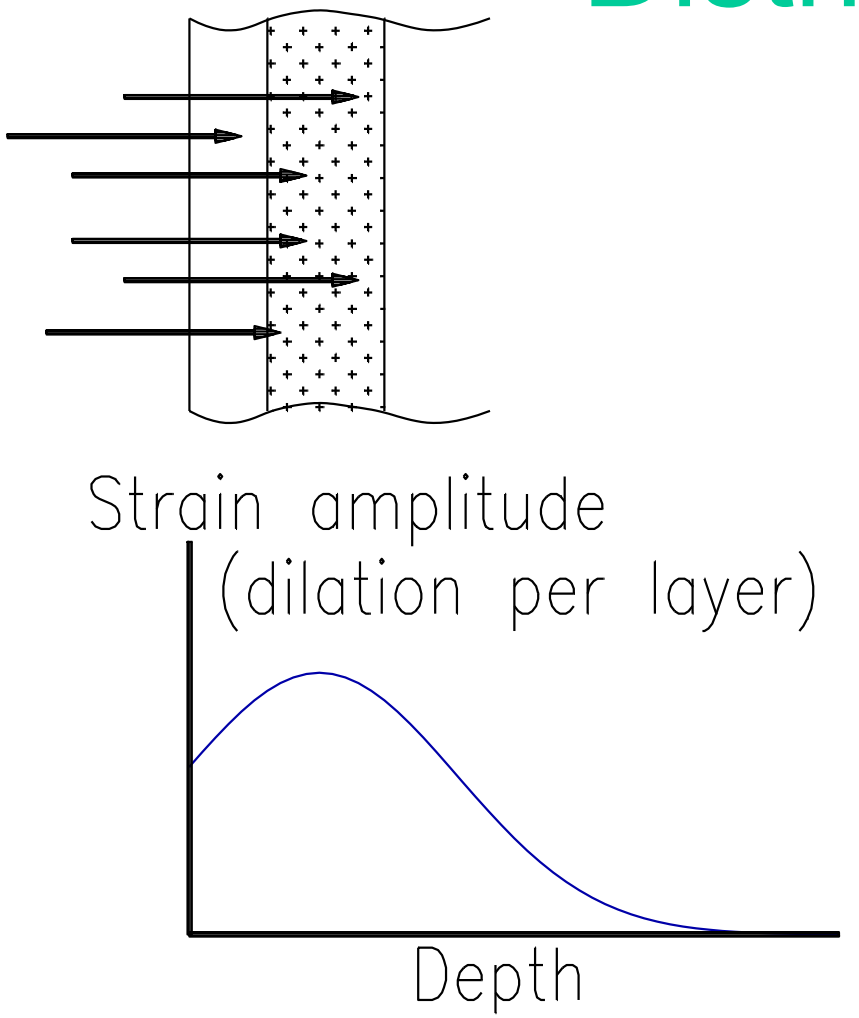
Damage profile



Implantation profile



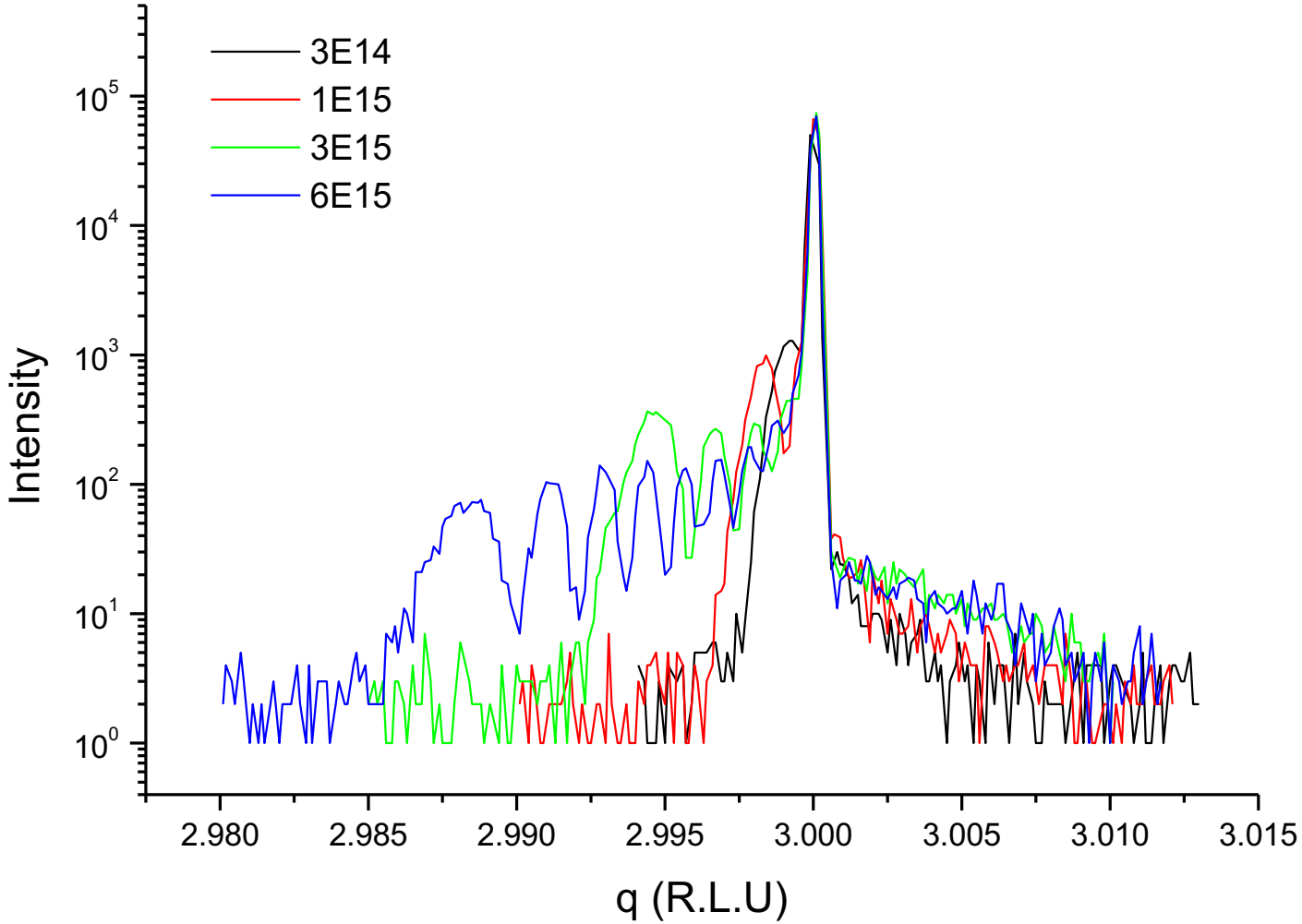
Gaussian Model of Strain Distribution



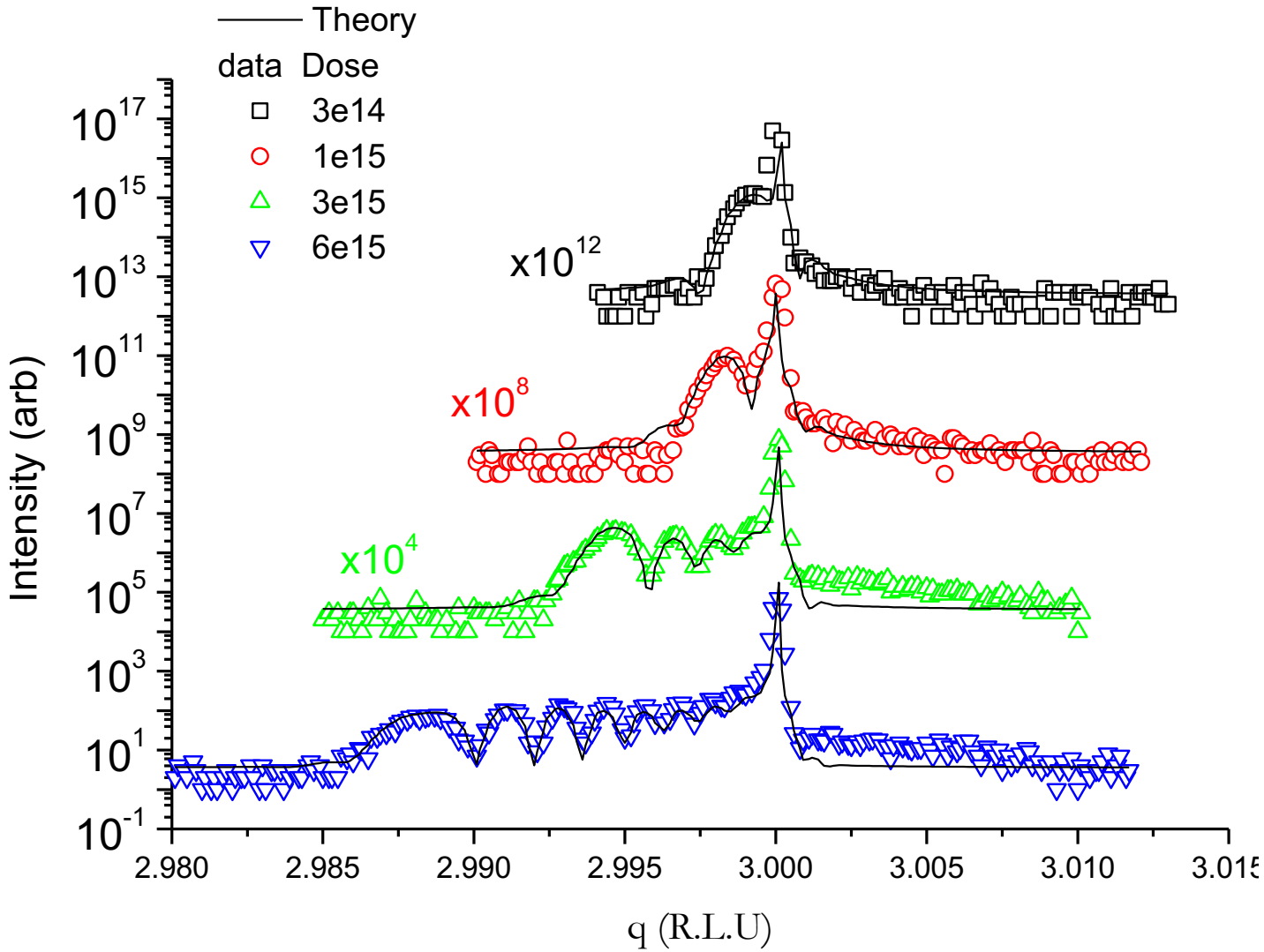
- Maximum at some characteristic depth
- Gaussian shape
- Strain is *per layer*
- Total displacement is integral of this curve

Dose dependence at Si(333)

