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Calculating and Mapping Unintentional Ion Channeling in Polycrystalline Materials*

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We propose here that it is important to include the effect of ion channeling when considering the equivalence of using ions accelerated to high energies to simulate the displacement damage produced by energetic neutrons

- Ions that channel will make less (maybe no) displacement damage.
- The primary knock-on atoms (PKAs) recoiled by neutrons are omnidirectional in the forward direction and of such low energies that they are unlikely to channel
- The monodirectional high energy ions implanted as PKAs will certainly channel if individual crystallites in the material are oriented with their crystallographic axes or planes aligned with the direction of the beam.
- This presentation will ameliorate this uncertainty in ion-neutron equivalence by combining:
  - theoretical calculations of axial and planar channeling ½ angles and dechanneling fractions
  - with orientation distribution measurements of polycrystalline samples performed on the TEM
- We will show how this approach quantitatively determines the probability that accelerated ions will channel in:
  - randomly oriented and
  - textured polycrystalline materials
  - and even map the position on the sample where such ion channeling occurs

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Ion channeling is usually thought of as a type of IBA where the Rutherford Backscattering of single crystal samples is measured as a function of tilt angle.

70 B. R. Appleton and G. Foti

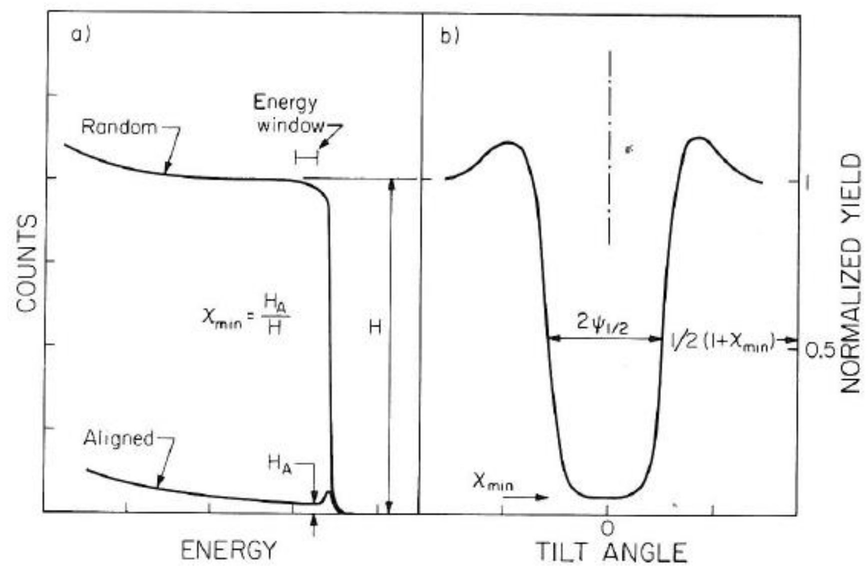

Figure 3.1 Backscattering spectra and angular yield profile.

...but this data also demonstrates that the small impact parameter collisions required for RBS, and the subsequent recoiling of target atoms, is significantly reduced for the channeling condition.

This is the premise of this paper.

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Outline

- Parameterizing the physics of ion channeling
- Representing axial and planar ion channeling as "equal angle projections"
- Calculating channeling probabilities for randomly oriented polycrystalline materials
- Including the effects of texture
  - crystallite orientation measurements
  - incorporating this data with equal angle projections
    - calculating channeling probability
    - mapping where ion channeling will occur
- Experiments

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Parameterizing Channeling

- A paper was written last year that detailed the calculation of RBS axial and planar channeling ½ angles and minimum yields for all ions at all energies on all bcc, fcc and diamond lattice crystals.
- This paper parameterized all of the charts generated by John Barrett (Phys. Rev. B3 (1973) 1782) used to improve the famous channeling theory of Jens Lindhard, Mat.-Fys. Medd, 34 (1965) 1.)

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Parameterization of ion channeling half-angles and minimum yields ☆

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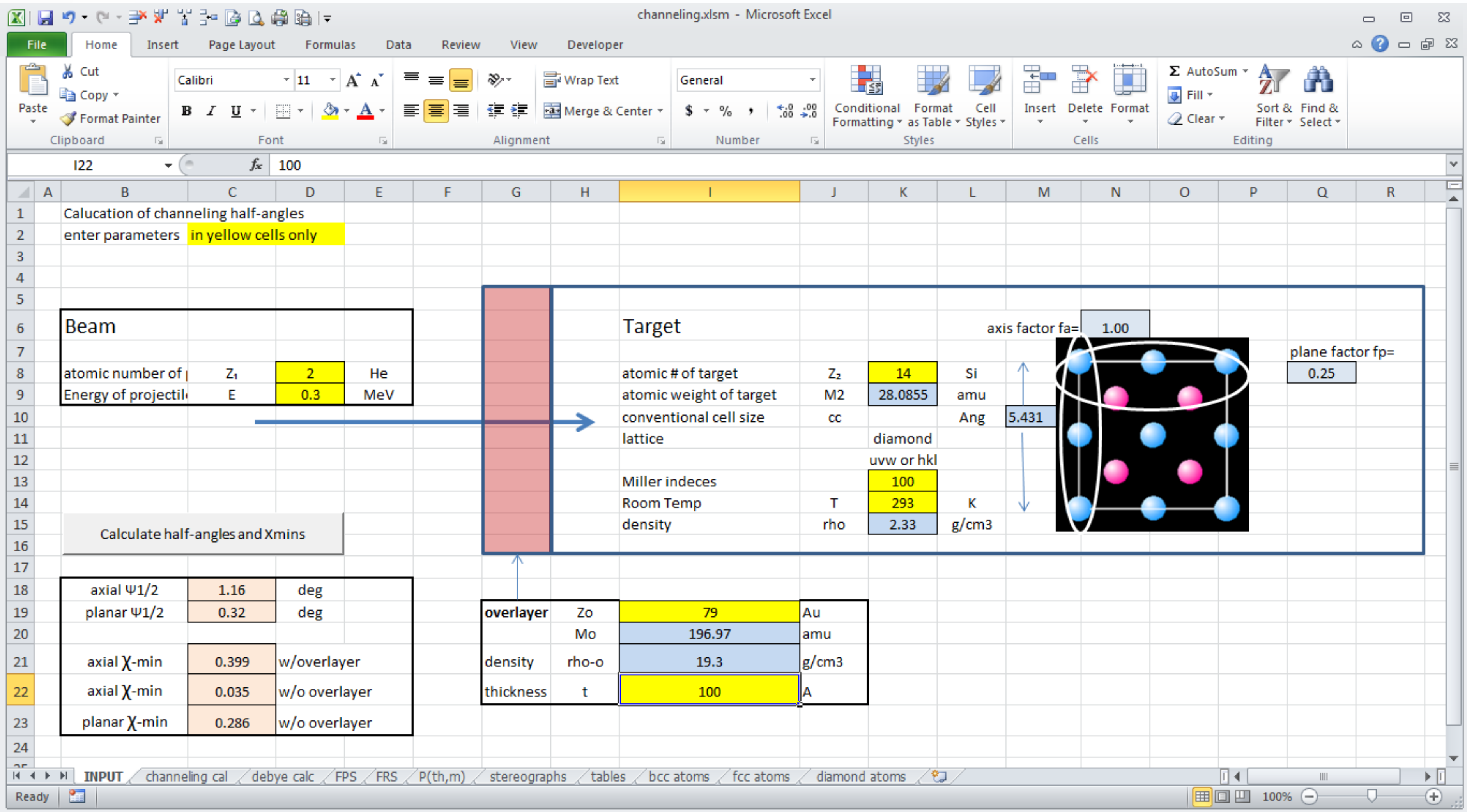
ABSTRACT

A MS Excel program has been written that calculates ion channeling half-angles and minimum yields in cubic bcc, fcc and diamond lattice crystals. All of the tables and graphs in the three Ion Beam Analysis Handbooks that previously had to be manually looked up and read from were programed into Excel in handy lookup tables, or parameterized, for the case of the graphs, using rather simple exponential functions with different power functions of the arguments. The program then offers an extremely convenient way to calculate axial and planar half-angles, minimum yields, effects on half-angles and minimum yields of amorphous overlayers. The program can calculate these half-angles and minimum yields for ⟨*uvw*⟩ axes and [*hkl*] planes up to (555). The program is open source and available at http://www.sandia.gov/pcnsc/departments/iba/ibatable.html.

- The paper above describes an Excel program that makes this calculation of channeling parameters quite easy. The program can be found at:

  http://www.sandia.gov/pcnsc/departments/iba/ibatable.html

channeling.xlsm program



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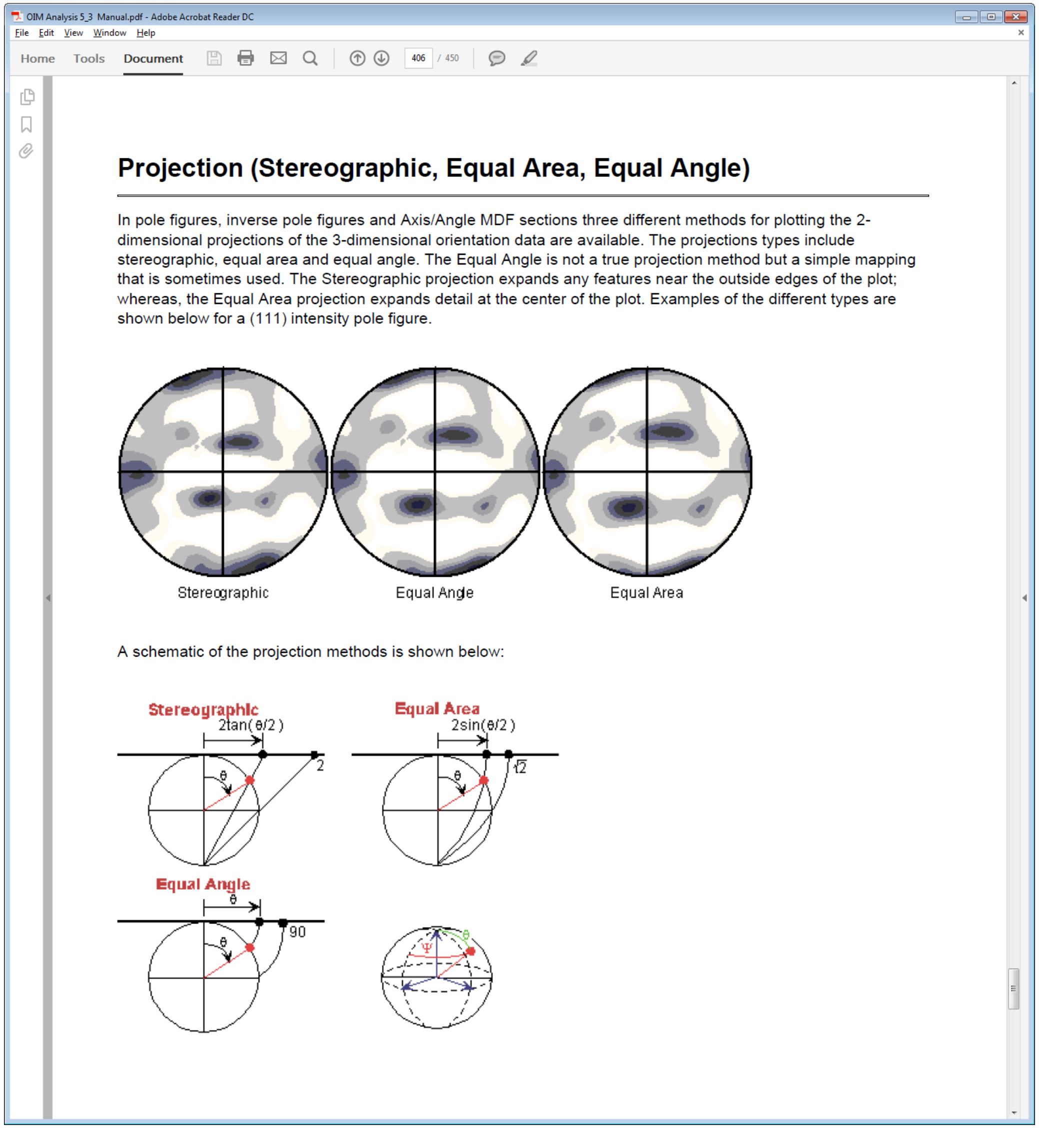
Equal Angle Projections are commonly used for displaying texture, but here we show how projecting plots of axial and planar channeling is also benefitted by this type of projection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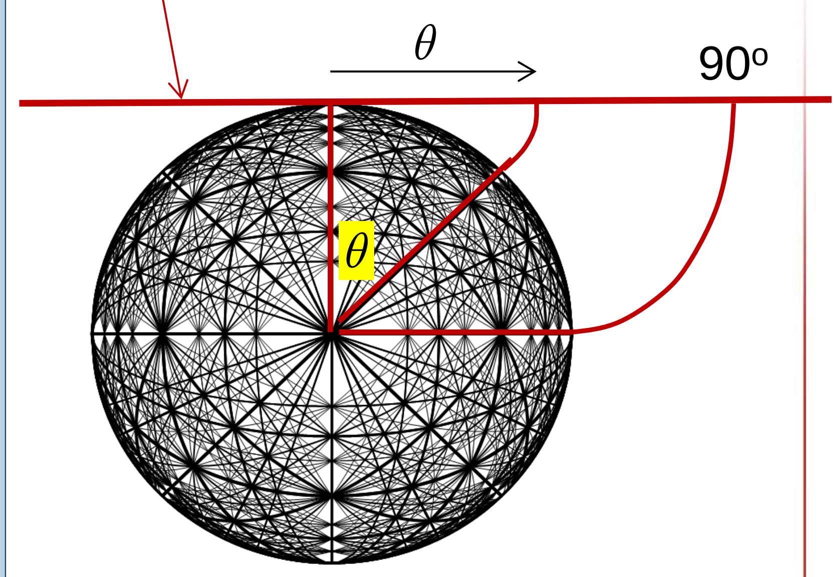
Projection (Stereographic, Equal Area, Equal Angle)

In pole figures, inverse pole figures and Axis/Angle MDF sections three different methods for plotting the 2-dimensional projections of the 3-dimensional orientation data are available. The projections types include stereographic, equal area and equal angle. The Equal Angle is not a true projection method but a simple mapping that is sometimes used. The Stereographic projection expands any features near the outside edges of the plot; whereas, the Equal Area projection expands detail at the center of the plot. Examples of the different types are shown below for a (111) intensity pole figure.