50keV Irradiation

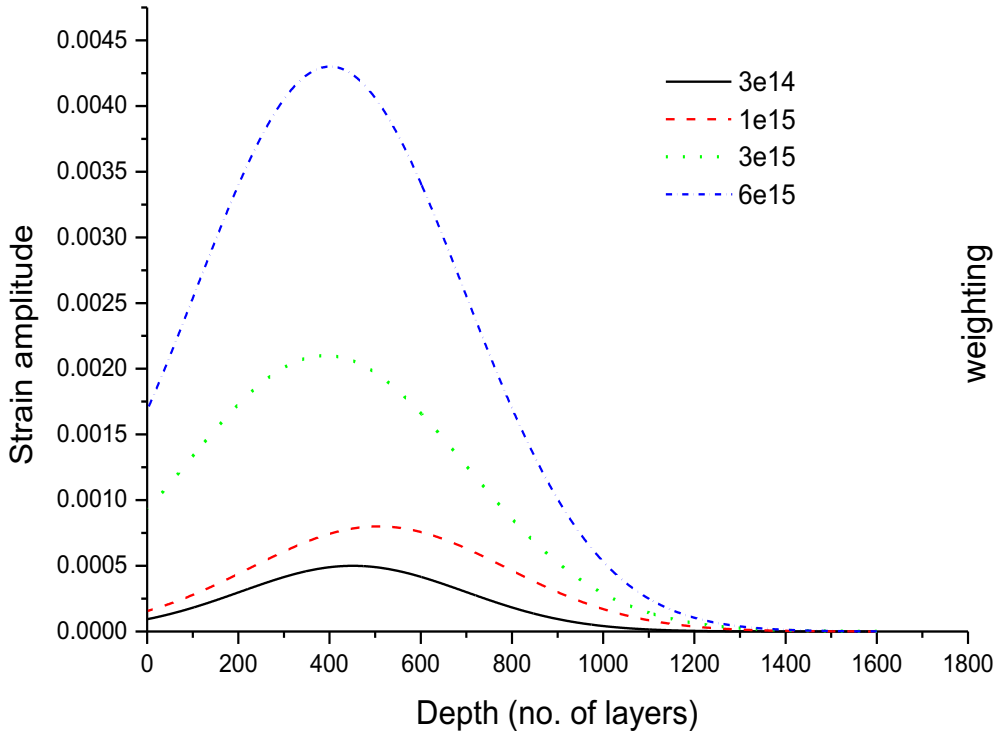


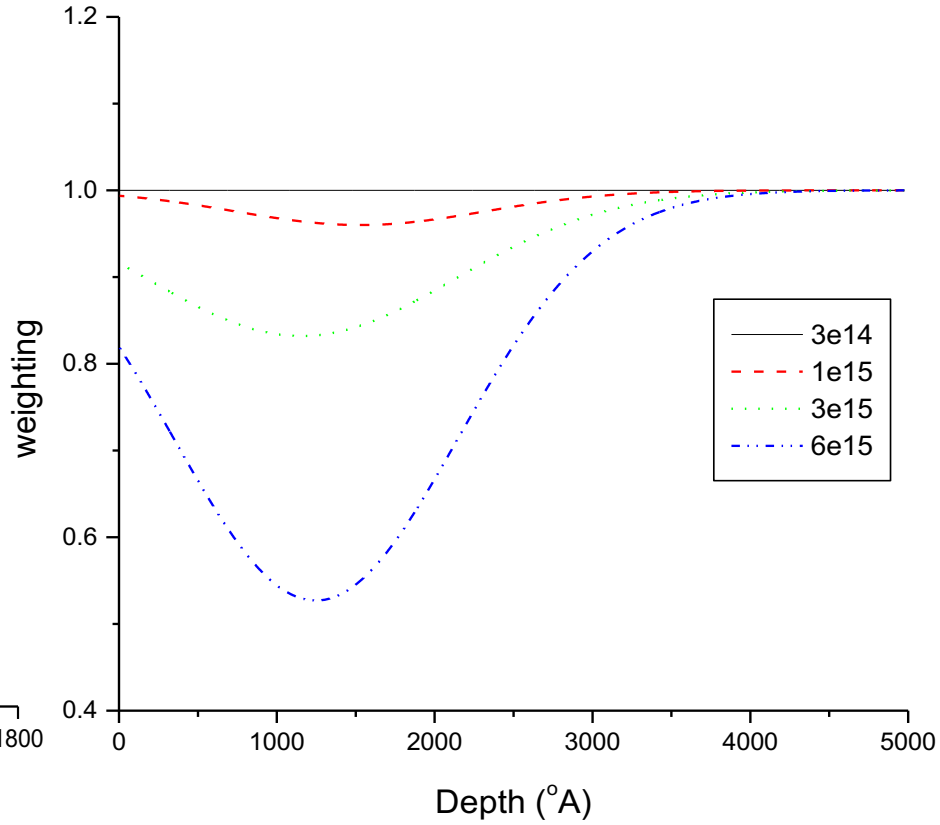
Fits of Dose Dependence



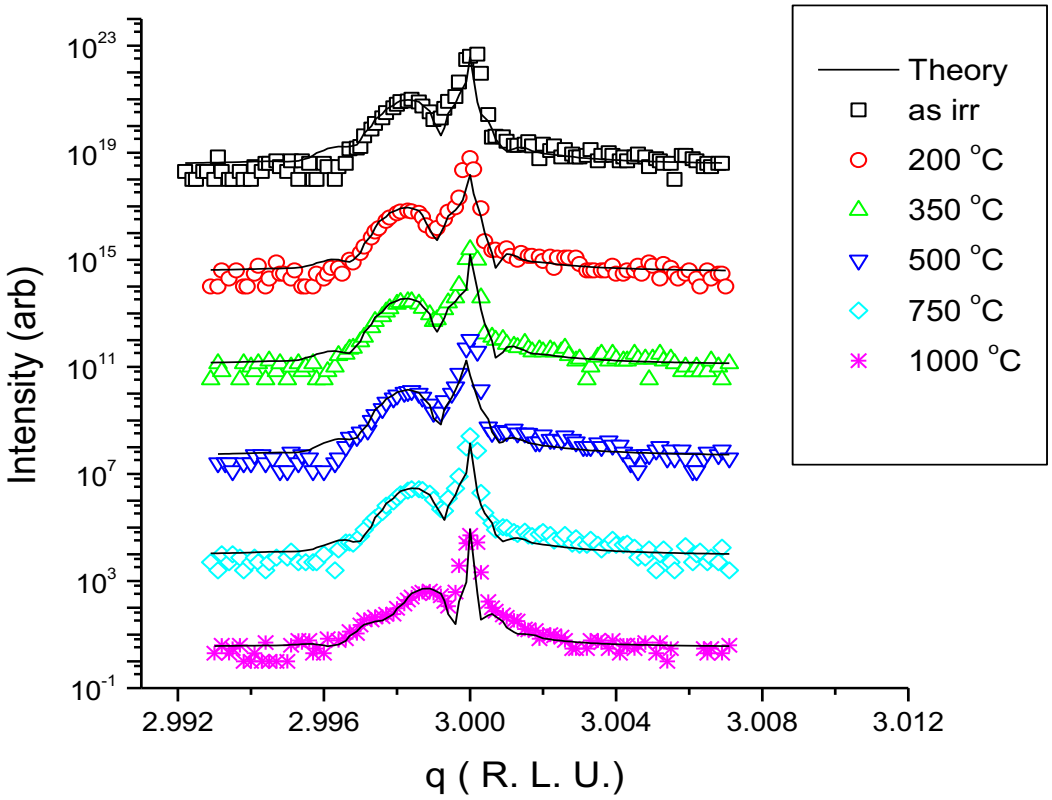
Fit of Dose Dependence

50keV Irradiation

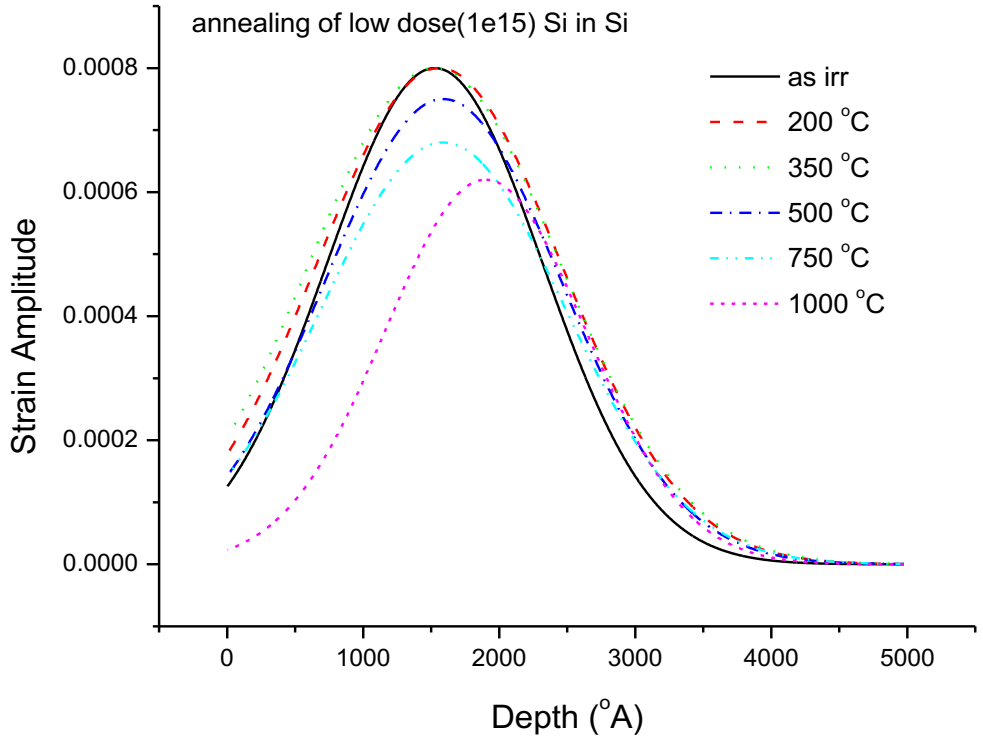


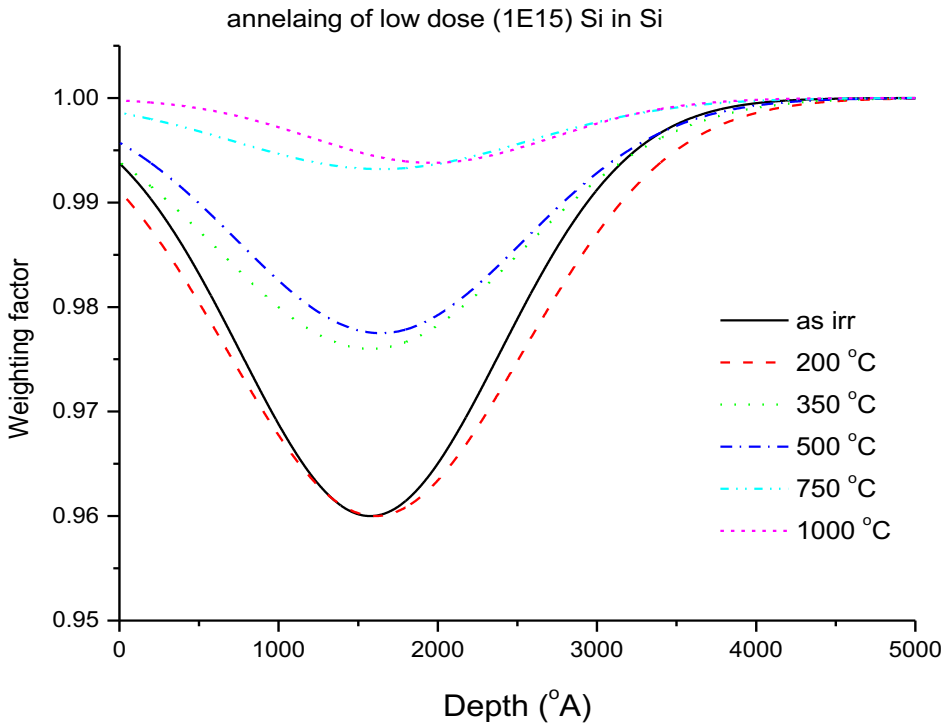


Low Dose Annealing

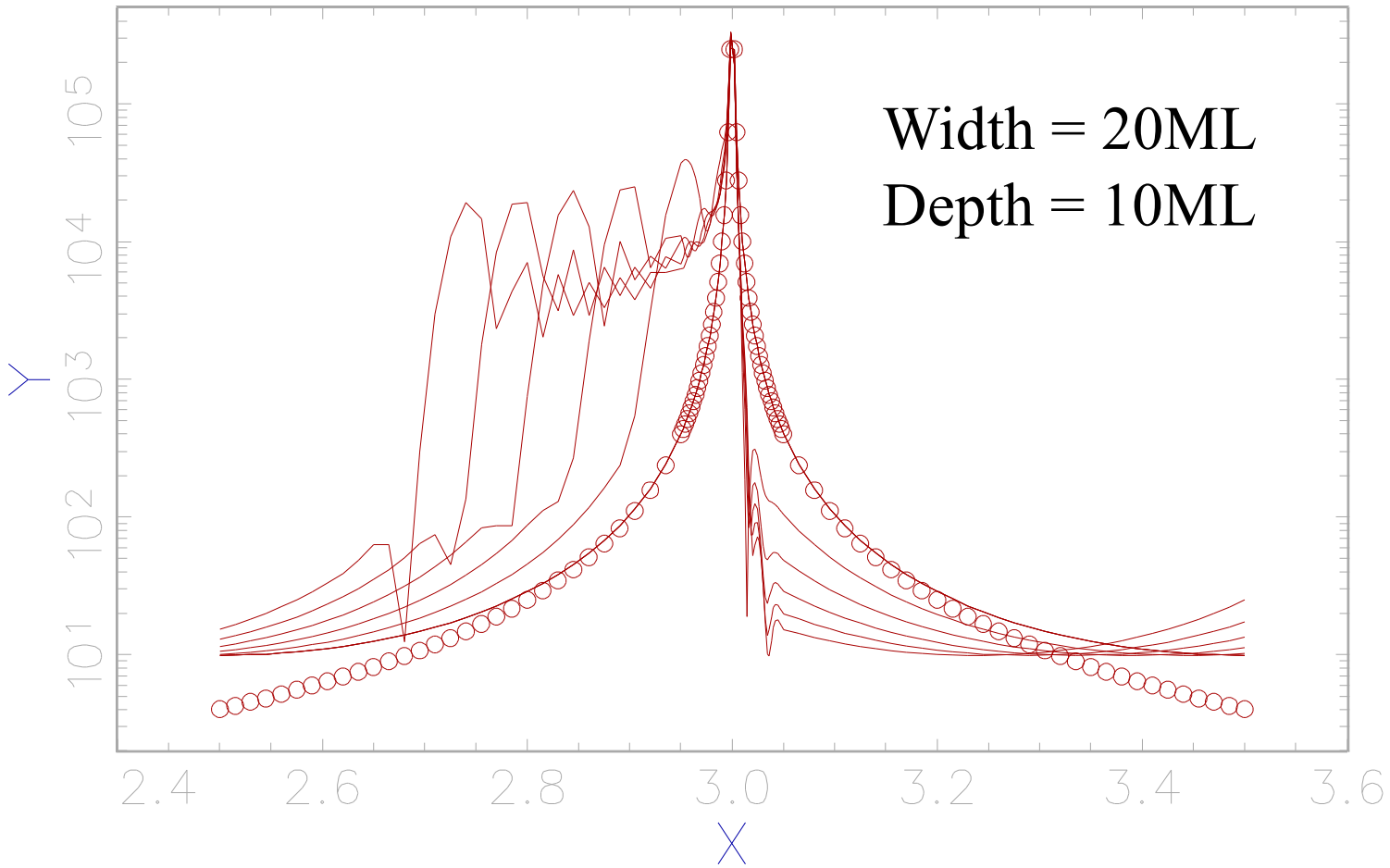


Fit of Low-dose Annealing

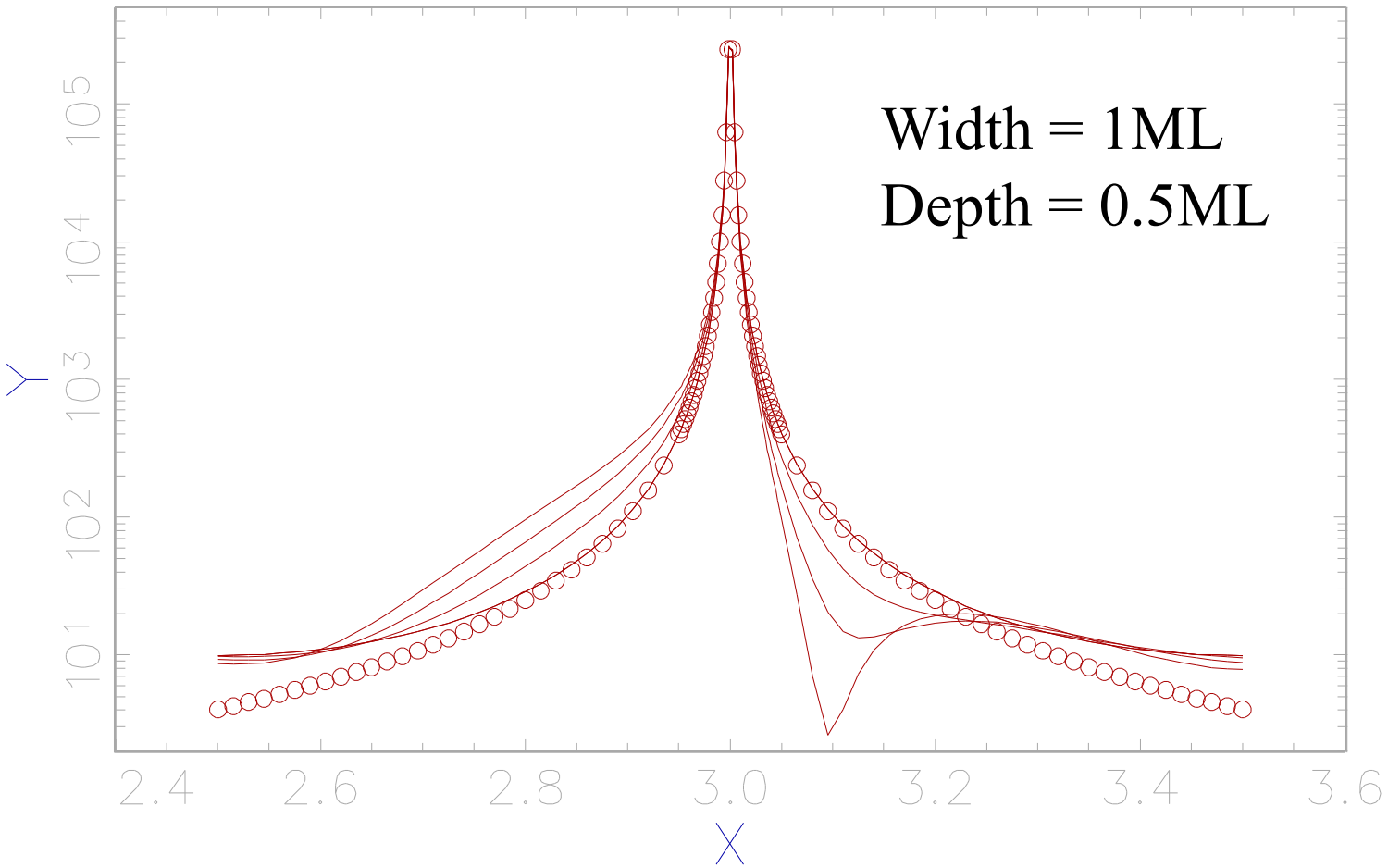




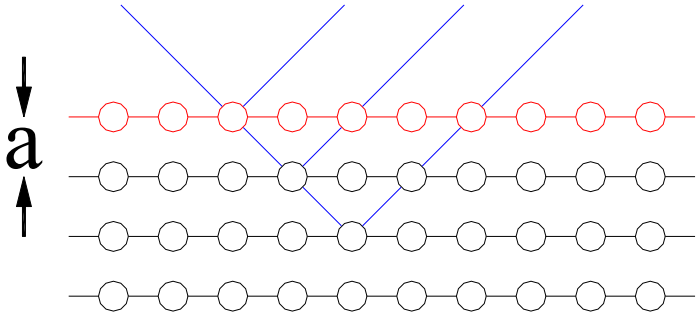