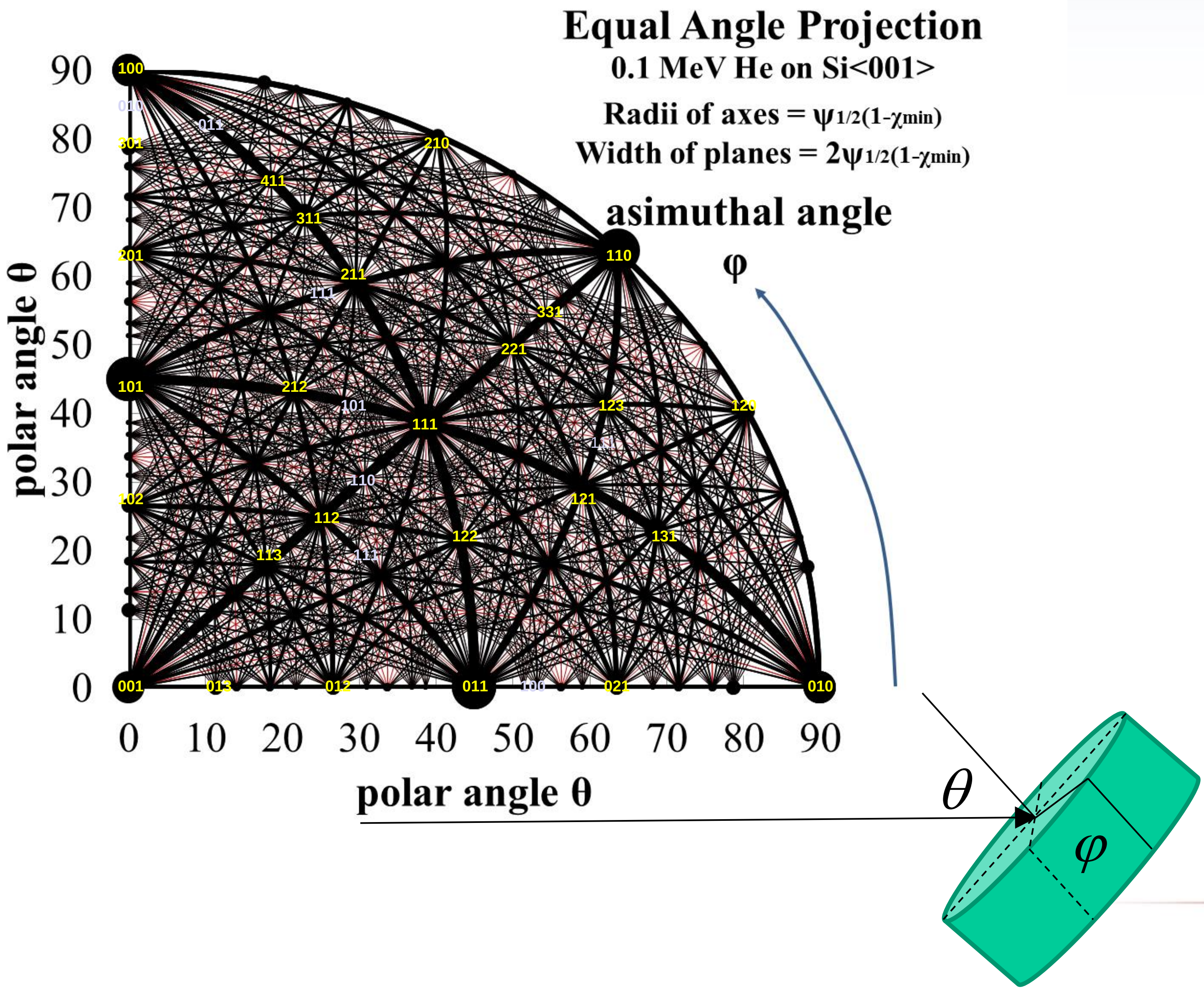
Stereographic Equal Angle Equal Area

A schematic of the projection methods is shown below:

By projecting channeling onto this plane this way, axes can be plotted as circles with a radius of $\Psi^{a}_{1/2}$, and planes as lines of constant width $2\Psi^{p}_{1/2}$.



Geometry used to represent ion channeling



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1.7 MeV Au on Au channeling half angles

axial channeling		1/2 angles	
e^2		1.44E-05	MeV-A
atomic number of projectile	Z_1	79	Au
atomic # of target	Z_2	79	Au
atomic weight of target	M2	196.9665	amu
Energy of projectile	E	1.7	MeV
conventional cell size	cc	4.078	Ang
lattice		fcc	
lattice type		1	u
Miller indeces		111	1
axis lattice factor	fa	1.73	loo
lattice spacing	d	7.06330319	Ang
Following the EQUATIONSL FOR CHANNELING in the IBA Handbook, p645			
		0.4685*C6^-(1/3)	
thomas fermi screening length	a	0.10918607	Ang
Debye Temp	theat-D	170	K
Room Temp	T	293	K
x"=Theta-D/T	x"	0.58020478	
debye fn	phi-D	0.8737759	
rms thermal amplitude	u1	0.08762425	Ang
characteristic axial channeling angle	Ψ_1	6.99901754	deg
		0.1221469	rad
ratio of a to d	a/d	0.01096125	
parameter to use in Frs	x'	1.35811809	
adimentional axial channeling Fn	Frs	0.71301132	
channeling 1/2 angle for Ψ_1<a/d	Ψ1/2	4.34162952	deg
channeling 1/2 angle for Ψ_1>a/d	Ψ1/2	2.09673967	deg
channeling 1/2 angle to use	Ψ1/2	2.10	deg

planar channeling			
atomic number of projectile	Z_1	79	
atomic # of target	Z_2	79	
atomic weight of target	M2	196.9665	
Energy of projectile	E	1.7	MeV
conventional cell size	cc	4.078	Ang
lattice		fcc	
lattice type		1	h
Miller indeces		11	0
plane lattice factor	f' or fp	0.35355339	
avg atomic spacing between planes	dp	1.44179073	Ang
density	rho	19.3	g/cm3
Avagodros number	Nav	6.02E+23	at/mole
target atoms/cm3	N	5.9017E+22	atoms/cm3
		0.05901709	atoms/A3
characteristic planer channeling angle	Ψa	2.68E+00	deg
Fps parameters			
	x'	1.81082411	
	y'	18.6223376	
adimentional planar channeling function	Fps	0.82413568	
Planar channeling 1/2 angle	Ψ1/2	1.44	deg

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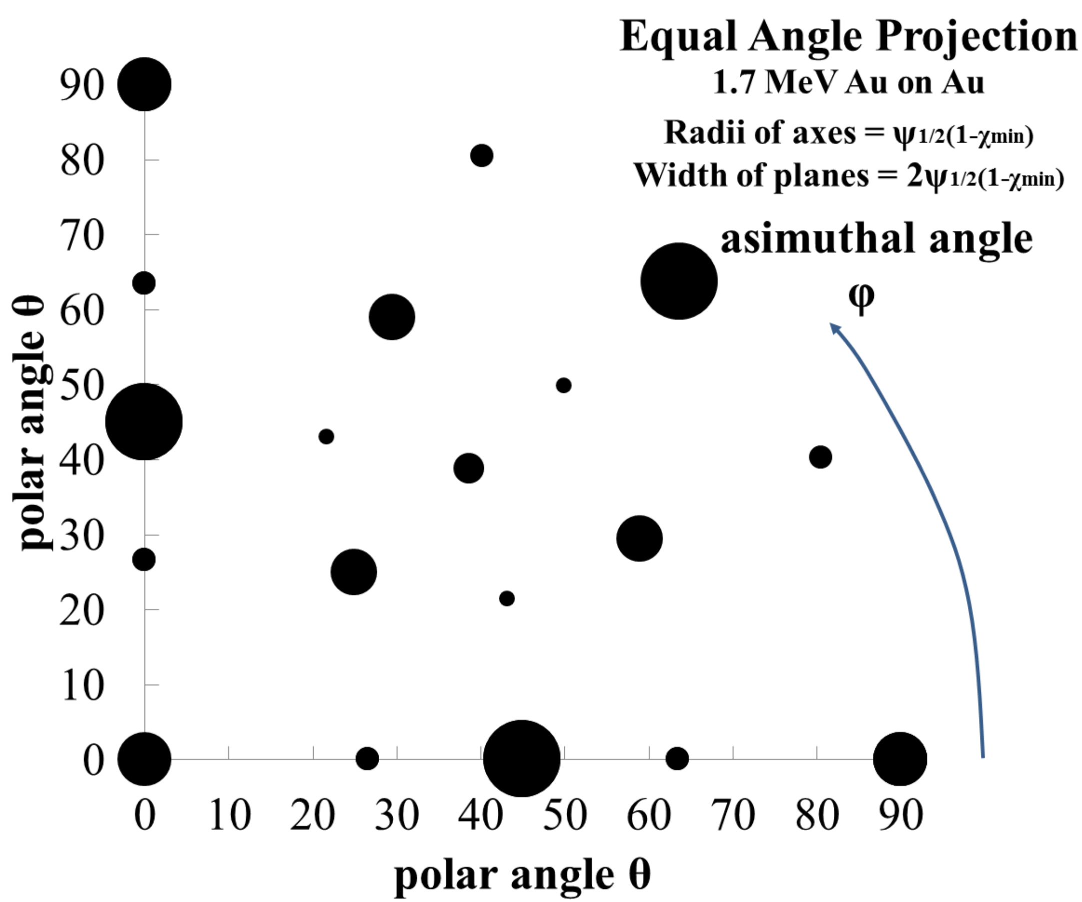
Equal Angle Projection - axes

To plot solid circles at position (x,y) to represent an (h,k,l) channeling axes:

1. $radius = \Psi_{1/2}^{a-hkl}(1-\chi_{\min})$
2. $\theta = \cos^{-1}(l/(h^2+k^2+l^2)^{1/2})$
3. $\varphi = \tan^{-1}(k/l)$
4. $x = \theta\cos(\varphi)$
5. $y = \theta\sin(\varphi)$



equal angle projection of planes

first parameterize circle representing plane

for standard Miller indices h, k, l

The normal to this plane is defined by:

$$n_z = l/(h^2+k^2+l^2)^{1/2}, n_y = k/(h^2+k^2+l^2)^{1/2}, n_x = h/(h^2+k^2+l^2)^{1/2}$$

or

$$\hat{n} = \begin{pmatrix} \cos(\varphi_n)\sin(\theta_n) \\ \sin(\theta_n)\sin(\varphi_n) \\ \cos(\theta_n) \end{pmatrix}$$

$$\theta_n = \cos^{-1}(n_z)$$

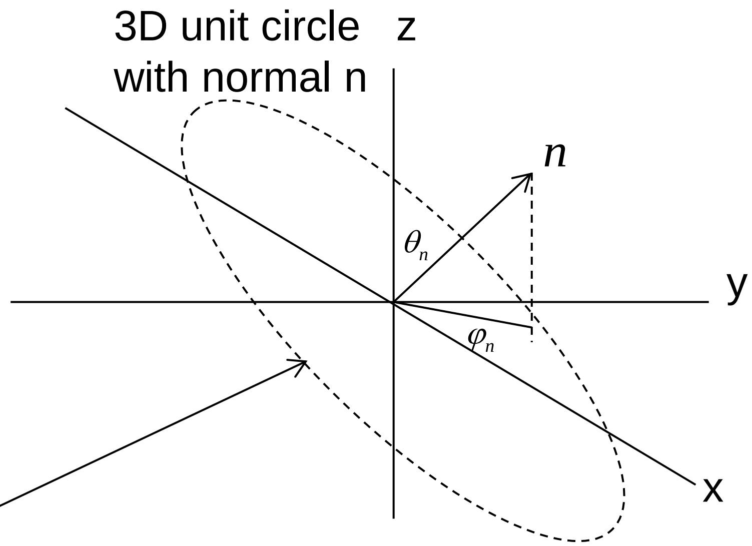
$$\varphi_n = \tan^{-1}(k/l)$$

The vector û is defined as:

$$\hat{u} = \begin{pmatrix} -\sin(\varphi_n) \\ \cos(\varphi_n) \\ 0 \end{pmatrix} \text{ and then } \hat{n} \times \hat{u} = \begin{pmatrix} \cos(\theta_n)\cos(\varphi_n) \\ \cos(\theta_n)\sin(\varphi_n) \\ -\sin(\theta_n) \end{pmatrix}$$

The parametric form of a 3D unit circle with normal $\hat{n}$ is:

$$\vec{P}(t) = \cos(t)\hat{u} + \sin(t)\hat{n} \times \hat{u}$$



equal angle projection of planes

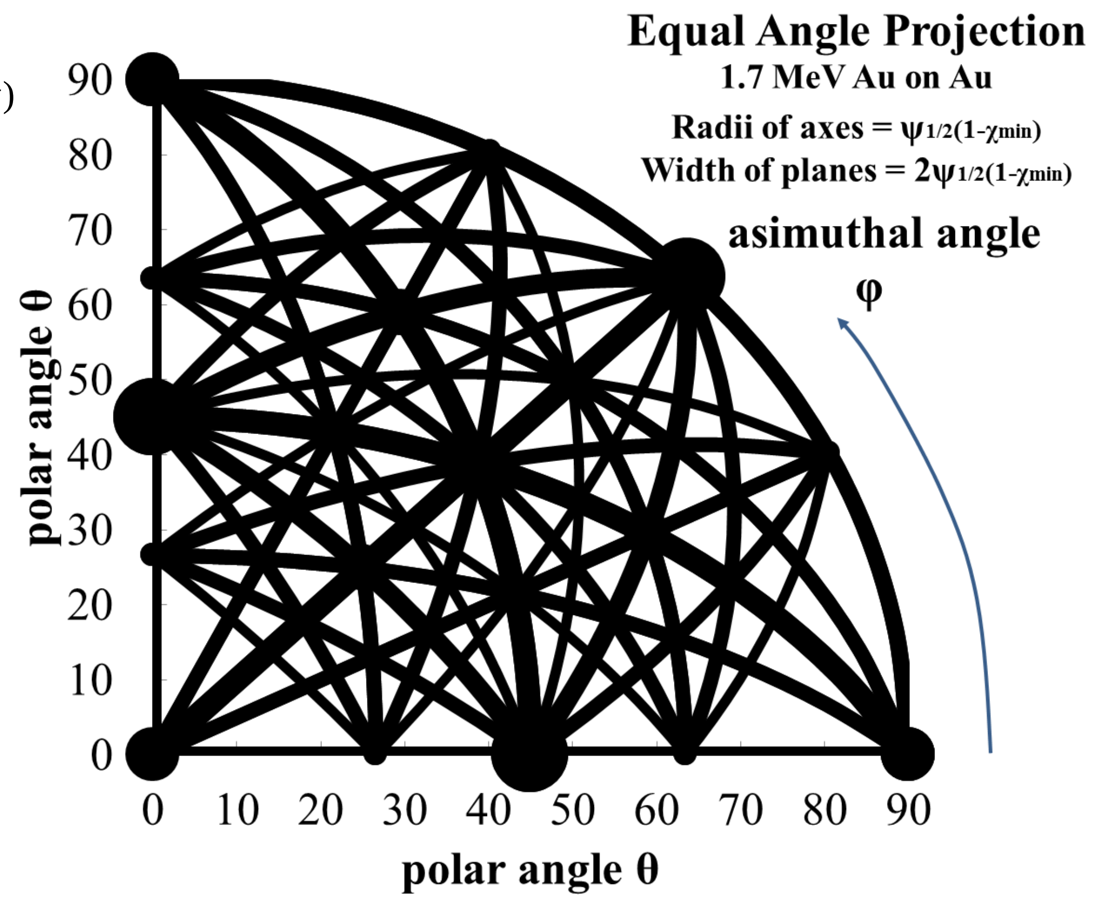
Then project this circle using equal angle projection

for a set of t values {t} calculate the $P_x(t), P_y(t), P_z(t)$ using:

1. $\vec{P}(t) = \cos(t)\hat{u} + \sin(t)\hat{n} \times \hat{u}$

The equal angle projection is then made by calculating x(t) and y(t)

2. $\theta(t) = \cos^{-1}(P_z / (P_x(t)^2 + P_y(t)^2 + P_z(t)^2)^{1/2})$
3. $\varphi(t) = \tan^{-1}(P_y(t) / P_x(t))$
4. $x(t) = \theta(t)\cos(\varphi(t))$
5. $y(t) = \theta(t)\sin(\varphi(t))$
6. the set of (x(t),y(t)) points are plotted and connected with a line of width $= \Psi_{1/2}^{p-hkl}(1-\chi_{min})$



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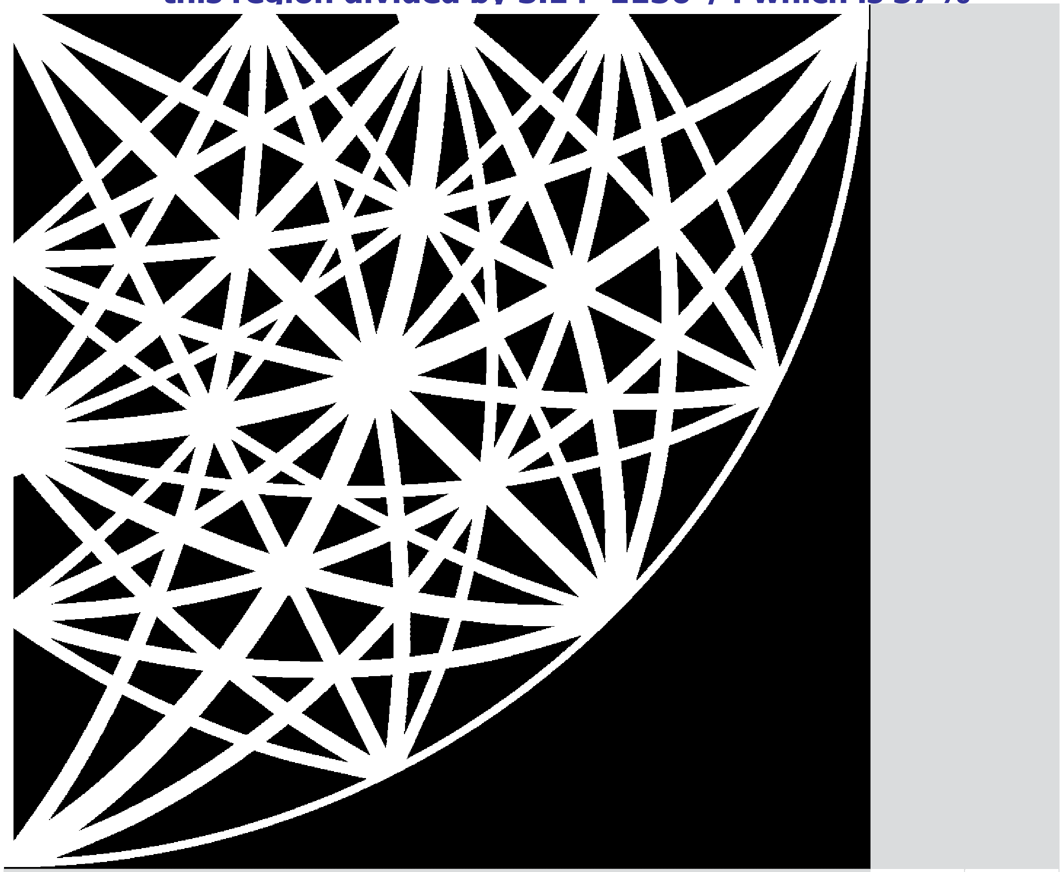
to calculate the channeling probability for randomly oriented polycrystalline materials:

1. the equal angle projections plotted in excel are saved as bitmap files.
2. then read into a 2D array of 1's and 0's
3. in plot below white areas are 1's and indicate channeling, black areas are 0's and indicate dechanneling
4. this quadrant of equal angle space has a 1136 cell radius
5. the channeling probability is then the sum of all the 1's in this region divided by $3.14*1136^2/4$ which is 57%



sum=	574892
total=	1013552
C-Prob	0.5672

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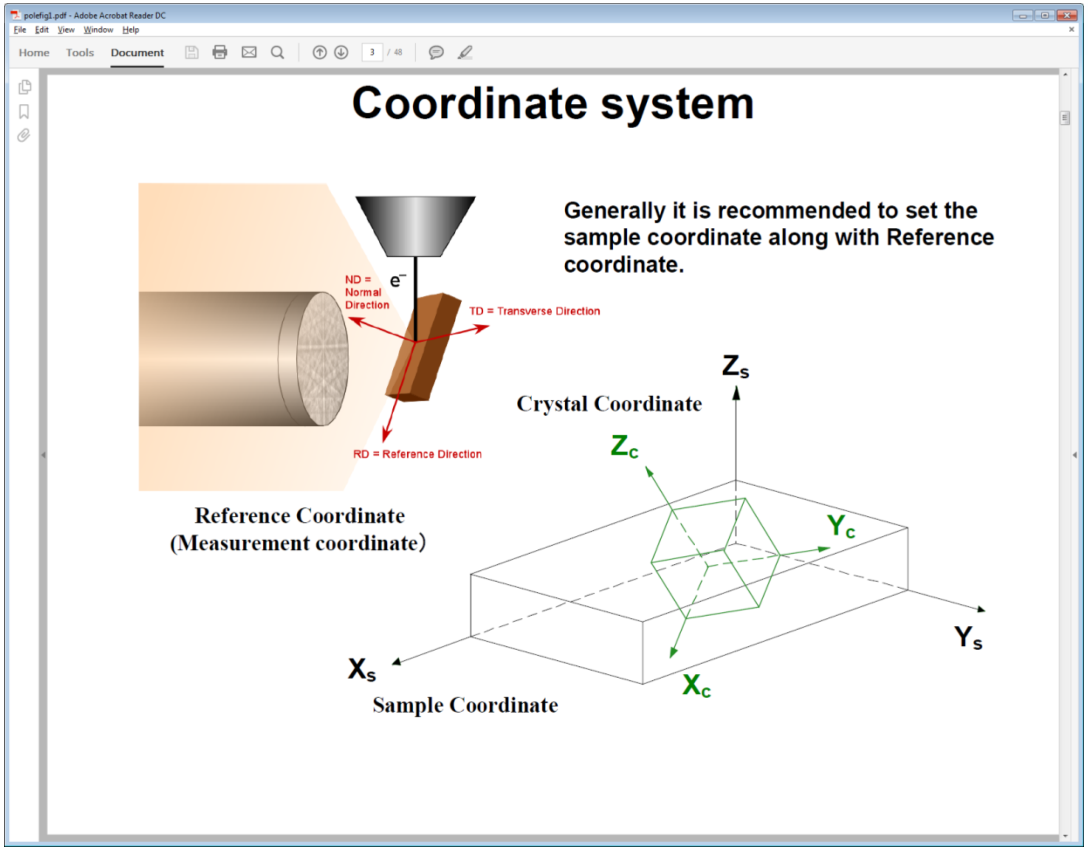
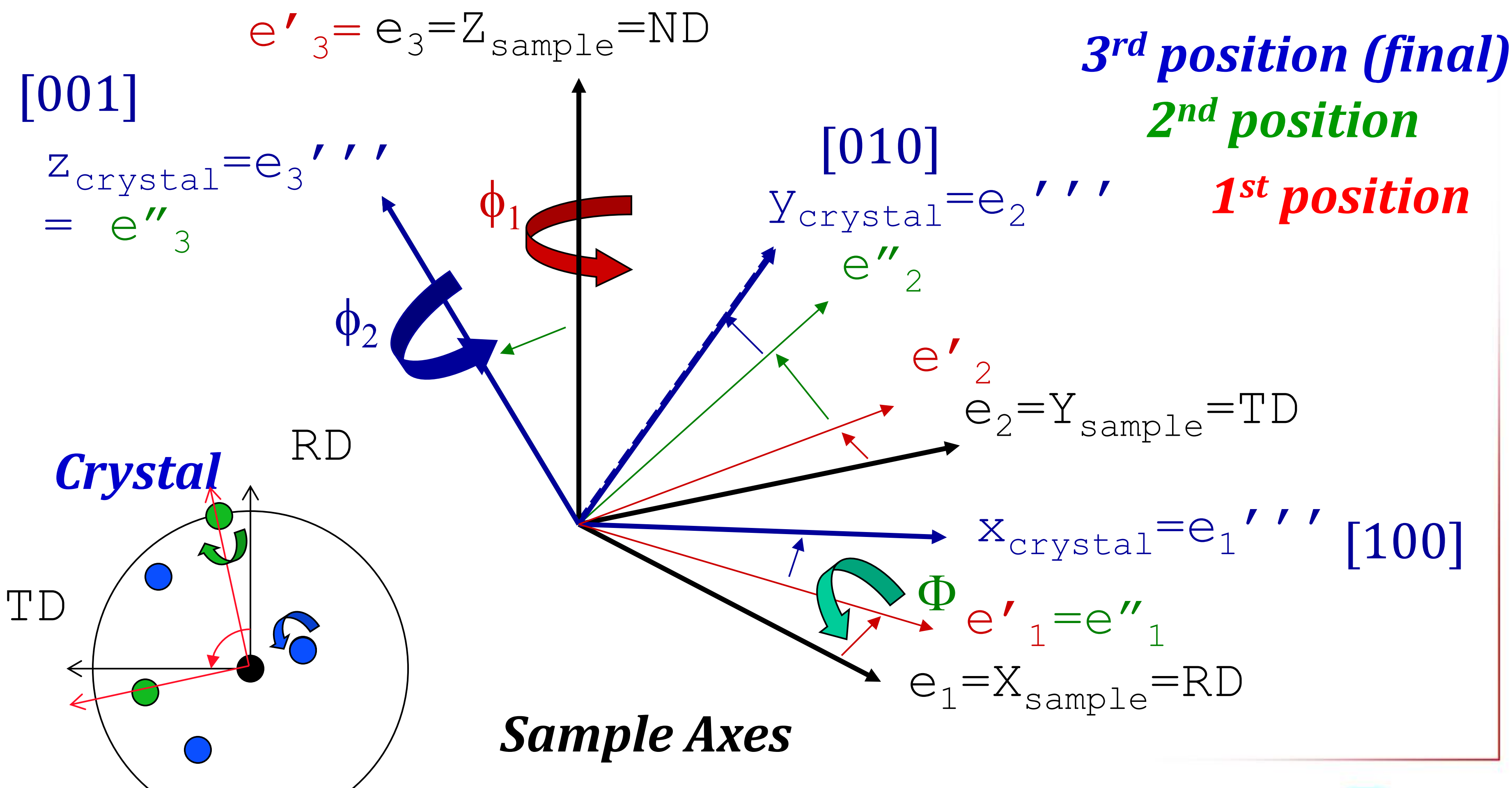
Definitions of Sample, Crystallite and Reference-Measurement coordinate systems for EBSD or Precession TEM



As the e-beam scans across the sample it scatters producing Kikuchi bands for EBSD and diffraction spots for Precession TEM yielding the standard Euler angles $(\varphi_1, \Phi, \varphi_2)$ of each polycrystal's orientation