Theoretical Profile for Strain



Extrapolation to Single Layer



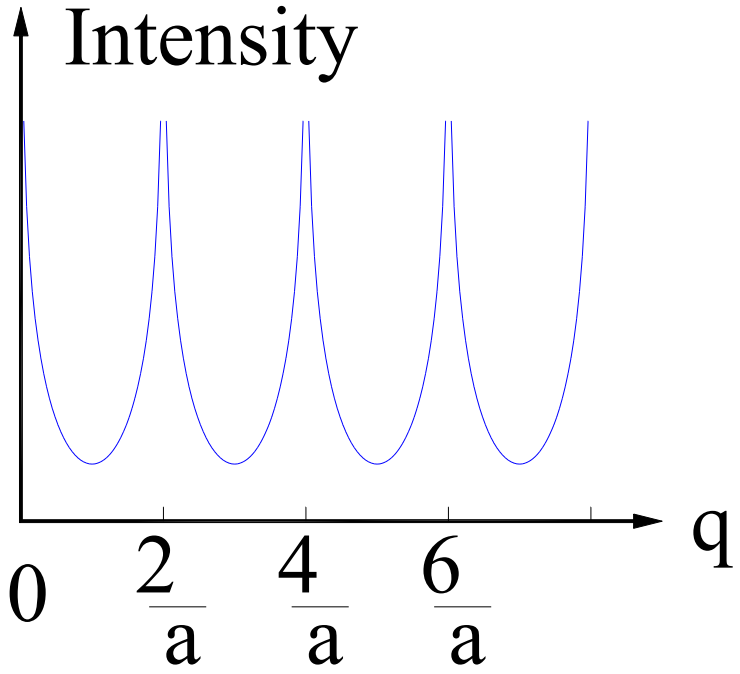
Origin of Truncation Rods



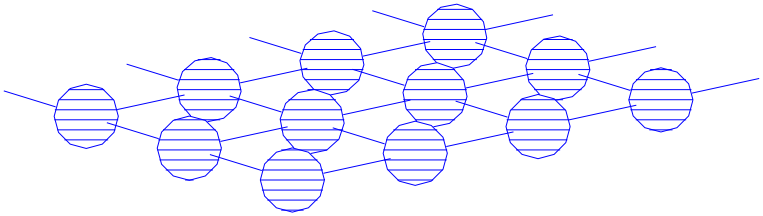
$$F_{CTR} = \sum_{n=0}^{\infty} A_n$$

$$= \sum_{n=0}^{\infty} f_L \; e^{inqa}$$

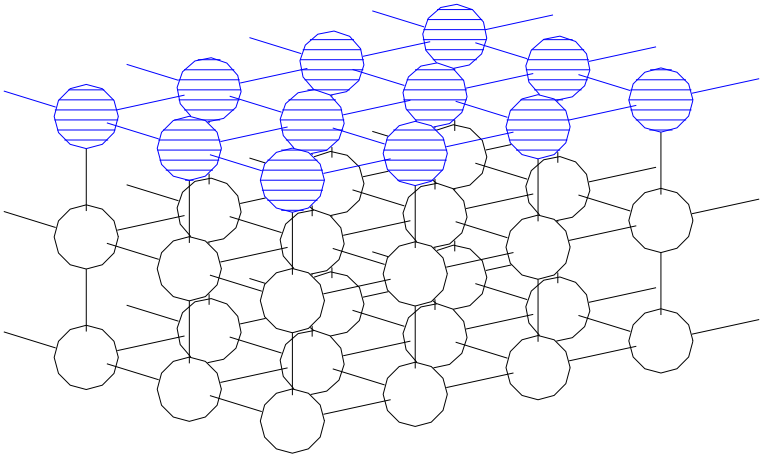
$$= \frac{f_L}{1 - e^{iqa}}$$



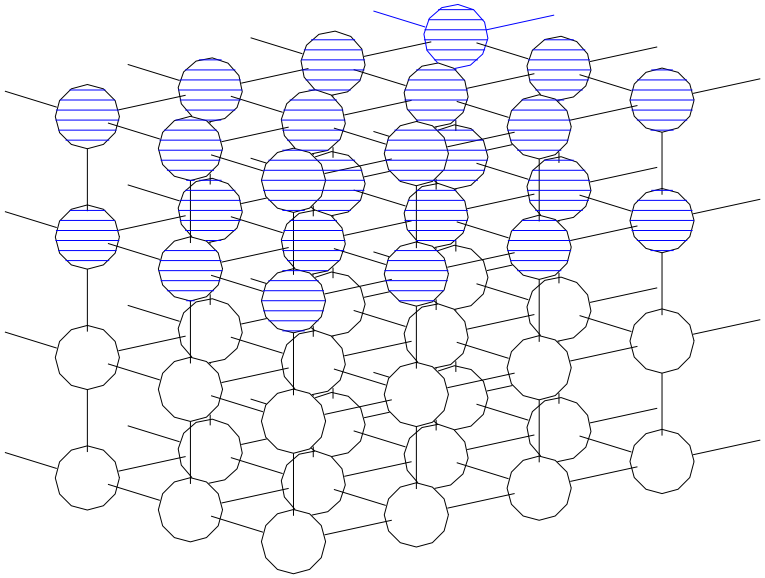
Surfaces and Interfaces



Isolated monolayer

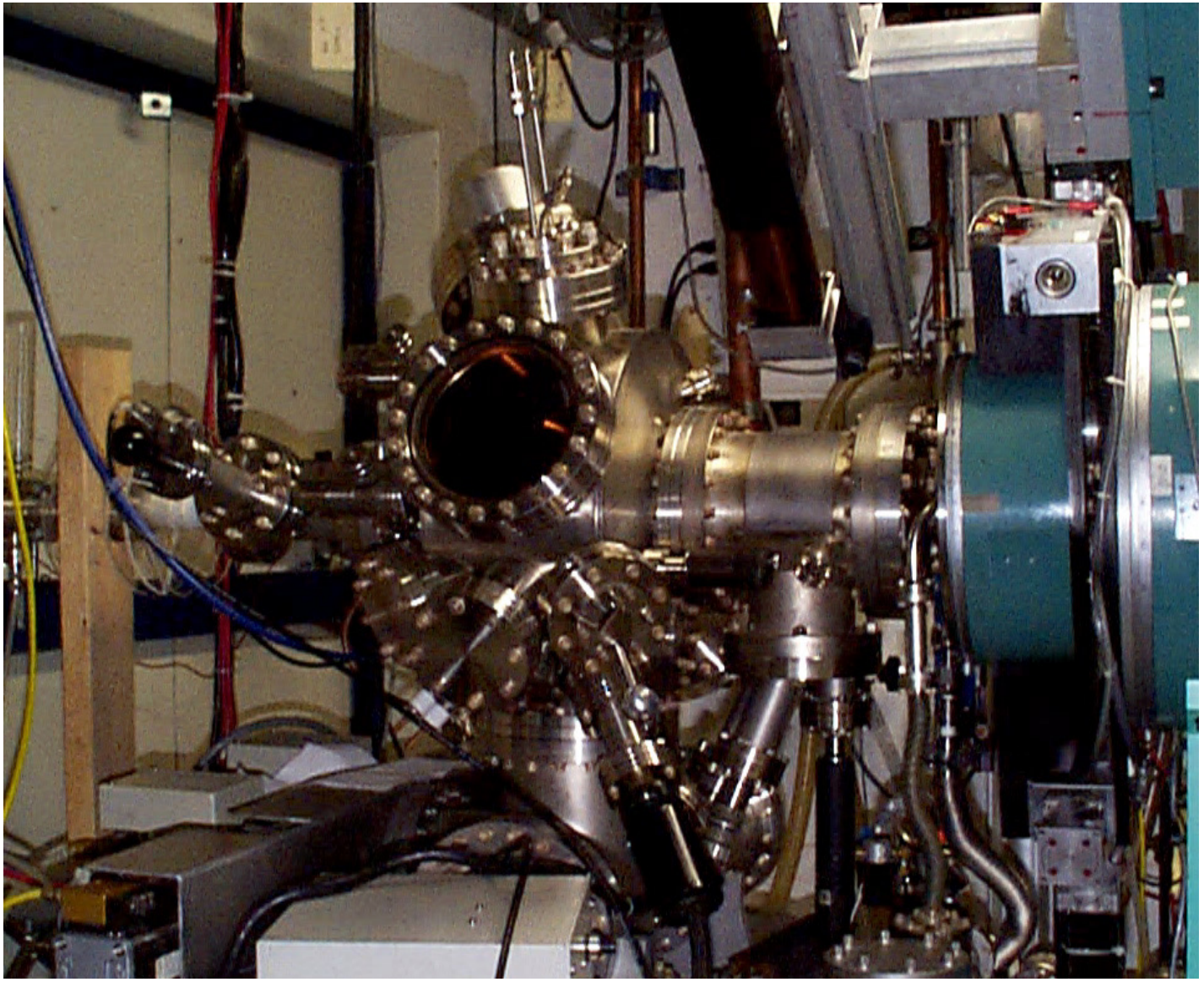


Surface of Crystal

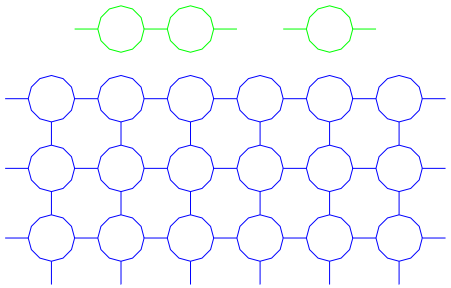


Crystal-Crystal Interface

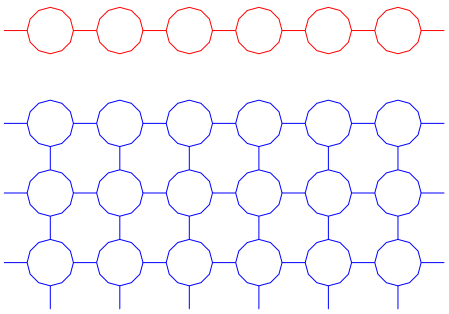
Surface X-ray Diffractometer



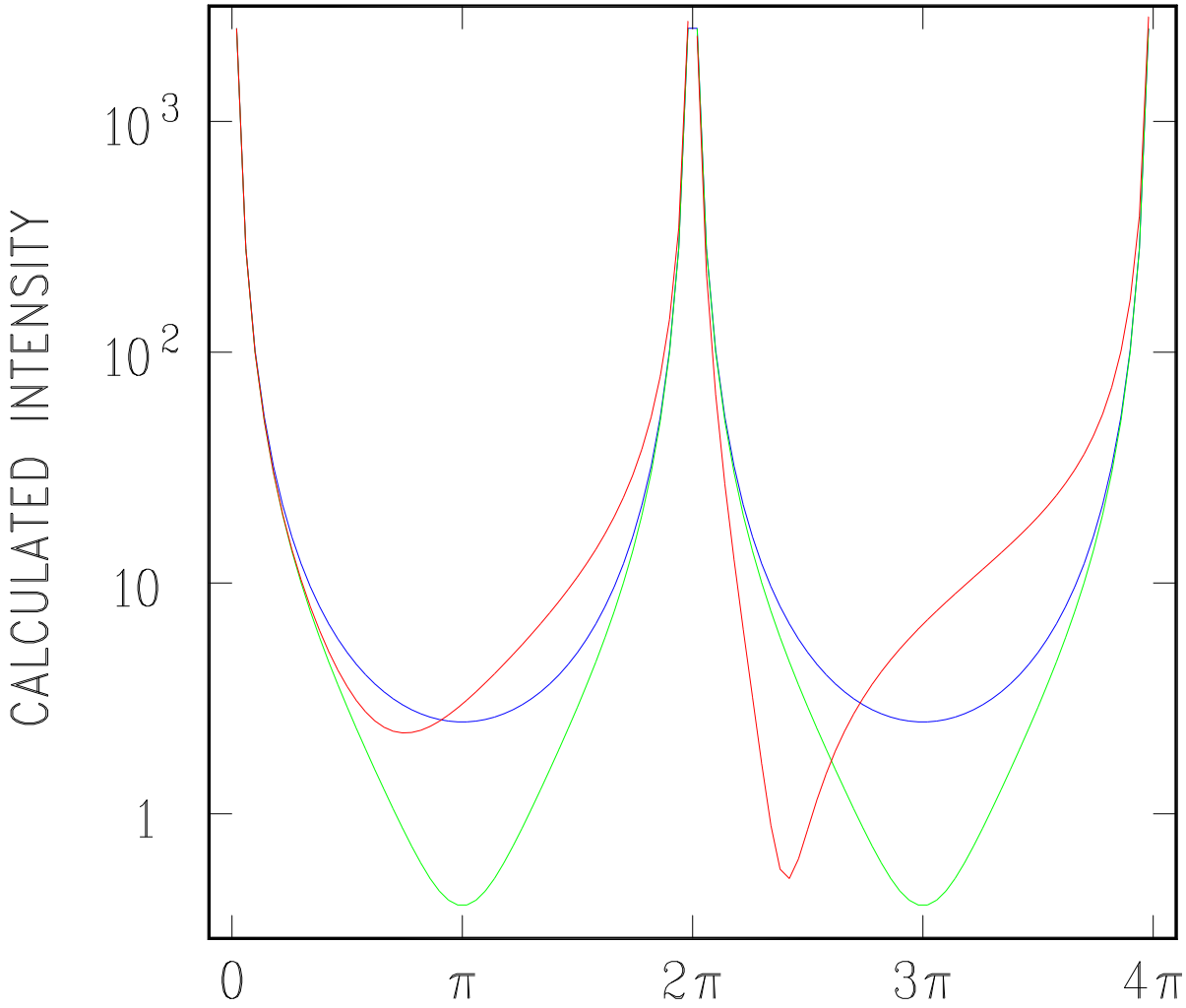
CTR and Surface Structure



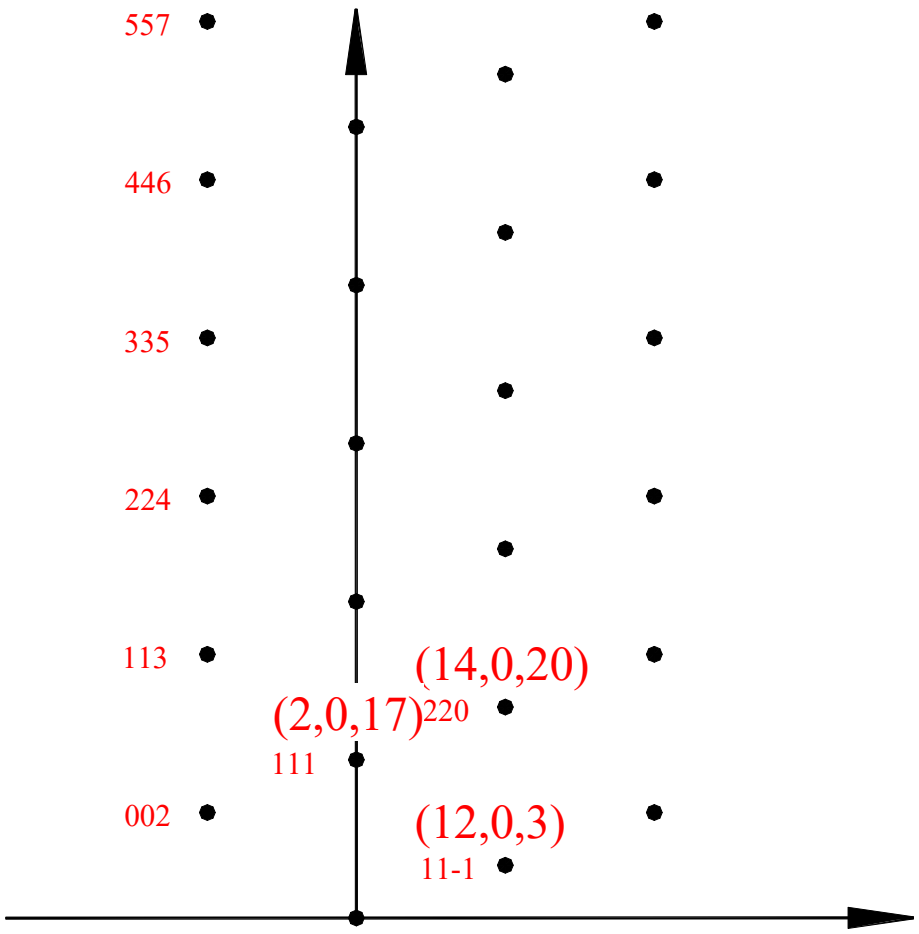
ROUGH SURFACE



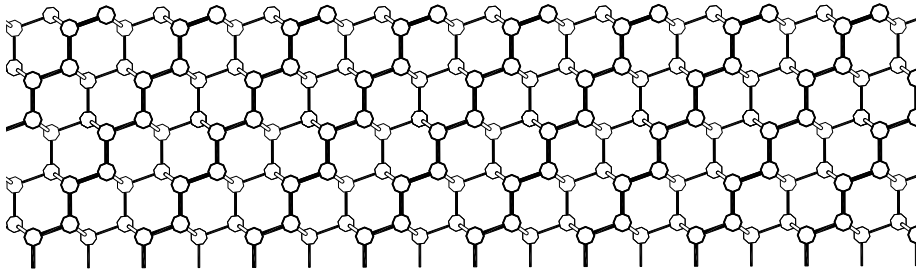
EXPANDED LAYER

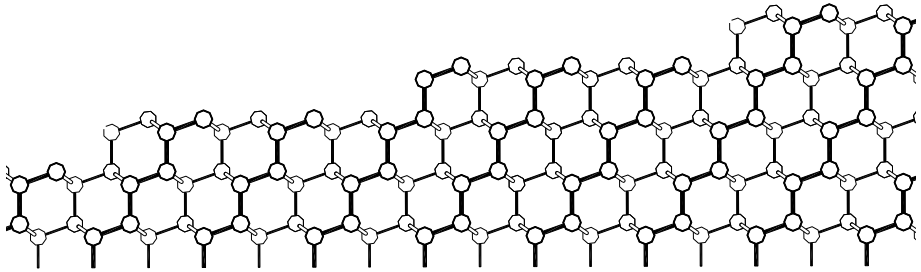


Crystallography of Steps



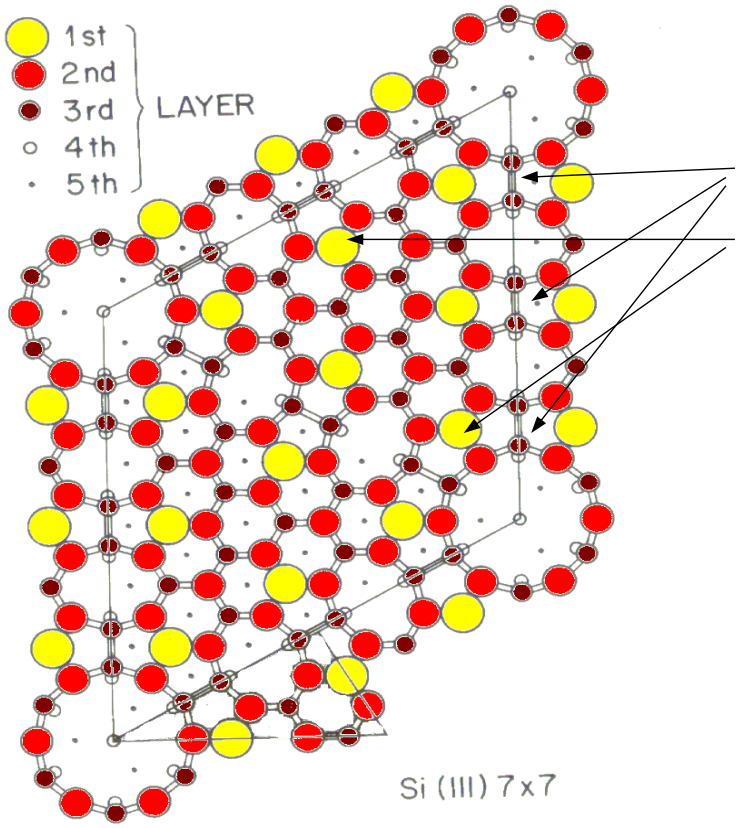
Silicon (111)