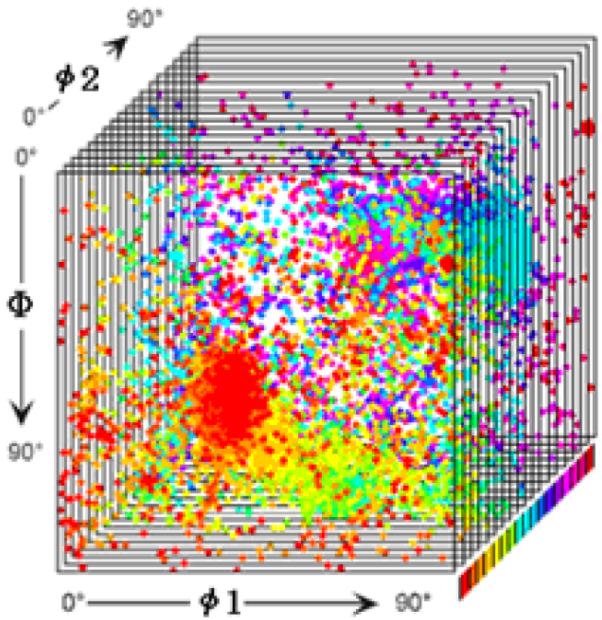
Euler Angles, Animated

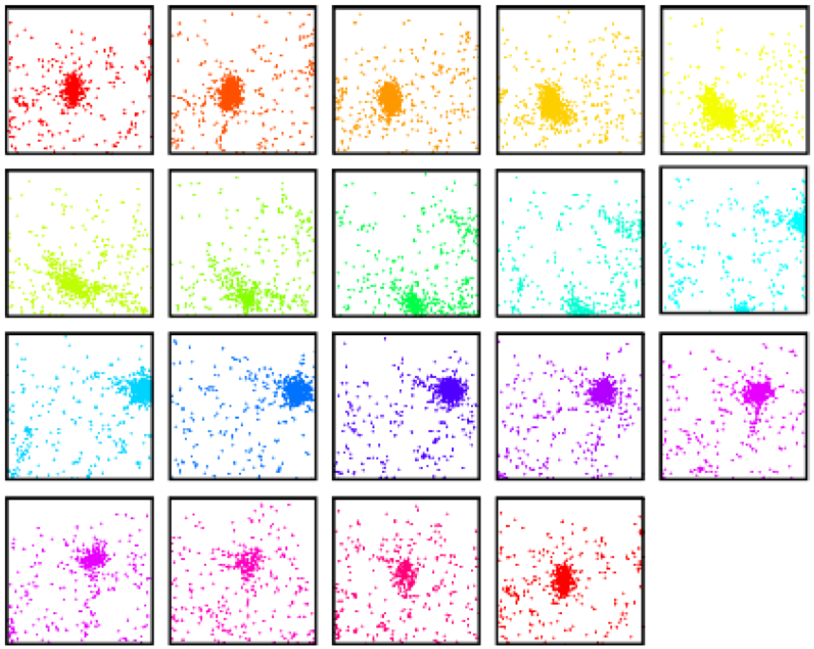


Obj/notation AxisTransformation Matrix EulerAngles Components

Euler Space Sections

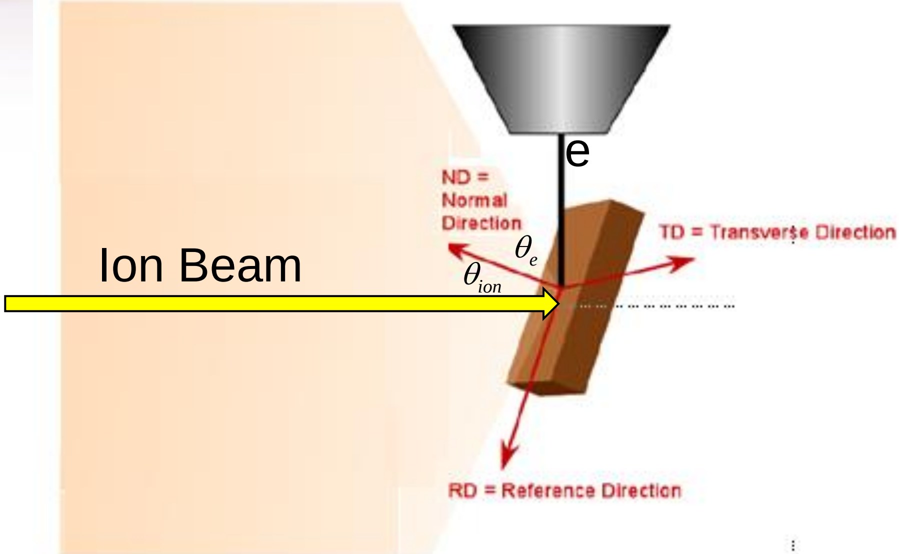
For orientation presentation, it is possible to plot Euler angle (φ1, Φ, φ2) directly. It is generally said as ODF (Orientation Distribution Function).

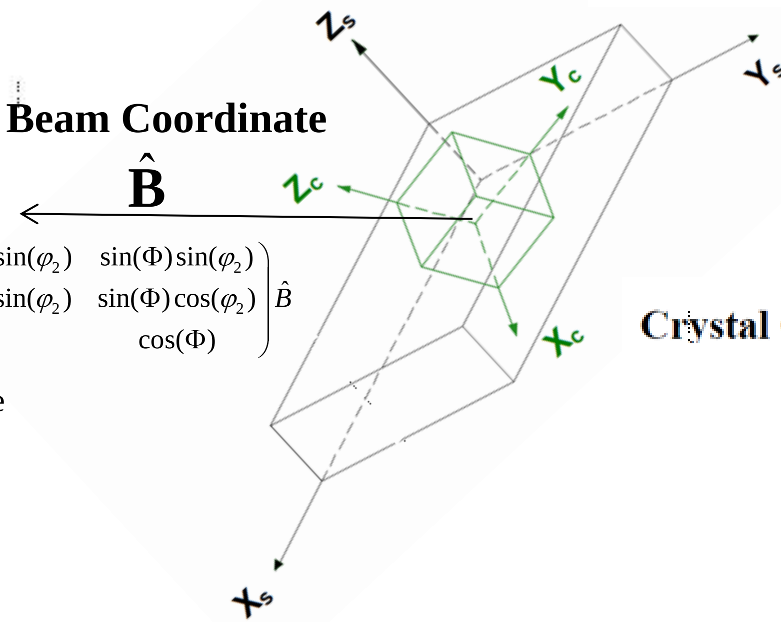




In Precession TEM, a diffraction pattern is measured for each scanned position of the beam and the three standard Euler angles $(\varphi_1, \Phi, \varphi_2)$ recorded. The sample is usually perpendicular to the electron beam.

At Sandia the ion beam is perpendicular to the TEM beam, and therefore samples must be tilted. The direction of the ion beam must then be transformed into the coordinate system of each polycrystal to see if channeling occurs.





$$\hat{B}' = \begin{pmatrix} \cos(\varphi_1)\cos(\varphi_2) - \cos(\Phi)\sin(\varphi_1)\sin(\varphi_2) & \cos(\varphi_2)\sin(\varphi_1) + \cos(\Phi)\cos(\varphi_1)\sin(\varphi_2) & \sin(\Phi)\sin(\varphi_2) \\ -\cos(\Phi)\cos(\varphi_2)\sin(\varphi_1) - \cos(\varphi_1)\sin(\varphi_2) & \cos(\Phi)\cos(\varphi_2)\cos(\varphi_1) - \sin(\varphi_1)\sin(\varphi_2) & \sin(\Phi)\cos(\varphi_2) \\ \sin(\Phi)\sin(\varphi_1) & -\sin(\Phi)\cos(\varphi_1) & \cos(\Phi) \end{pmatrix} \hat{B}$$

The θ and φ orientation of each polycrystallite with respect to the ion beam reference coordinate system is given by:

$$\theta = \cos^{-1}(B_z^{'})$$

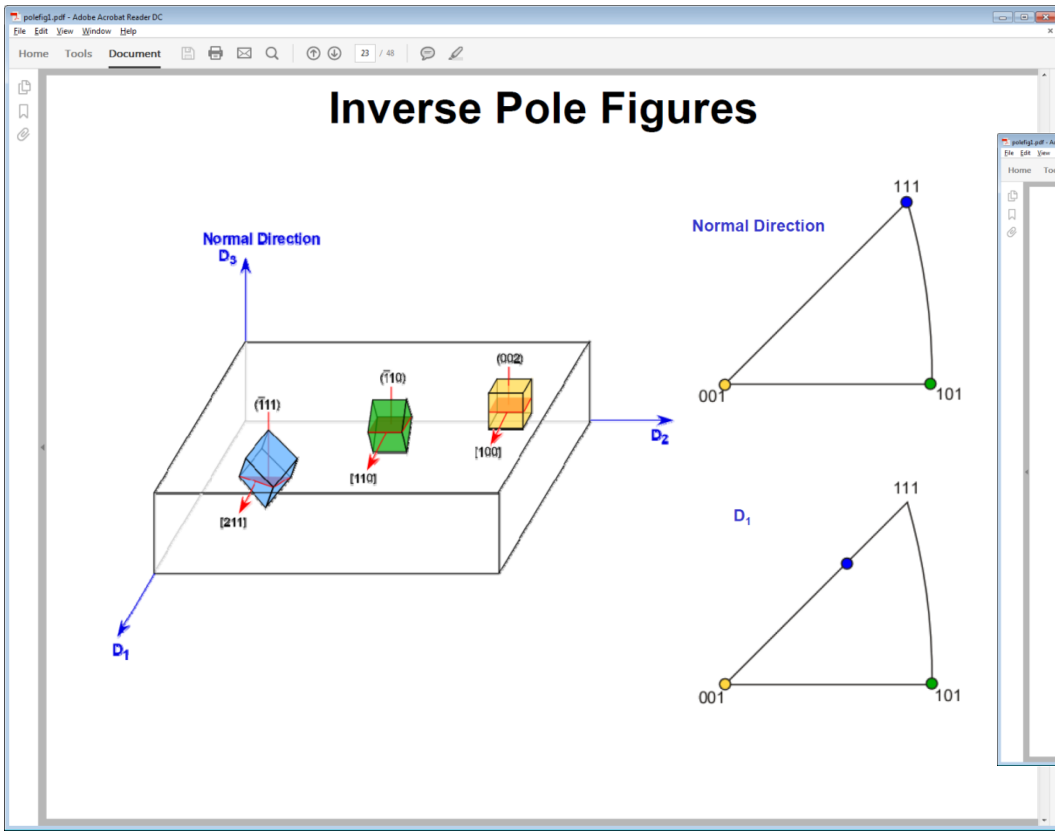
$$\varphi = \tan^{-1}(B_y^{'} / B_x^{'})$$

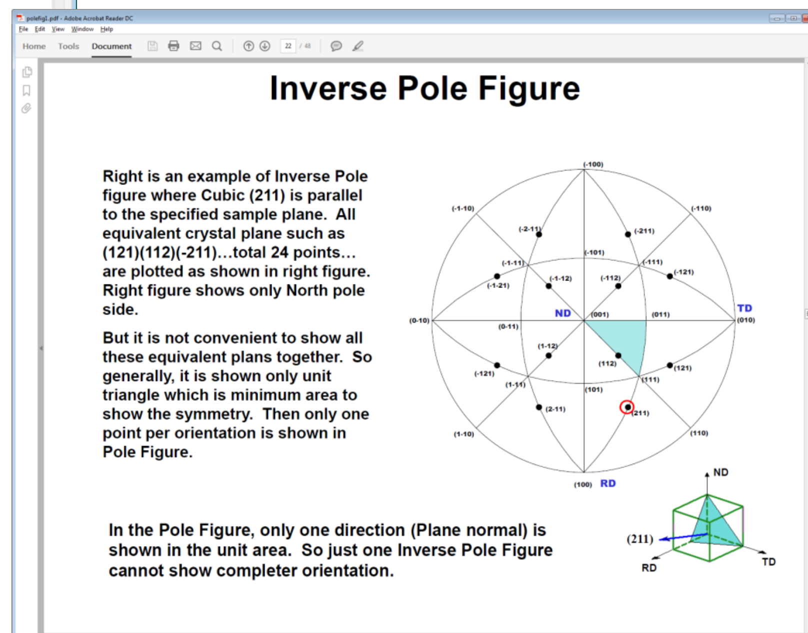
and then plotted as (x,y) dots using the equal angle projection:

$$x = \theta\cos(\varphi)$$

$$y = \theta\sin(\varphi)$$

This results in discrete "Ion Beam Direction" inverse pole figures (IPF) being made from the rotated-sample$(\varphi_1, \Phi, \varphi_2)$ orientation distributions measured by the TEM

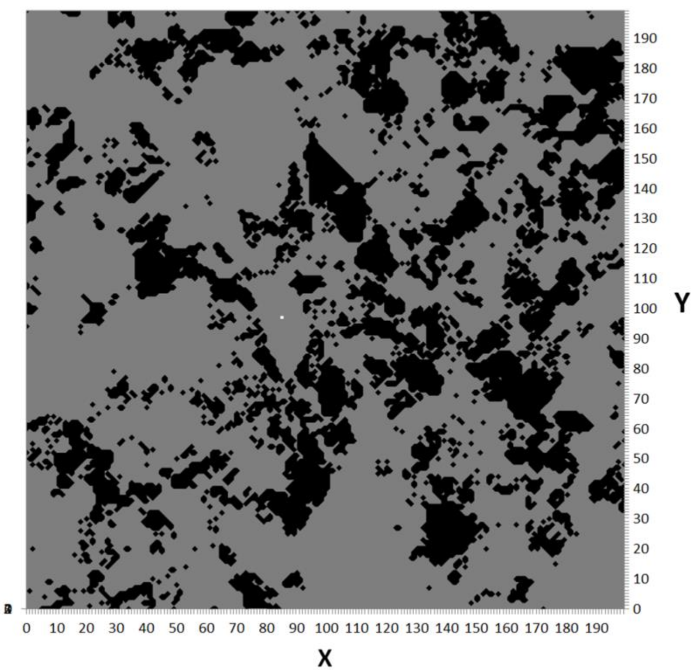


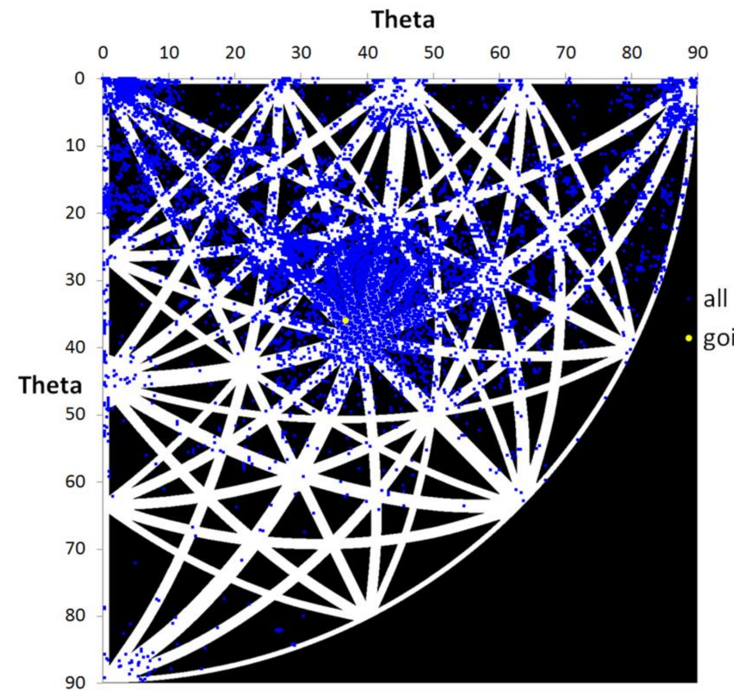


1.7 MeV Au exposure and Precession TEM of polycrystalline Au

The three Euler angles $(\varphi_1, \Phi, \varphi_2)$ for each polycrystal in the sample are recorded as a function of the (x,y) position of the electron beam.