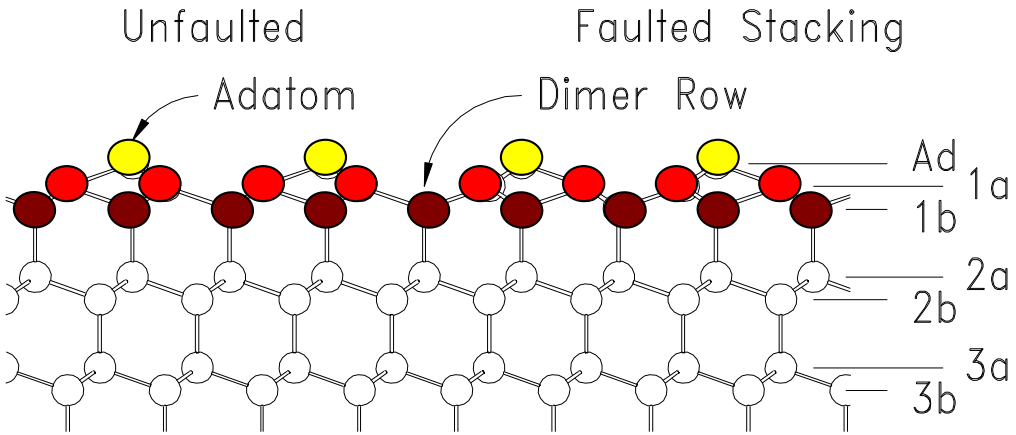


Si(557) surface

Si(111) 7x7

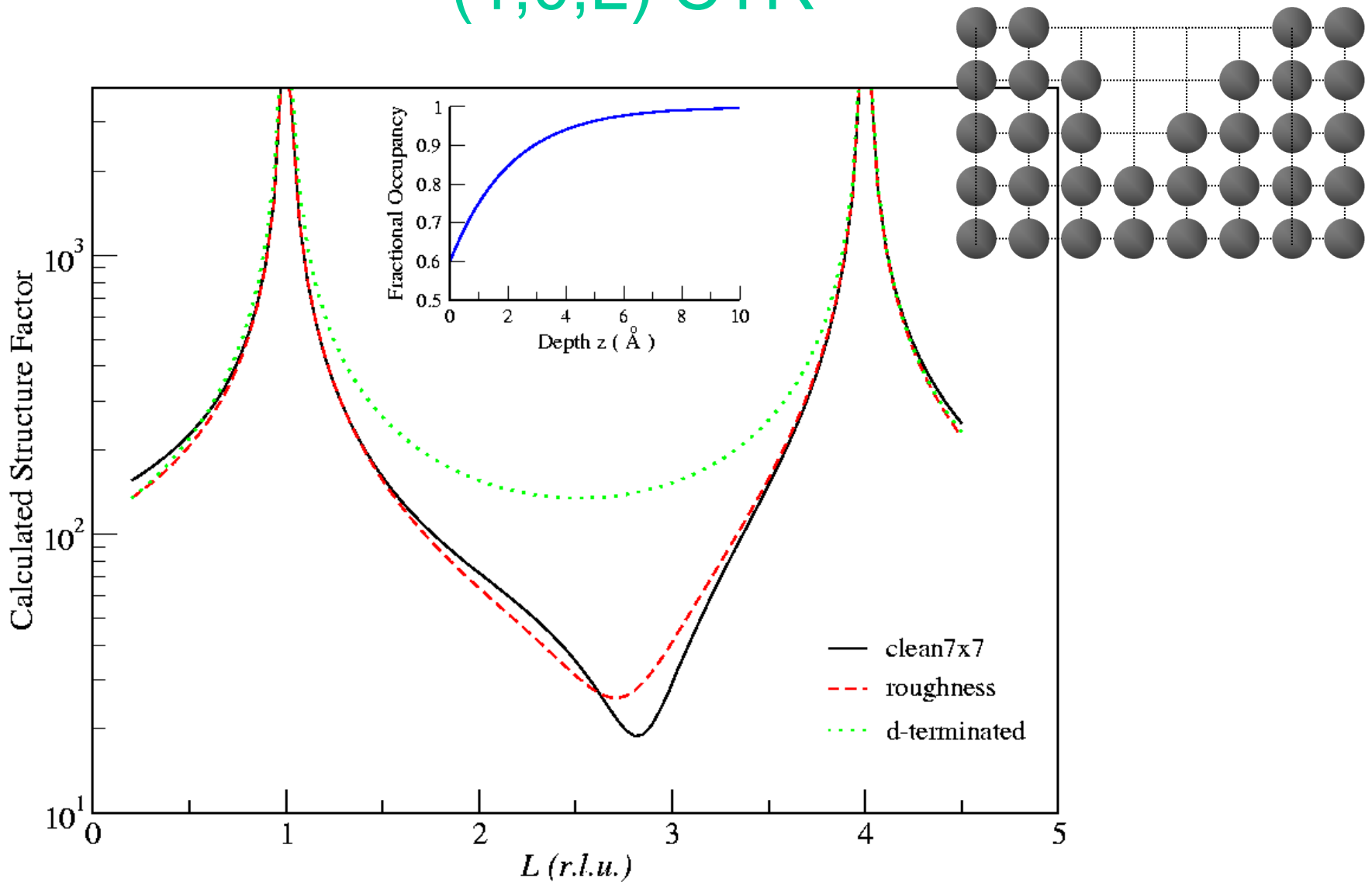


Dimers +
Adatoms +
Stacking Fault
= DAS model

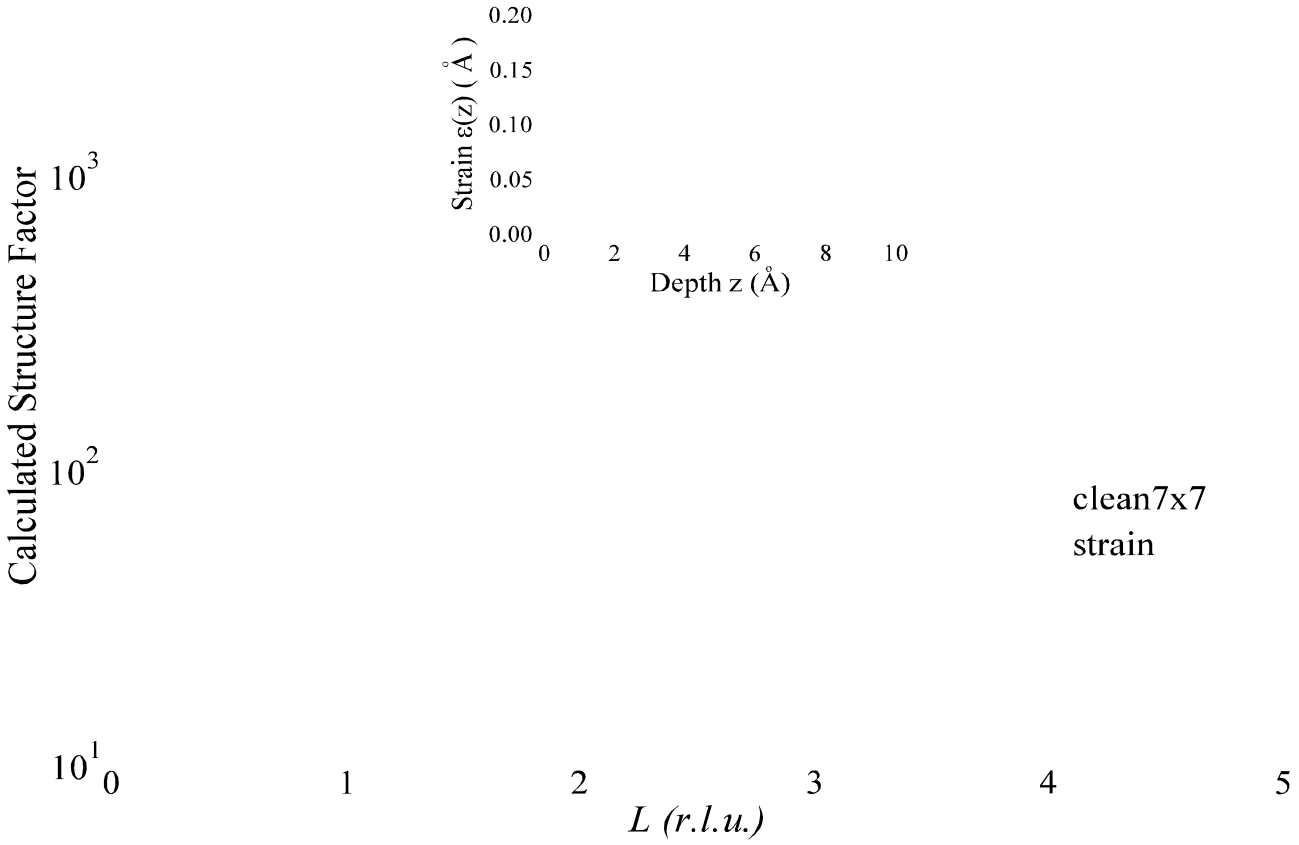


Effect of Roughness

(1,0,L) CTR

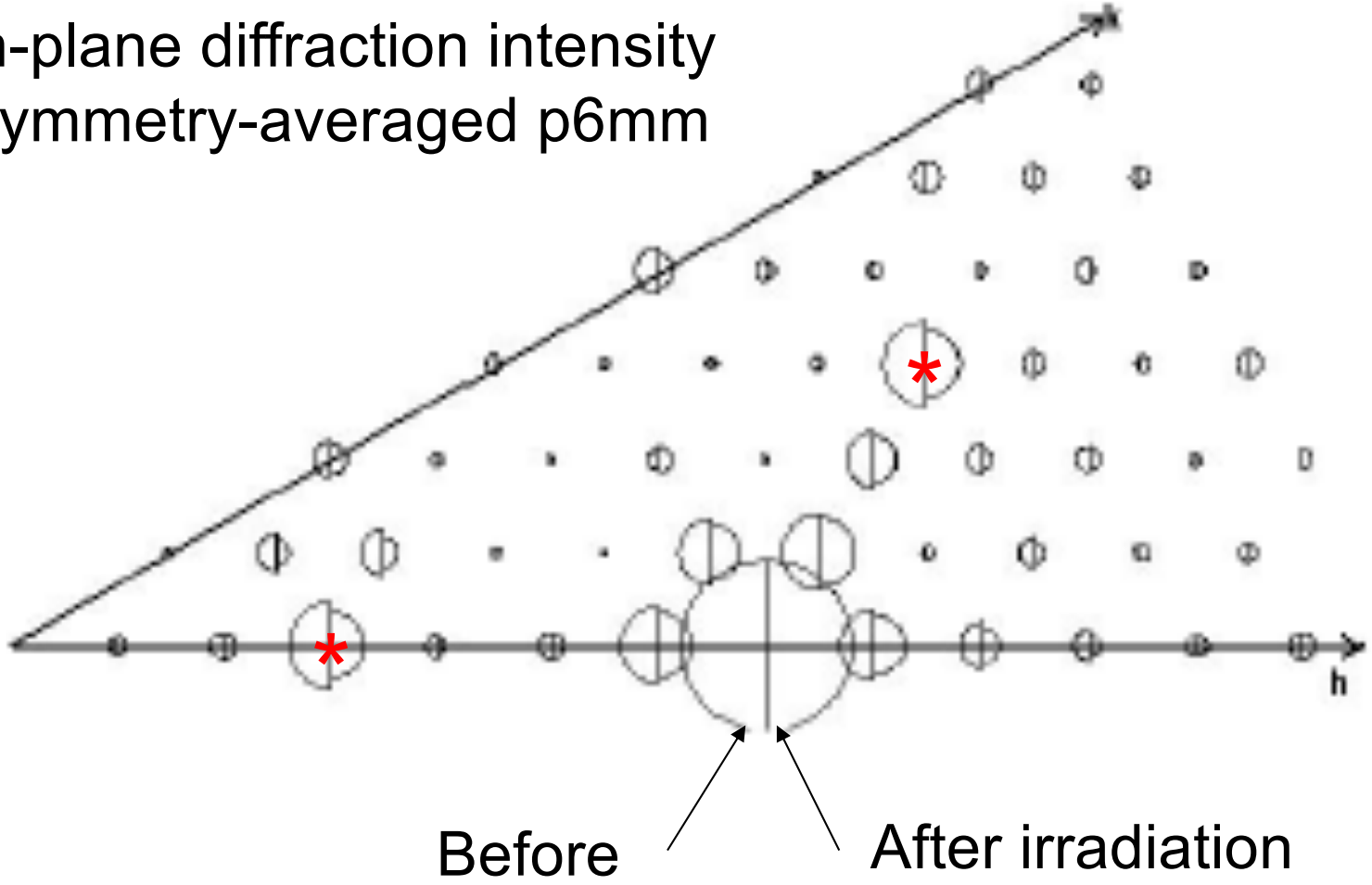


Surface Relaxation

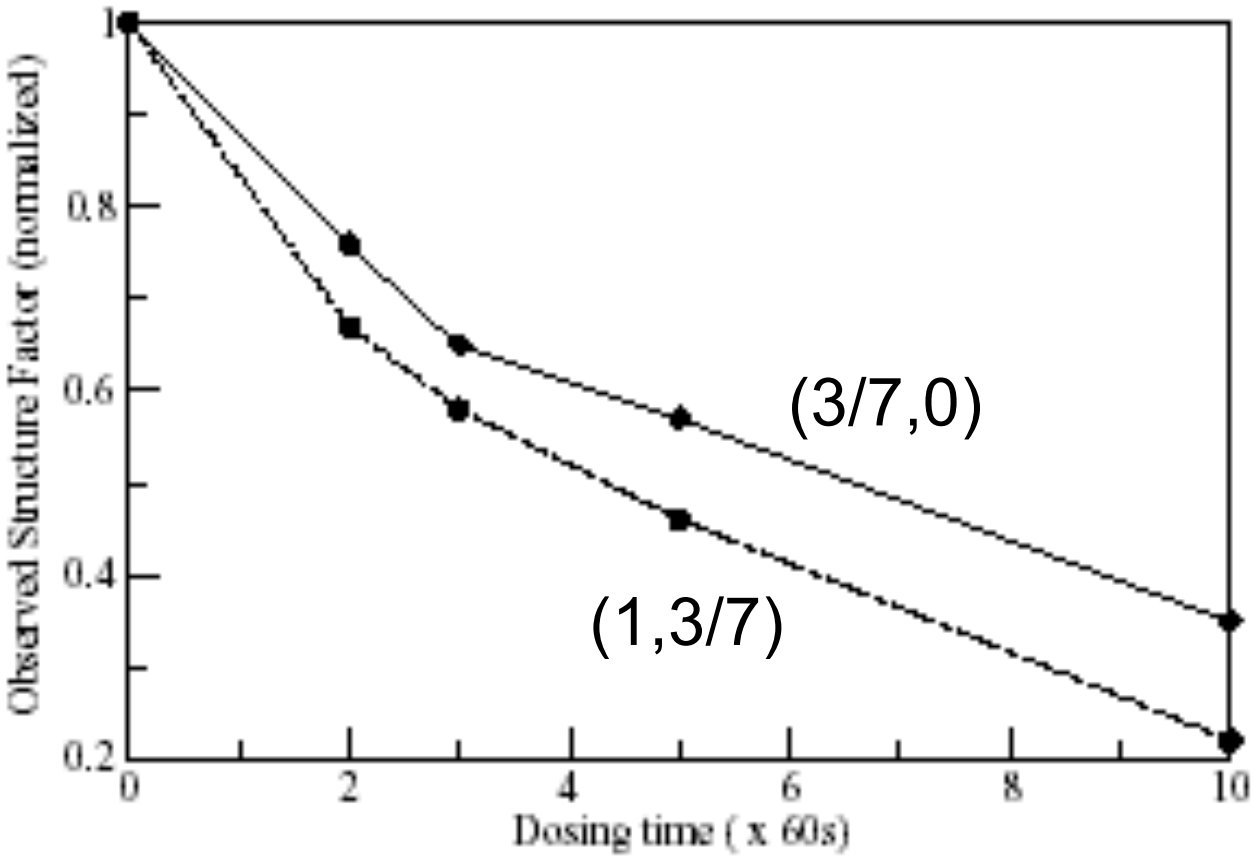


Low dose Irradiation (Ar^+)

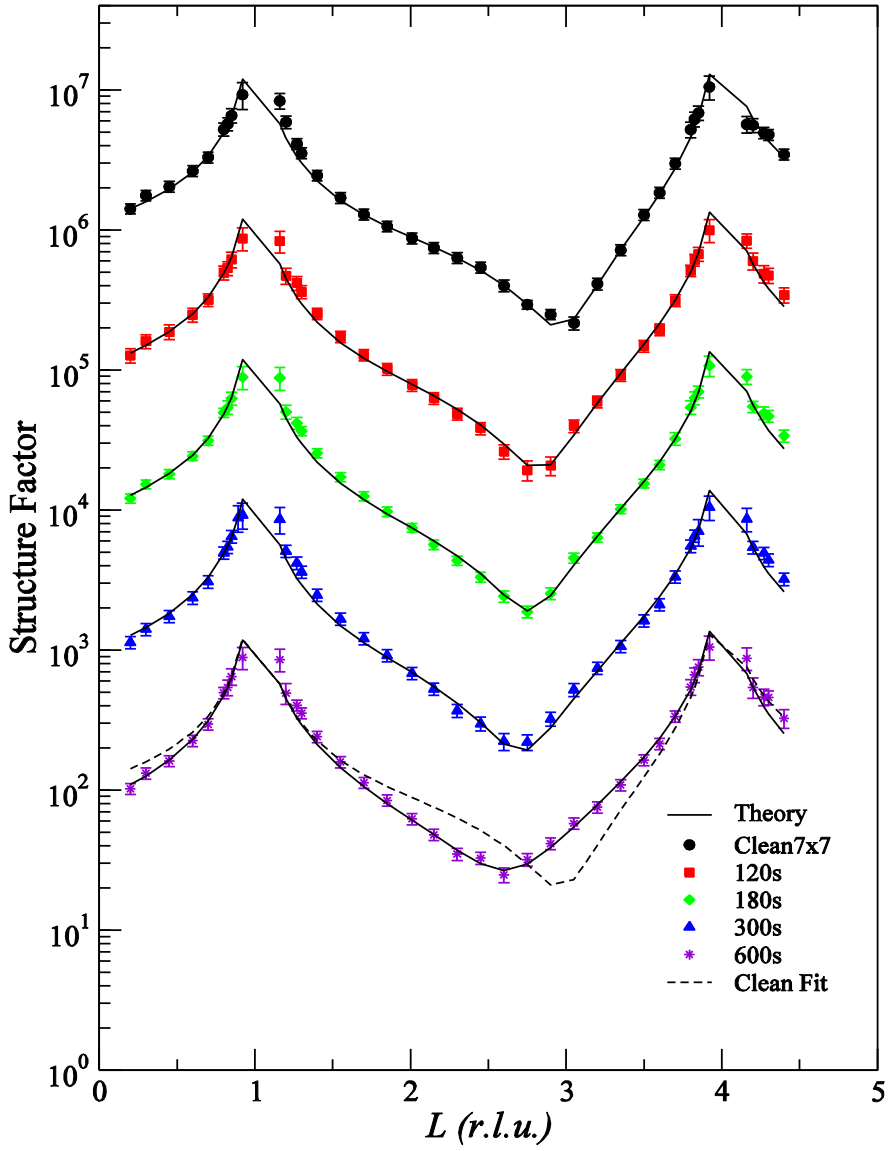
- 200eV Ar^+ irradiation
- In-plane diffraction intensity
- Symmetry-averaged p6mm