In the figure to the right, an equal angle plot of the discrete 001 IPF (i.e. for a sample not tilted) is plotted over the equal-angle projection of axial and planar channeling. If one of the discrete points corresponds to a white region, the theory contends that channeling will occur.





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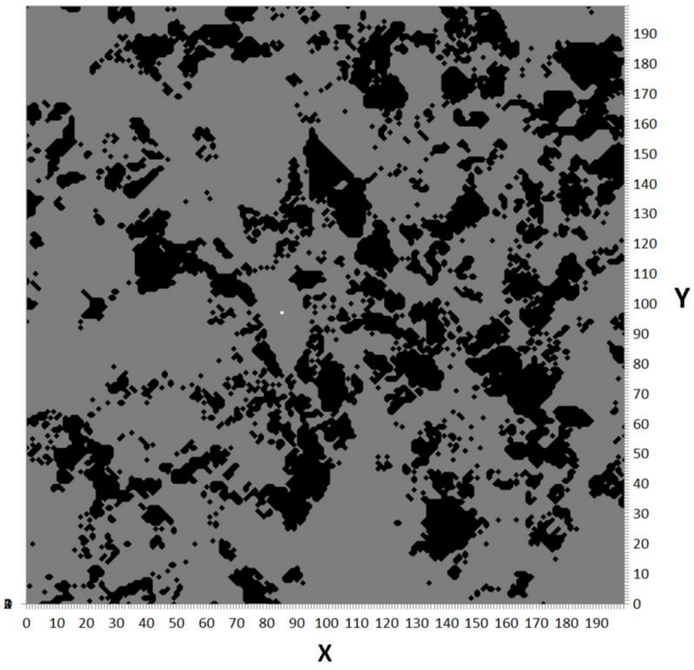
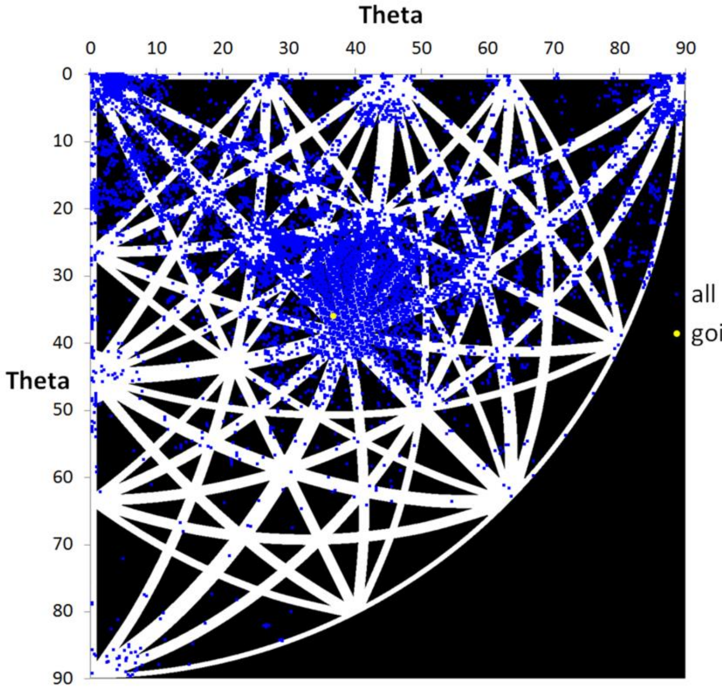
1.7 MeV Au exposure and Precession TEM of polycrystalline Au

The three Euler angles $(\varphi_1, \Phi, \varphi_2)$ for each polycrystal in the sample are recorded as a function of the (x,y) position of the electron beam.

The figure to the left records the position of the beam and points are plotted gray if their corresponding discreet IPF point is in a white channeled region of the plot to the right. For example, the yellow grain of interest (goi) point in the right figure indicates channeling, and the white point in the left figure shows where that grain is.

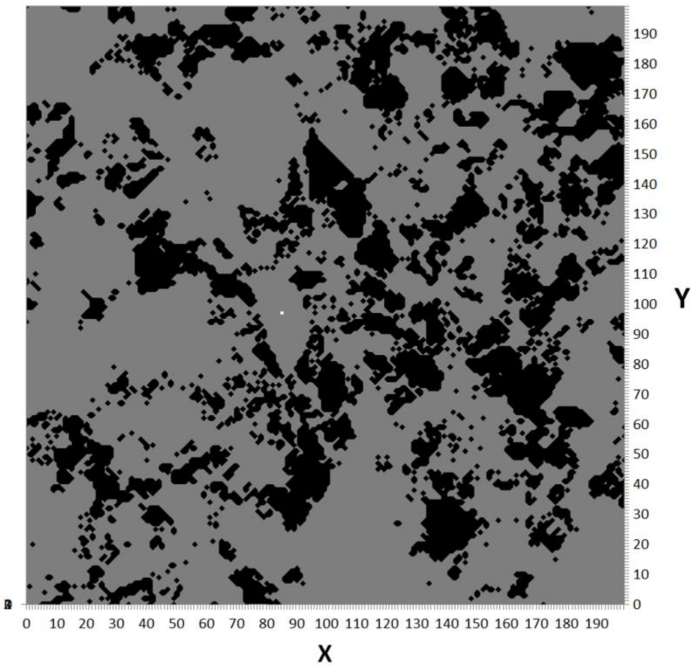


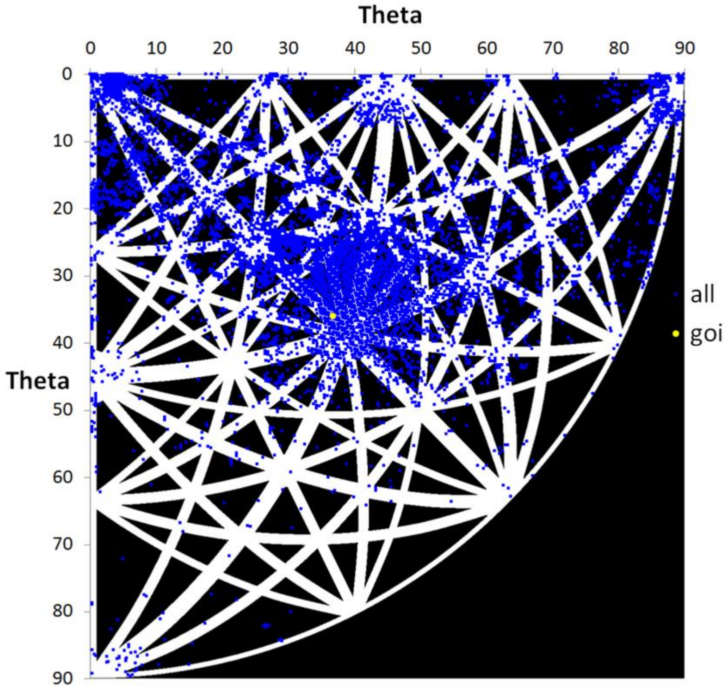


1.7 MeV Au exposure and Precession TEM of polycrystalline Au

The three Euler angles $(\varphi_1, \Phi, \varphi_2)$ for each polycrystal in the sample are recorded as a function of the (x,y) position of the electron beam.

The probability of channeling is determined by counting the number of discrete IPF points that are within the axial or planar channeling half angles (i.e. the white regions of the equal angle projected IPF plots), or just the fractional area of the gray regions on the left figure.

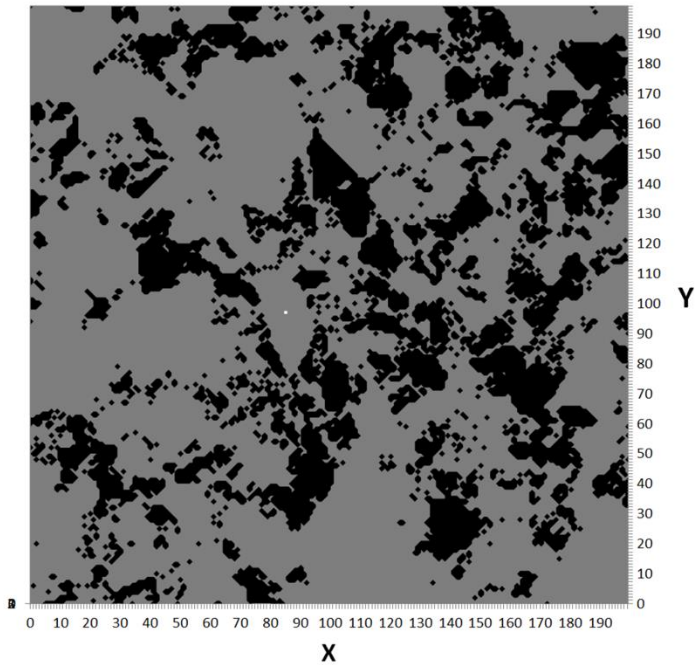


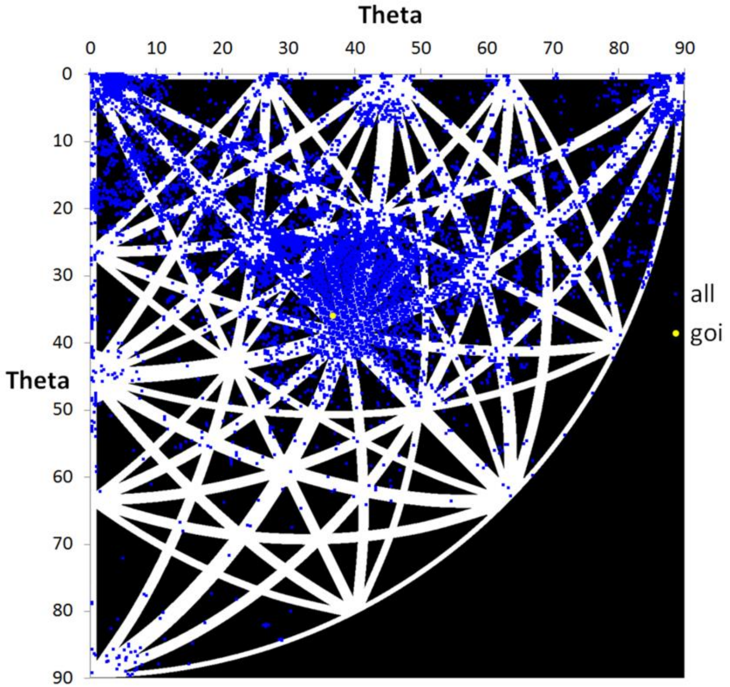


1.7 MeV Au exposure and Precession TEM of polycrystalline Au

The three Euler angles $(\varphi_1, \Phi, \varphi_2)$ for each polycrystal in the sample are recorded as a function of the (x,y) position of the electron beam.

The discrete 001 IPF of this sample clearly shows strong 111 texture, and for this untilted case, the ion beam would have to come in parallel to the electron beam. The channeling probability would be 79% which is higher than the 57% channeling calculated earlier for randomly oriented Au.





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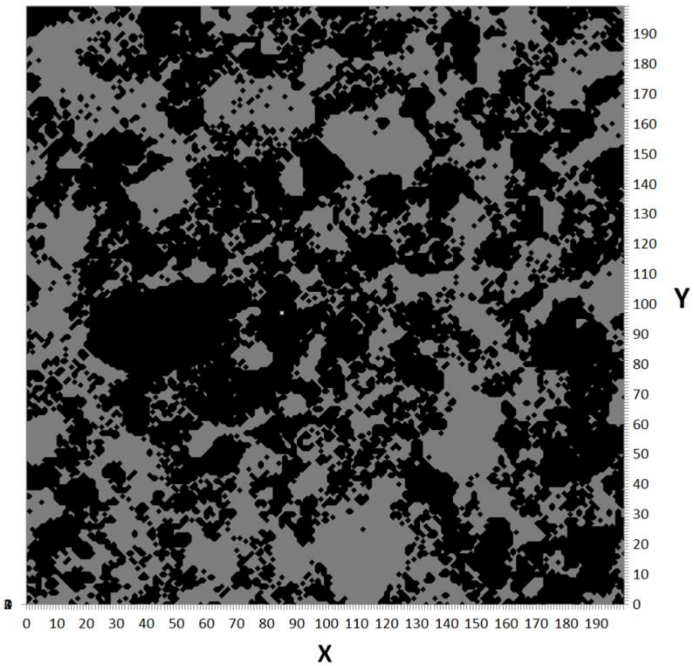
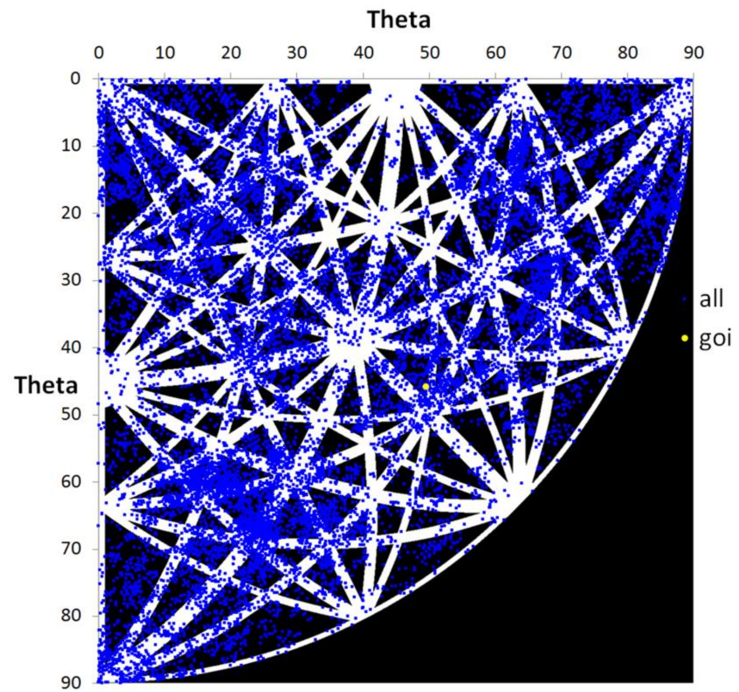
1.7 MeV Au exposure and Precession TEM of polycrystalline Au

The three Euler angles $(\varphi_1, \Phi, \varphi_2)$ for each polycrystal in the sample are recorded as a function of the (x,y) position of the electron beam.

Of course our ion beam can't have the same direction as the TEM beam, and in fact the stage is limited to a +/-30º rotation. This means that the tilt of the sample in the Beam system is 60º, and the Beam-IPF and corresponding channeling map are plotted below. Here the channeling probability is 57%, which is the same as random. Note that here the goi is not channeling.





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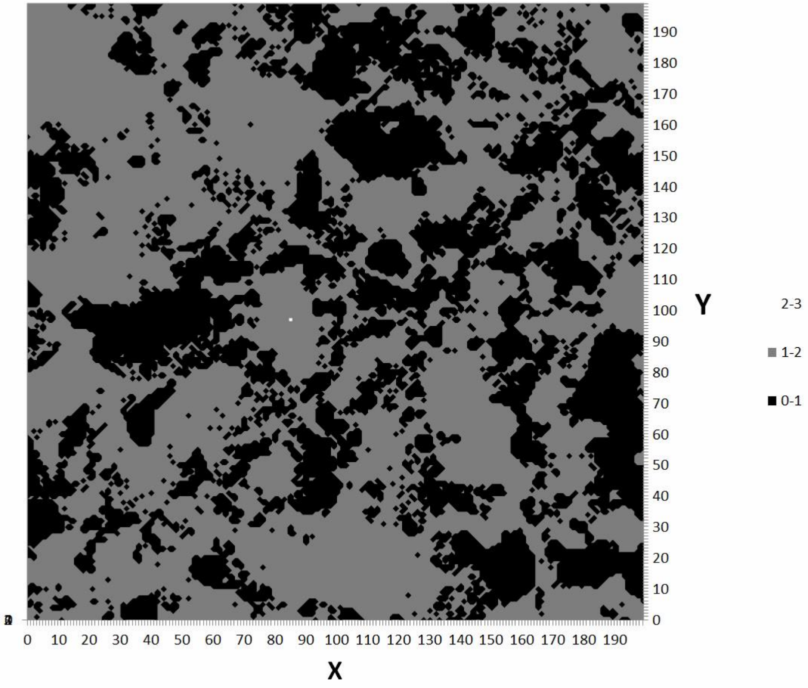
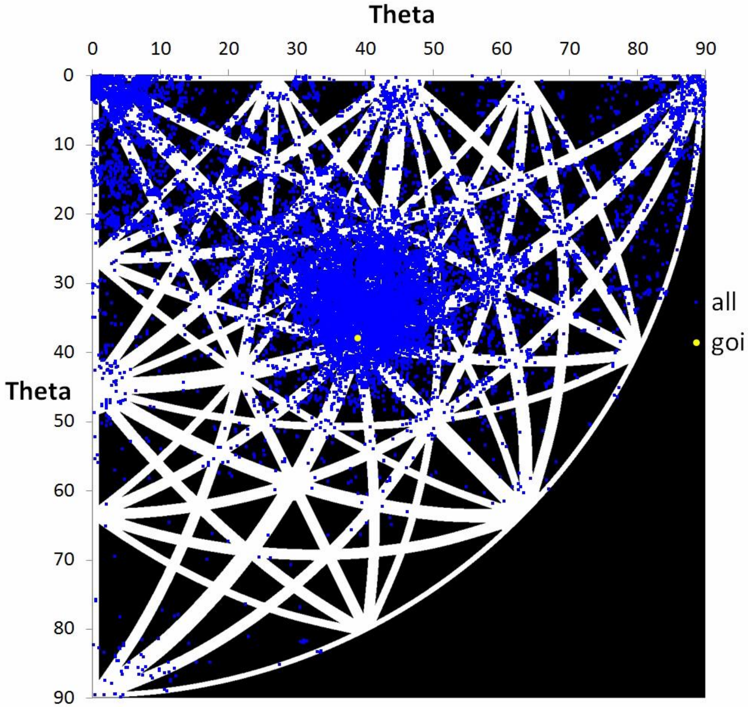
equal-angle Beam-IPF of poly Au with 1.7 MeV Au channeling for different tilts





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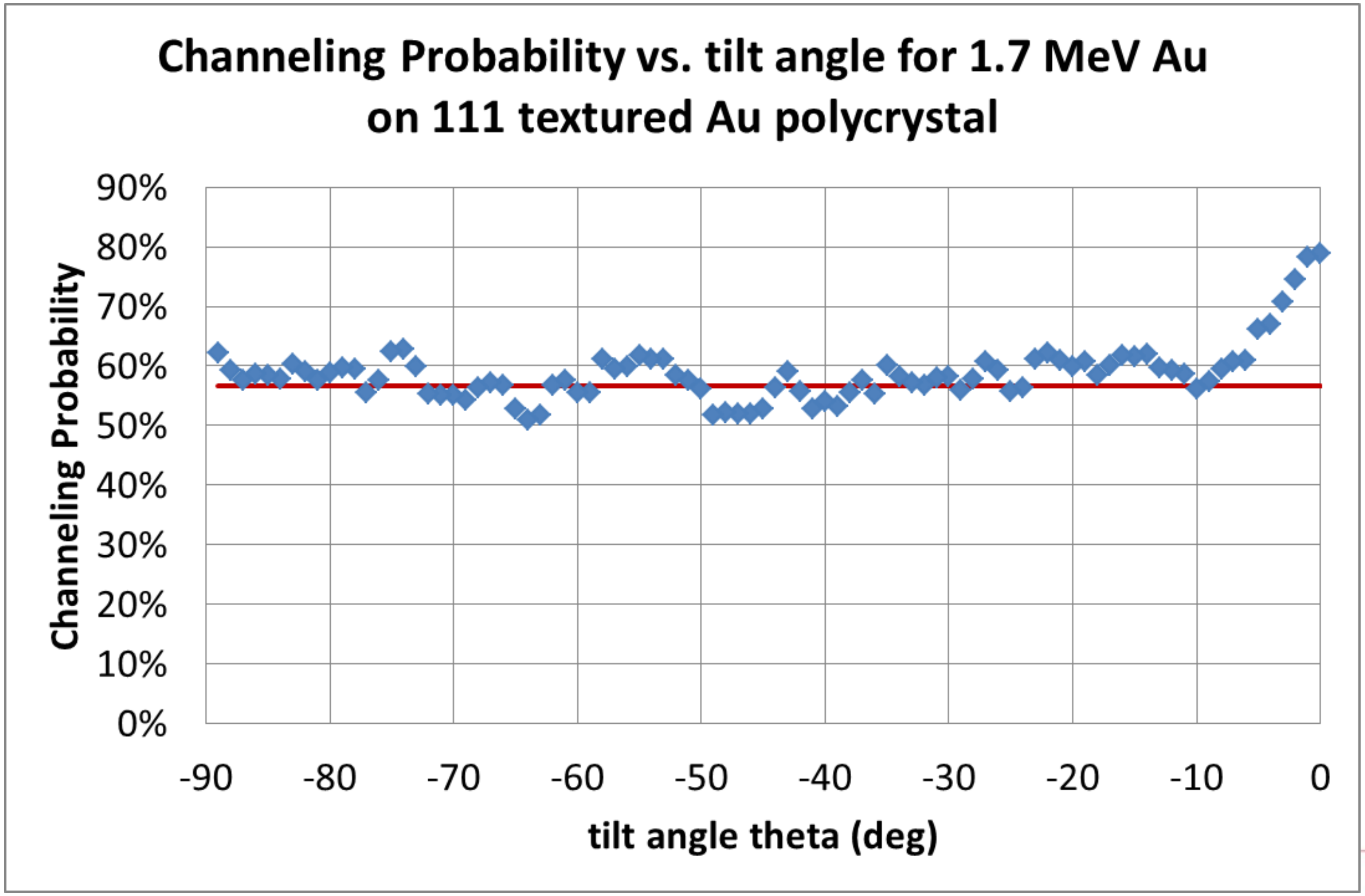
For this sample just about any tilt results in the channeling probability being ~ same as for random



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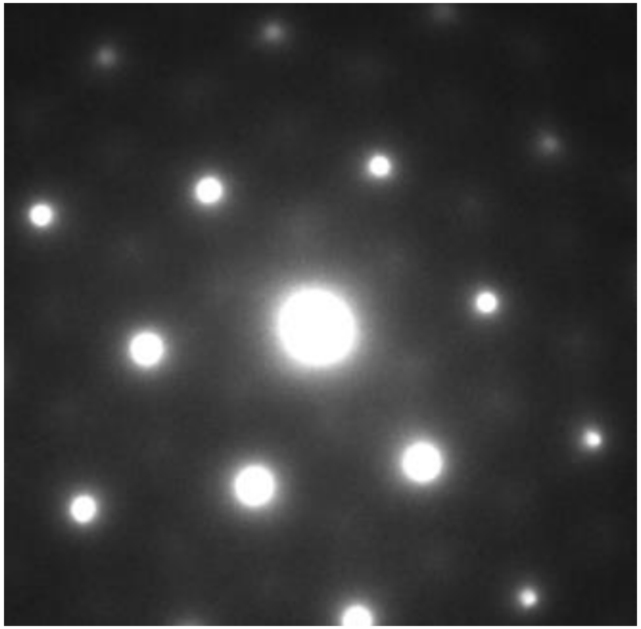
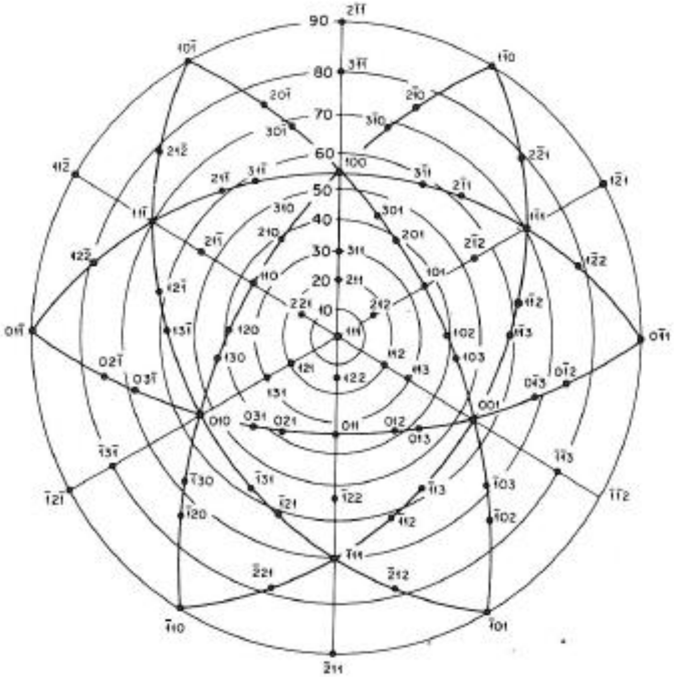
Process to find 111 axial channel for ions

1. precicely position one grain's 111 axis to be parallel with TEM beam using diffraction pattern

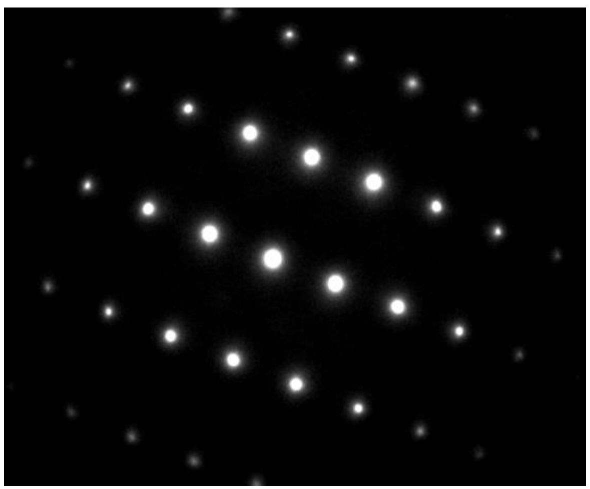
2. rotate sample so tilt will follow $1\bar{1}0$ plane toward 112 axis