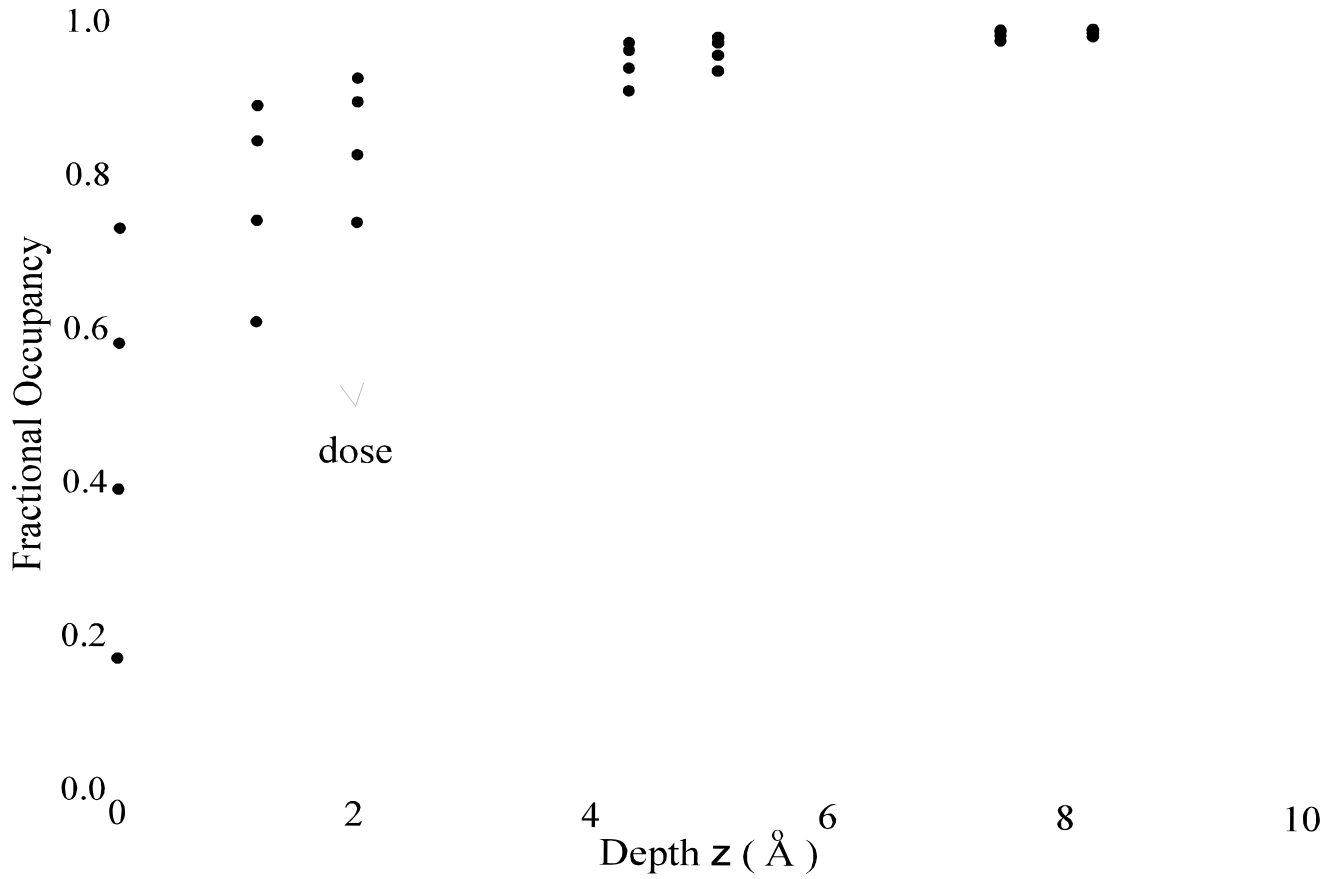
In-plane *vs* dosing time



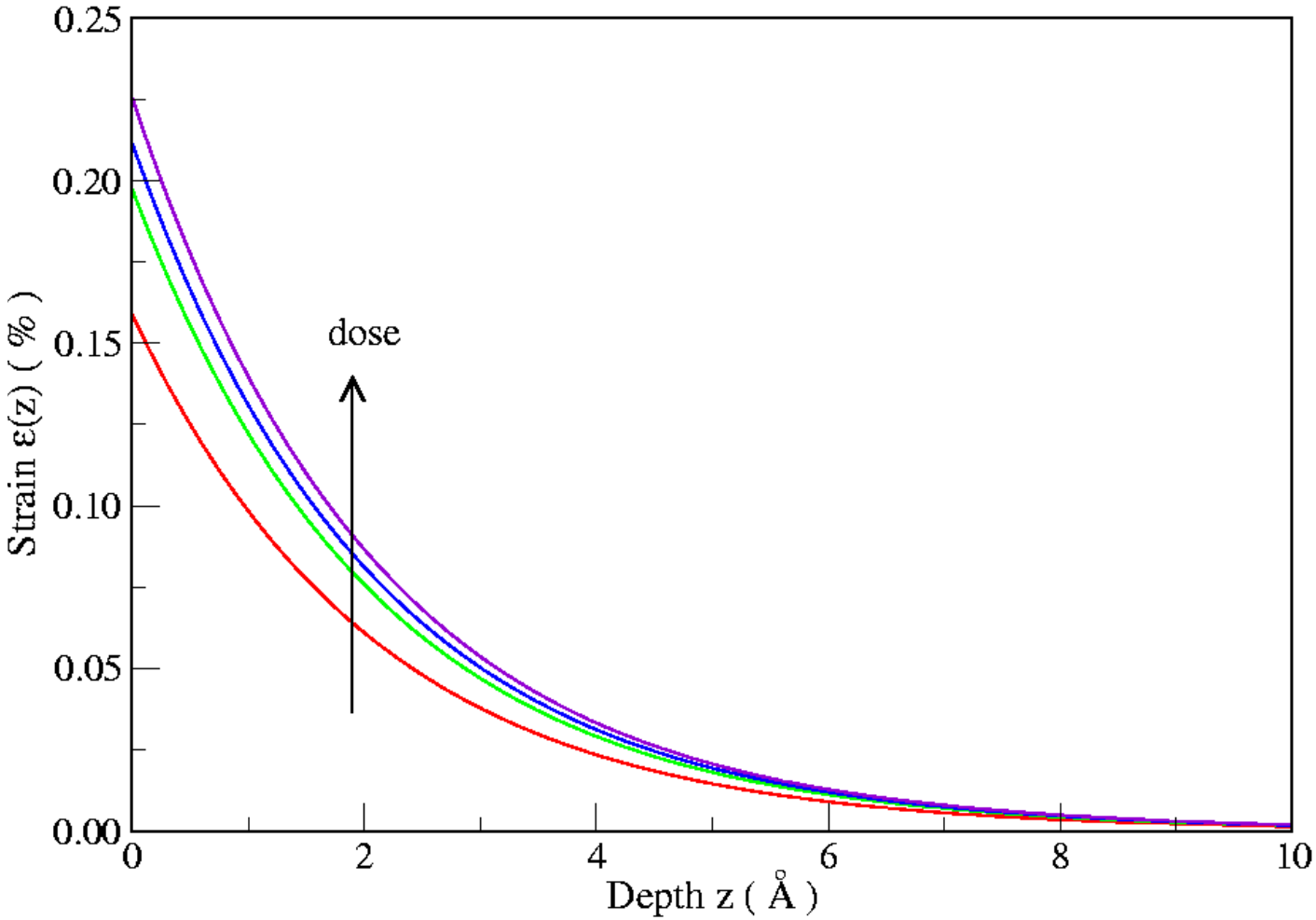
Measured CTR's *vs* dose



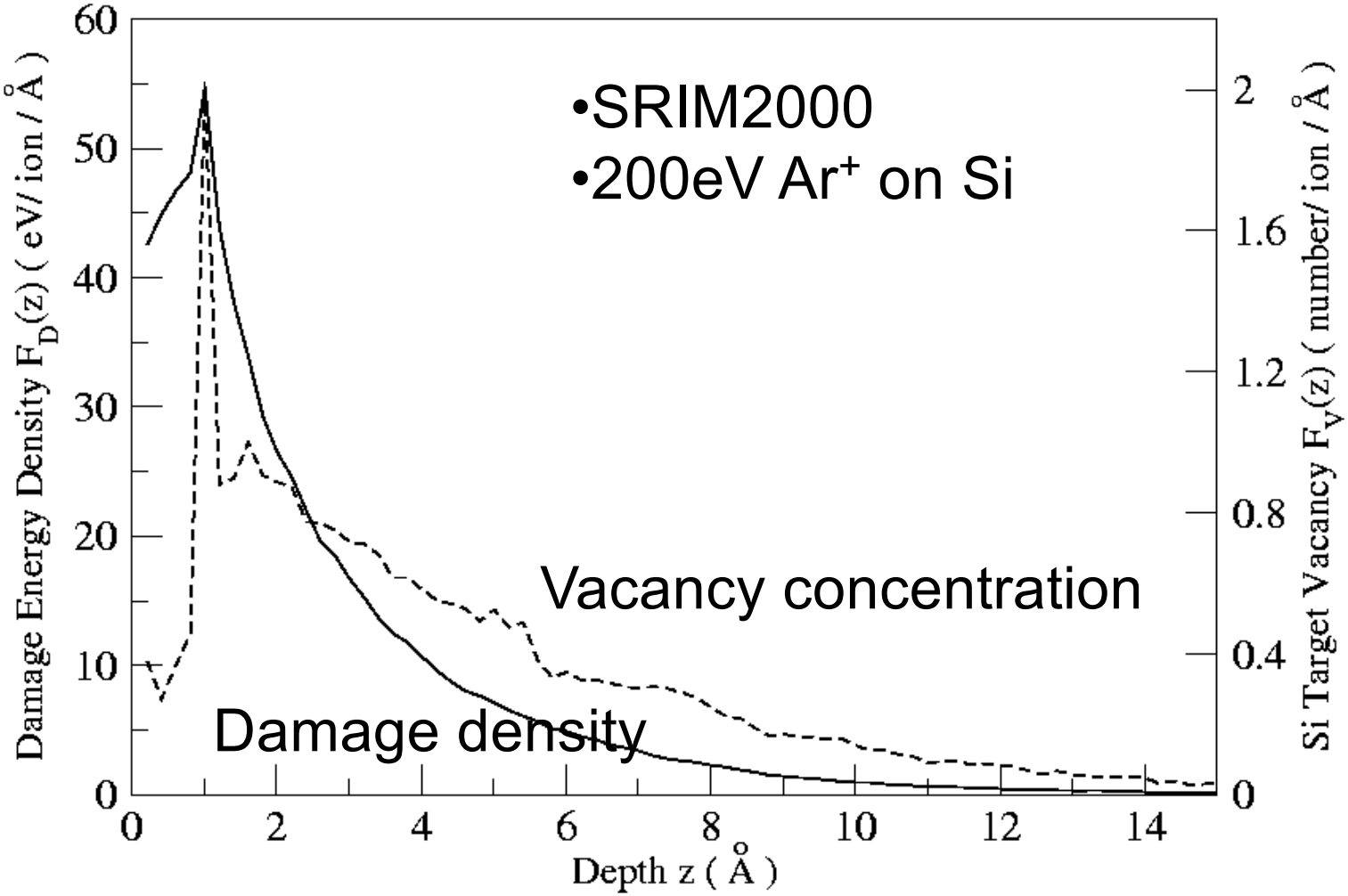
Occupancy Profiles



Strain Profiles



TRIM calculation

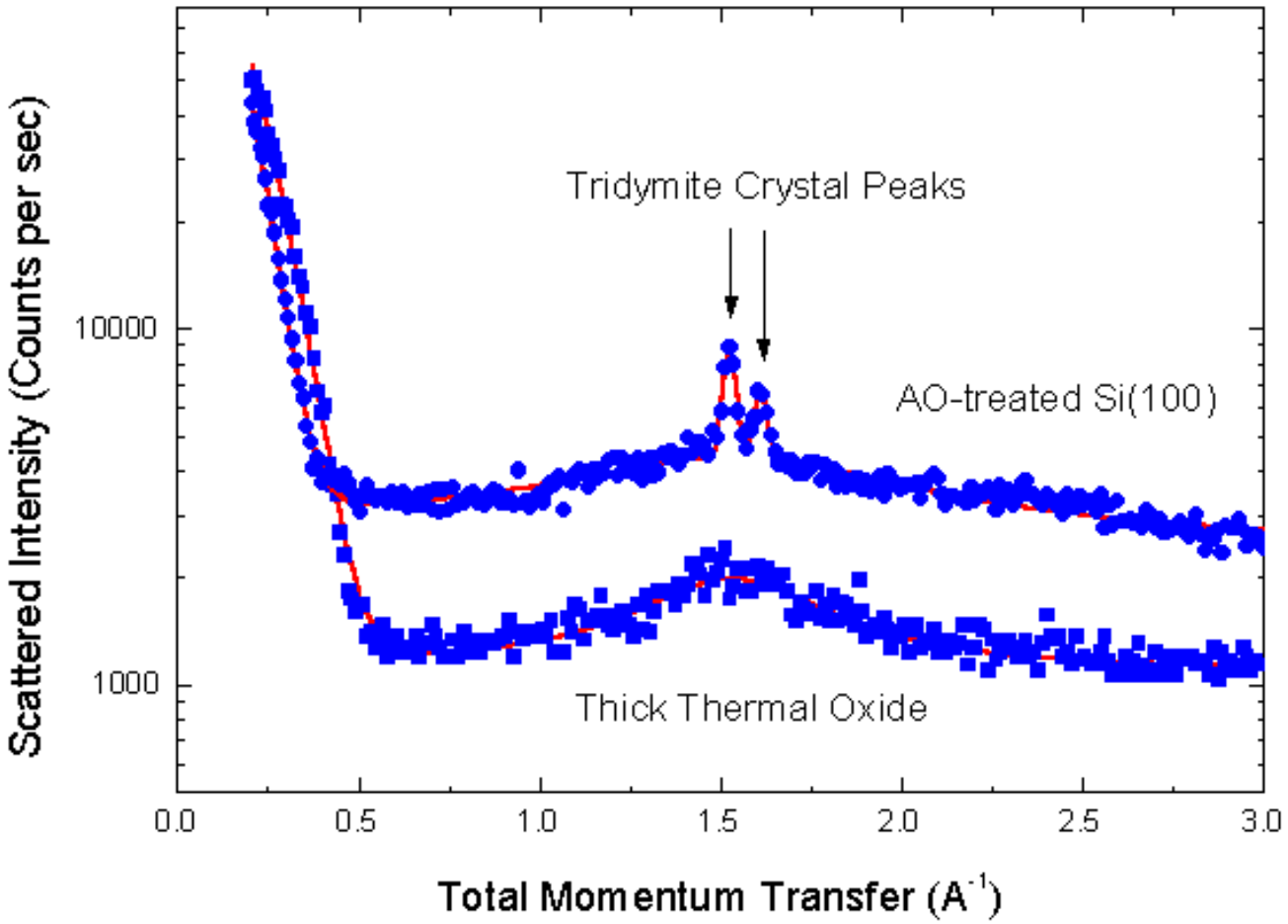


200 eV Ar^+ irradiation

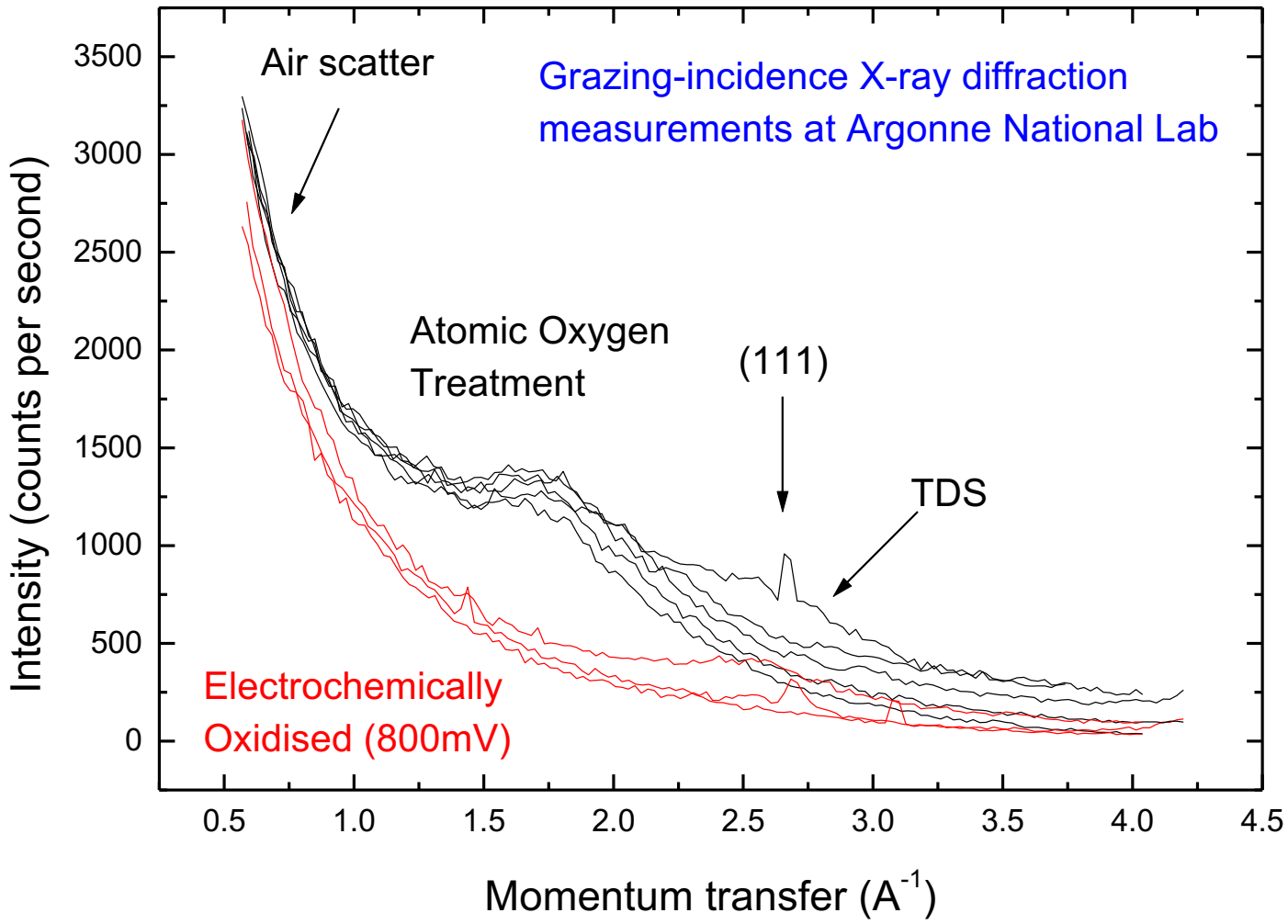
- Exponential occupation profile
- New model of roughness
- Accompanying strain profile
- Outwards relaxation of surface layers