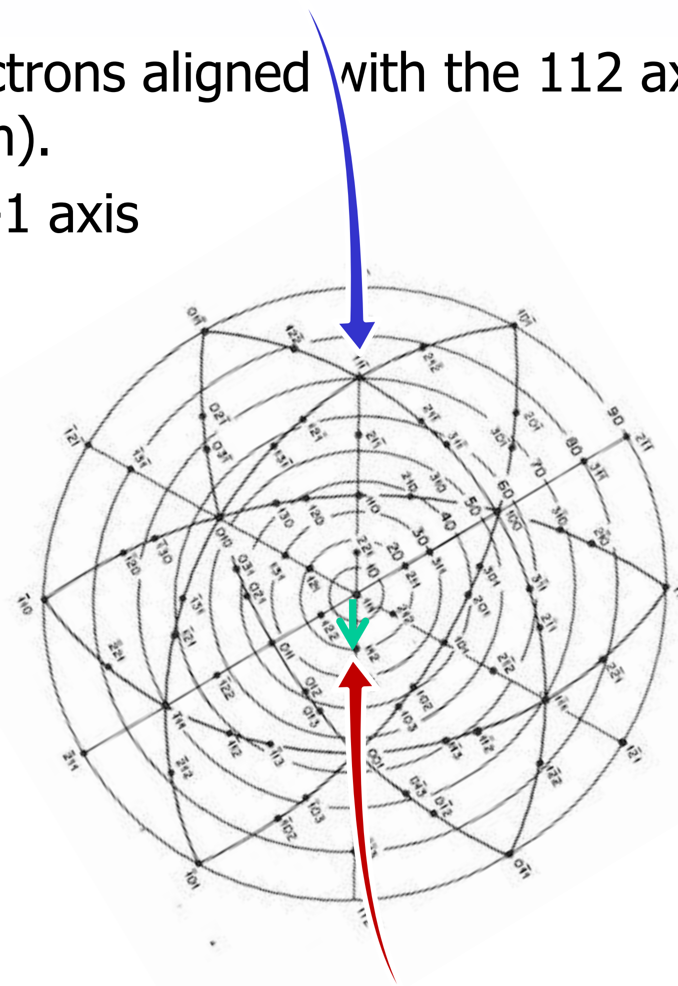




3. the sample is then tilted -19.47 from 0 degrees

- which orients the sample for electrons aligned with the 112 axis (as seen in the diffraction pattern).
- and ion channeling along the 11-1 axis





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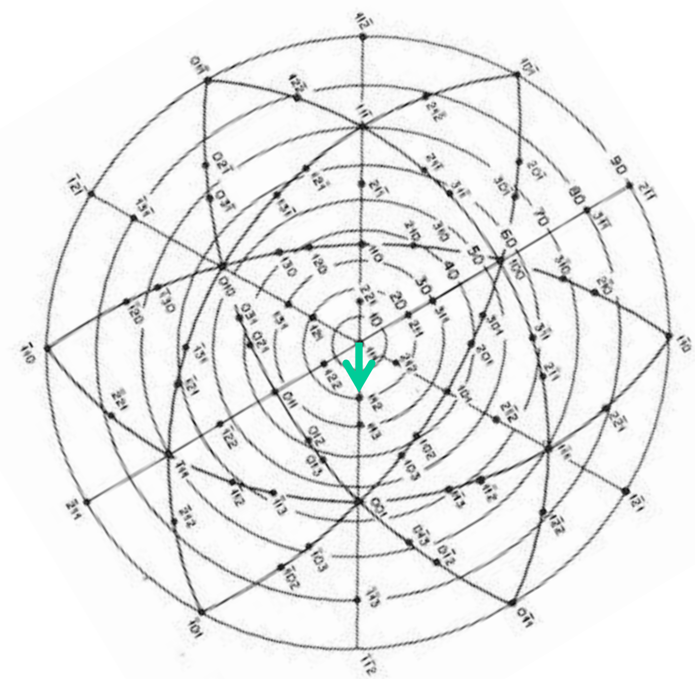
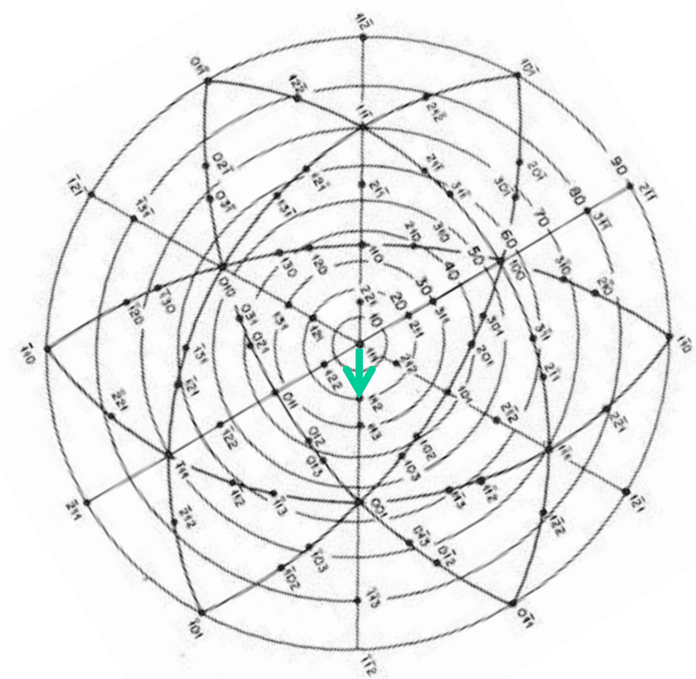
4. the sample is then implanted with the 1.7 MeV Au to a predetermined fluence.

- It is thought that the grain that has been aligned for channeling will suffer less displacement damage from nearby grains that are not so aligned.

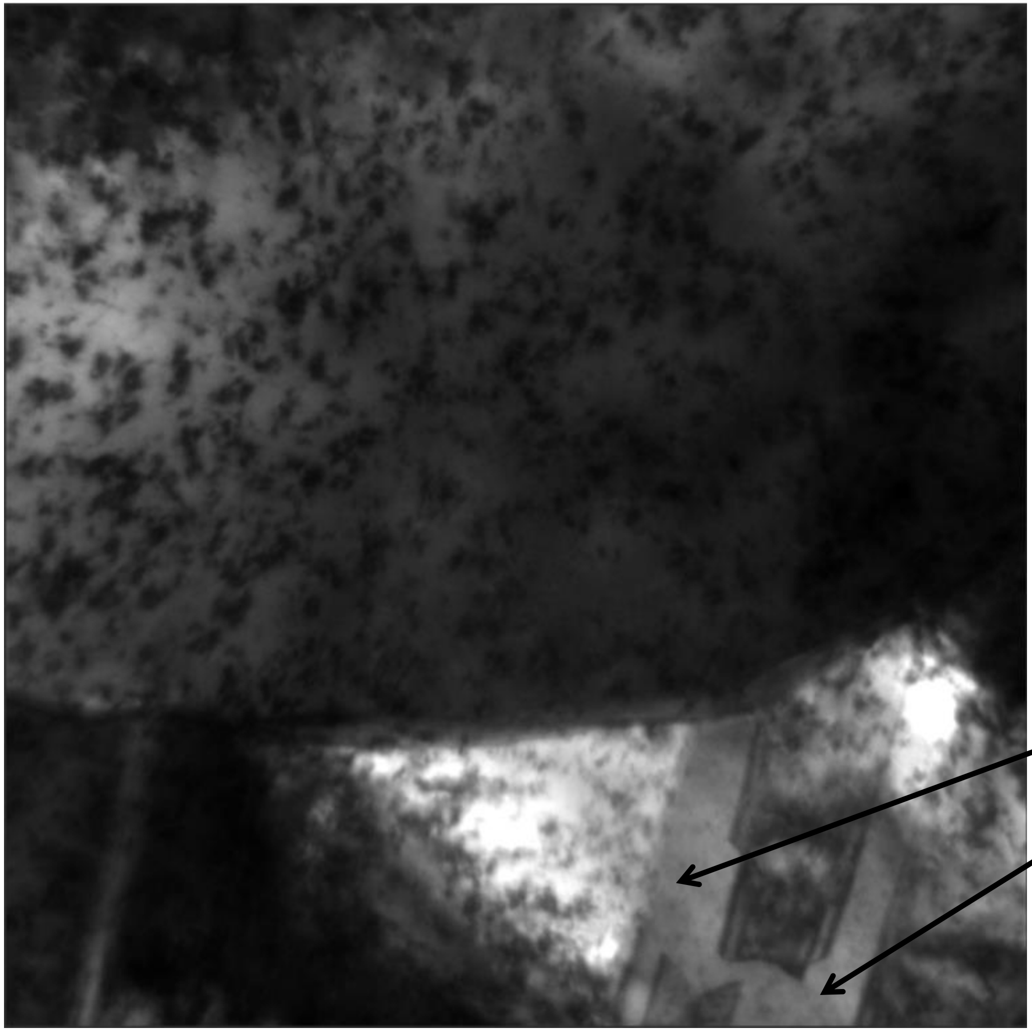


5. The TEM is then used to look for defects like SFTs and determine their density

- It is thought that the grain that has been aligned will have a lower density of SFTs, maybe 0.
- Neighboring grains that don't ion channel should have the highest denisty of SFTs.



Ion current was probably too high, as the damage seen below occurred in only about 10 seconds and is difficult to quantify differences between grains. However, there is no obvious difference between the oriented grain and the other grains in the sample

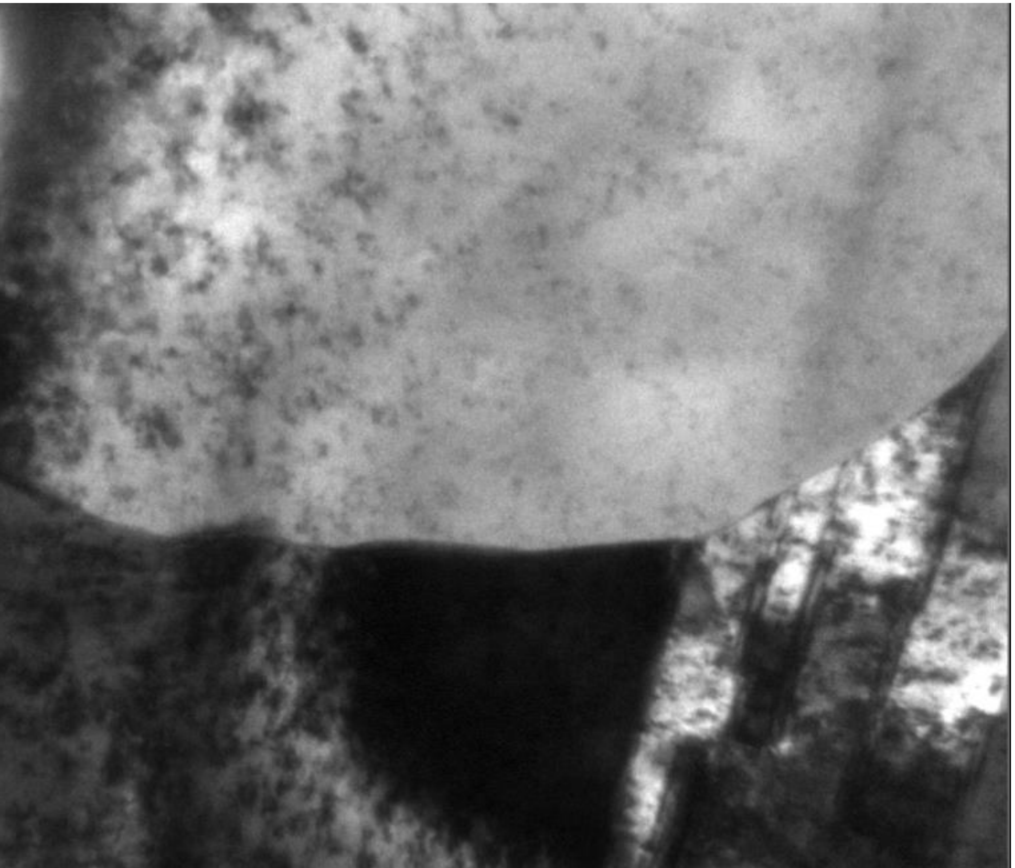


Grain oriented for channeling

At this tilt, this area appears to be less damaged.. I tilted approximately 1 degree away and imaged again (see next slide)

Randomly oriented grains

Only about one degree tilt from the previous image shows that these areas are actually heavily damaged. This is a nice example of why defect analysis in TEM is challenging and requires very precise imaging conditions.