- 3Å depth is consistent with TRIM

Grazing Incidence XRD

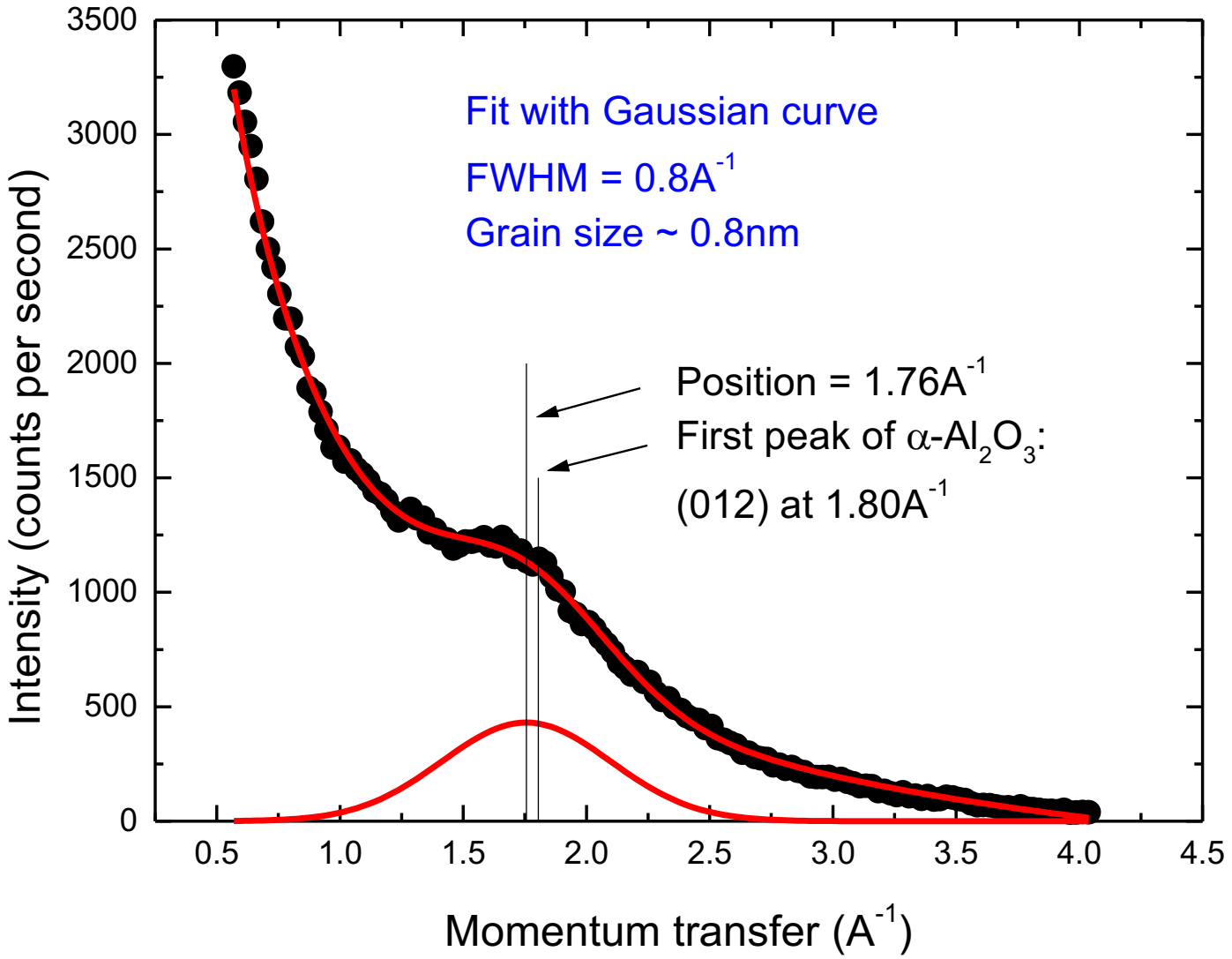
Atomic O oxidation by Tim Minton (Montana)
Consistent with Maja Kisa's TED result



Oxidation of Al(111) Crystals



Oxide Structural Properties



Future Goals

- Lower energy ions, closer to LEO
- He^+ different from Ar^+?
- Oxygen ECR (plasma) Source
- Ex-situ MURI samples by AO
- Passivation studies
- Real-time study of collision cascade