I think these experiments should be run again at a lower current so I can try to actually quantify defect density, but so far I do not see any obvious evidence of channeling…

2.7 MeV Si on Au Channeling Experiment

h	k	l	$\Psi_{1/2}^{a}$ axis-deg	$\Psi_{1/2}^{p}$ plane-deg
0	0	1	2.03	0.43
0	1	1	2.63	0.55
1	1	1	1.35	0.48

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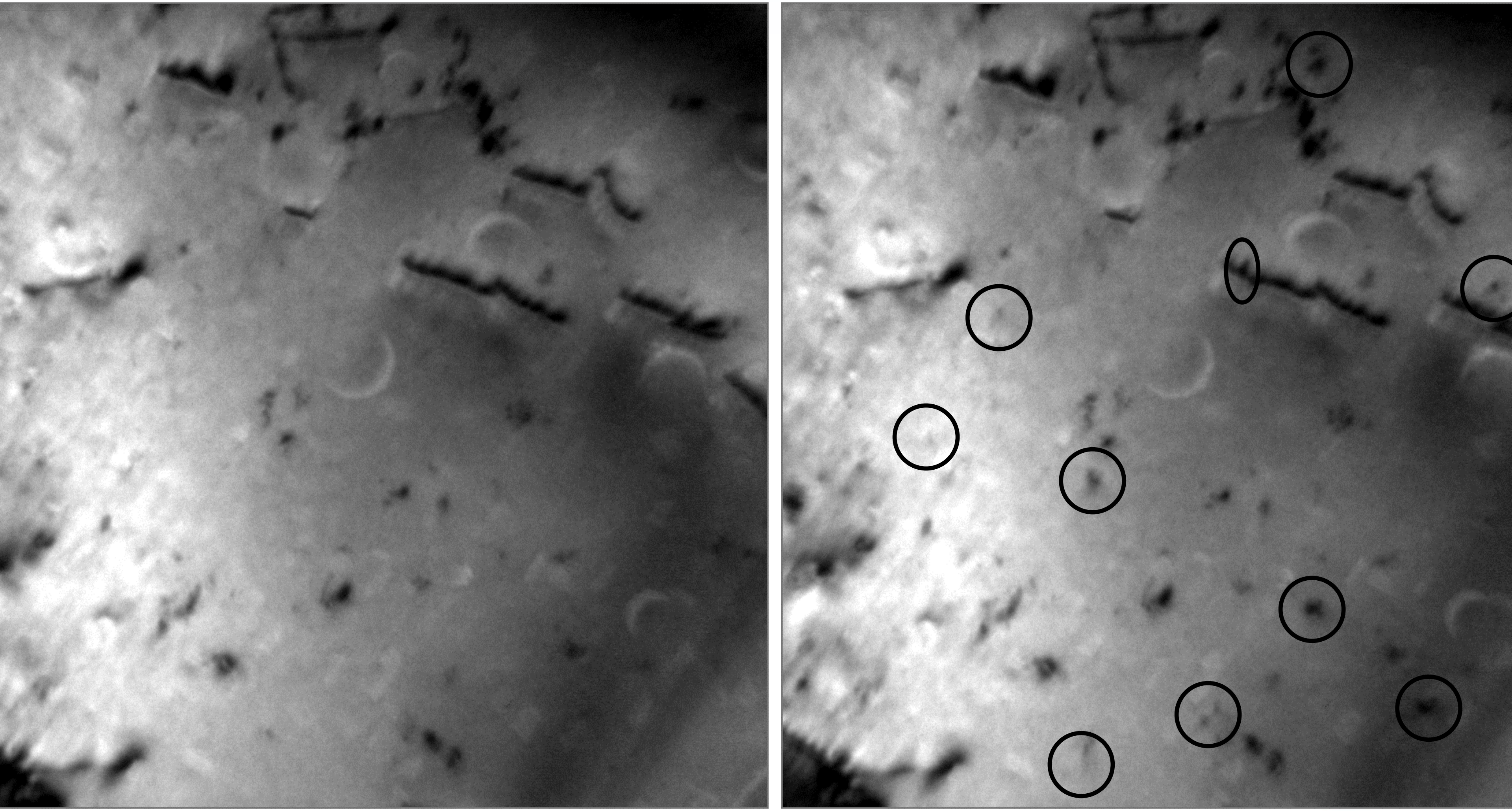
2.7 MeV Si on fcc Au 1) <111> channeled and then 2) random orientation for approximately the same ion fluence. The defects added are circled in the random micrograph, and we expected a lot more?



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Why are we not seeing channeling?

- Sample issues/contamination?
- Could we pick a different axis oriented for channeling which has a larger half angle than the <111>?
- Maybe try a different ion or energy?
- Maybe try a BCC metal so there is a lot more room for error in alignment
- Are we super certain the beam enters perfectly orthogonally to the stage?
- Are we sure the magnetic field in TEM doesn't change affect direction beyond half angle
- Do our tandem ions have energies below the minimum energy for channeling (ala Hobler)

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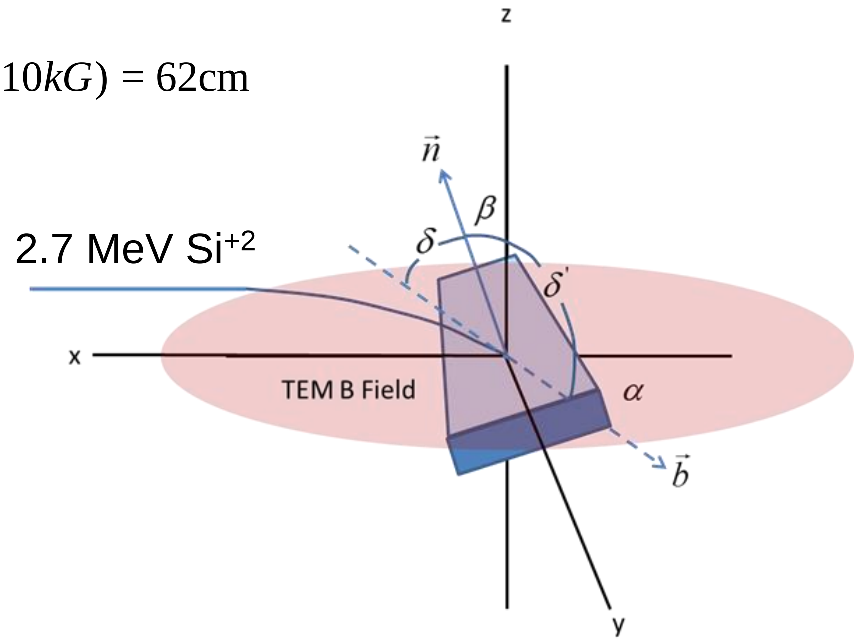
The B field in the TEM can change the angle of the beam ~ the same as the channeling ½ angles

$$R_T = \frac{\sqrt{2mE}}{B_T q} = \text{(for m=28, q=2, E=2.7 MeV, } B_T = 10kG\text{)} = 62\text{cm}$$

$$r_T = 2cm$$

$$\alpha = \tan^{-1}\left(\frac{dy}{dx}\right) = \tan^{-1}\left(\frac{r_T}{R_T}\sqrt{\frac{1+\frac{1}{2}\left(\frac{r_T}{R_T}\right)^2}{1-\frac{1}{2}\left(\frac{r_T}{R_T}\right)^2}}\right) = 1.8^0$$



h	k	l	$\Psi^{a}_{1/2}$ axis-deg	$\Psi^{p}_{1/2}$ plane-deg
0	0	1	2.03	0.43
0	1	1	2.63	0.55
1	1	1	1.35	0.48

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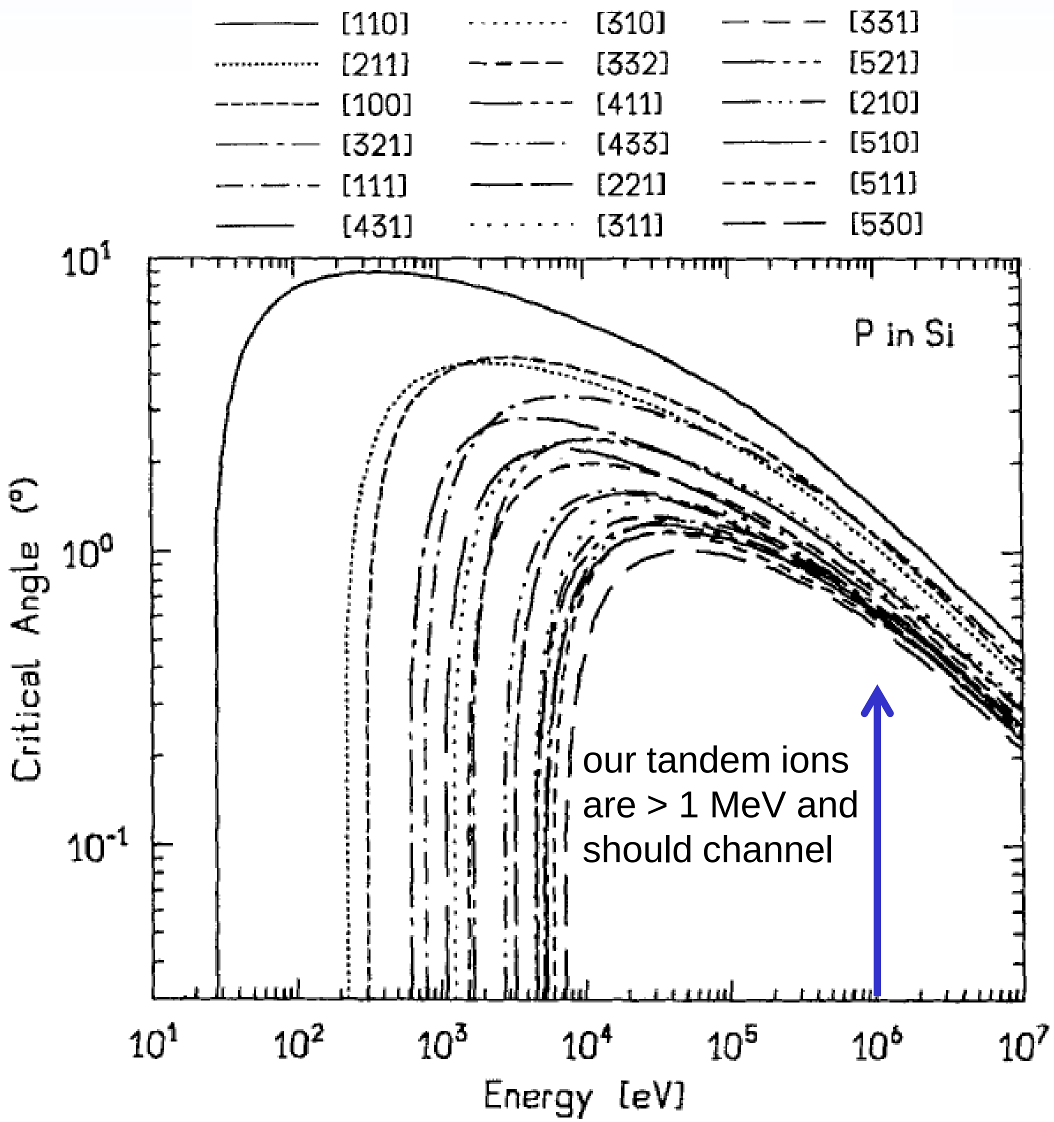
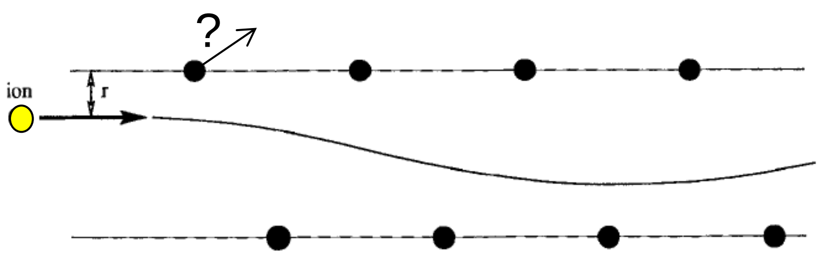
Hobler has calculated lower energy limits to ion channeling



Why are we not seeing channeling? (a more sinister possibility ☹)

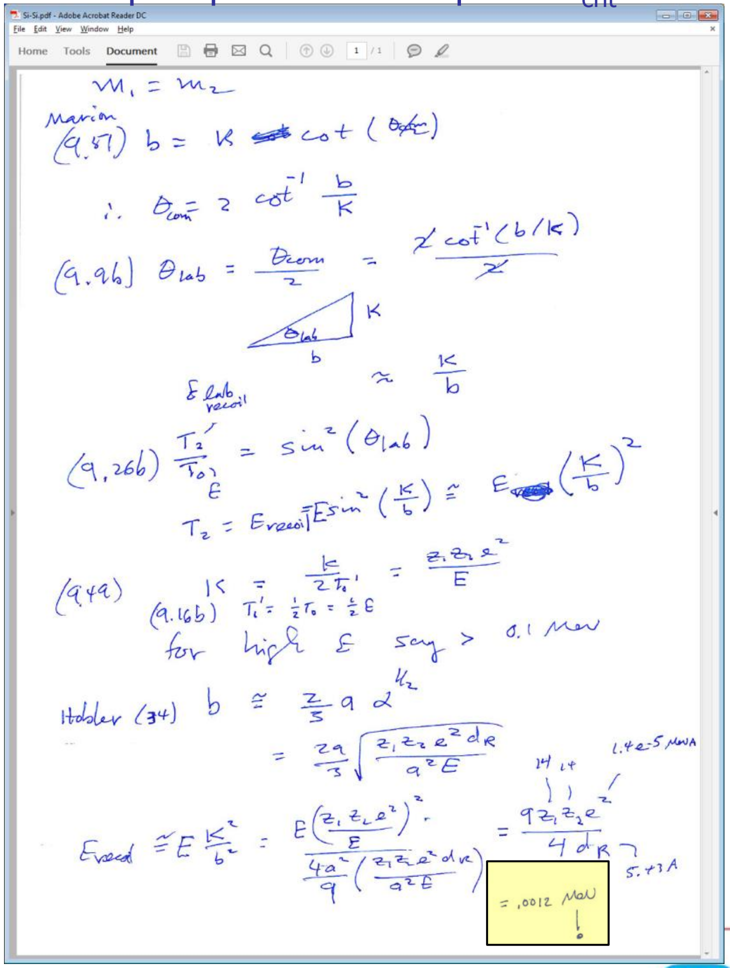
- The premise that RBS channeling doesn't displace atoms is wrong?
  - then the $\Psi_{1/2}$s are wrong
  - =>new "nondamaging" channeling theory

In the standard Lindhard and Hobler channeling theories, the target atoms are replaced by fixed lines of charge. …But do these atoms really remain fixed during the ion's closest approach?



$$r^0_{\text{crit}} = 2/3.a\sqrt{\alpha}(1 - \sqrt{\alpha}/19 + \alpha/700) \text{ with } \alpha = Z_1 Z_2 e^2 d_R / a^2 E$$

Binary collision of 1 MeV Si on Si with an impact parameter b equal to r_{crit}^{o}



Yikes!

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Summary

- Developed Excel program for calculating unintentional ion channeling probability in
  - randomly oriented polycrystalline materials
  - textured materials
    - need beam-sample geometry (including ion steering by TEM)
    - orientation microscopy data $(\varphi_1, \Phi, \varphi_2)$
- …but may need a new theory for axial and planar $\Psi_{1/2}$ where displaced atoms are not made
- …and if you are OK with the RBS $\Psi_{1/2}$s approach, I'll be glad to calculate channeling probabilities for you. bldoyle@sandia.gov

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