SAND2017-0635PE

EFFECTS OF SINGLE ION STRIKES INTO SI ON THE 3D RECIPROCAL SPACE - UPDATE

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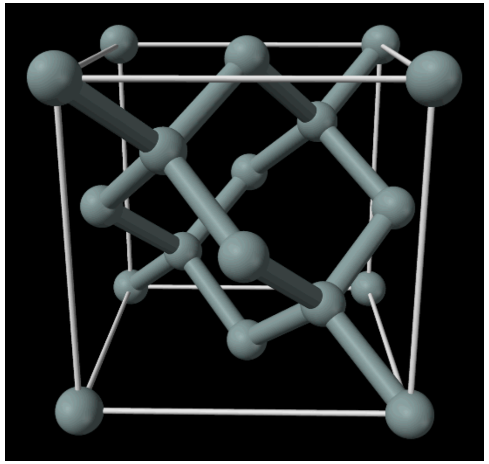
Question?

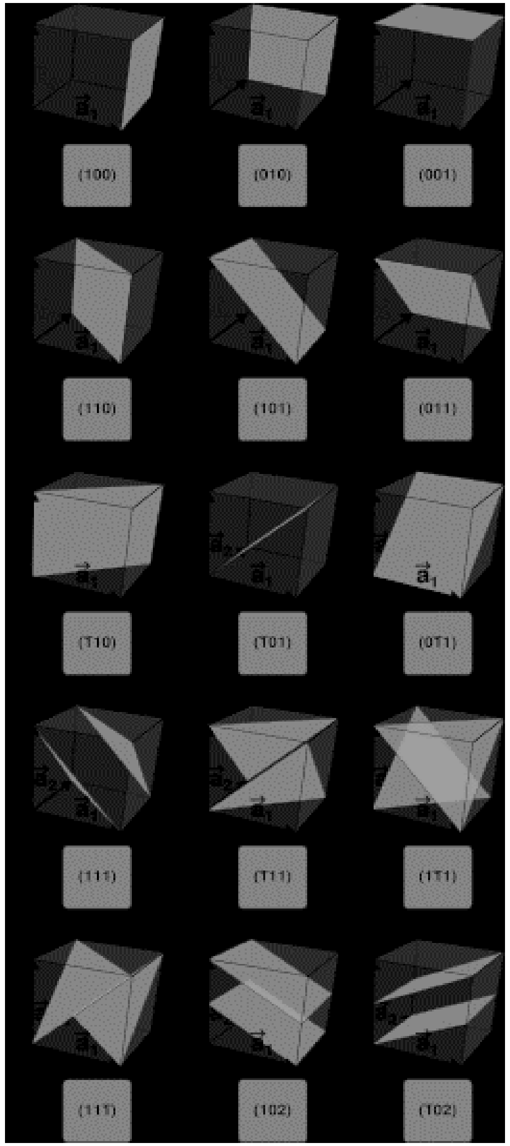
How does Si behave at the atomistic level during single ion strikes and how does this affect the 3D Reciprocal Space?

Real Space

- In Real Space a unit cell is made up of atoms
- With a real distance, $\dot{A}$
- You can look at different planes of the crystal according to the miller indices (hkl)
- In what way can we extract crystallographic information?
  - Electron Diffraction in a TEM



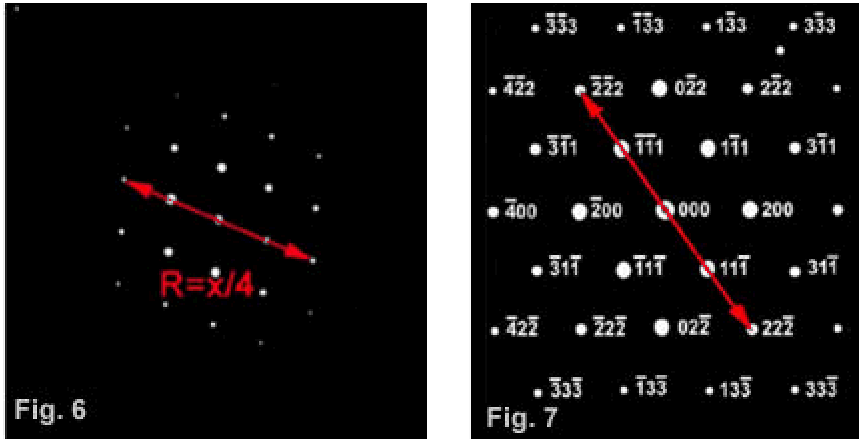
Real Space Unit Cell of Silicon [1]



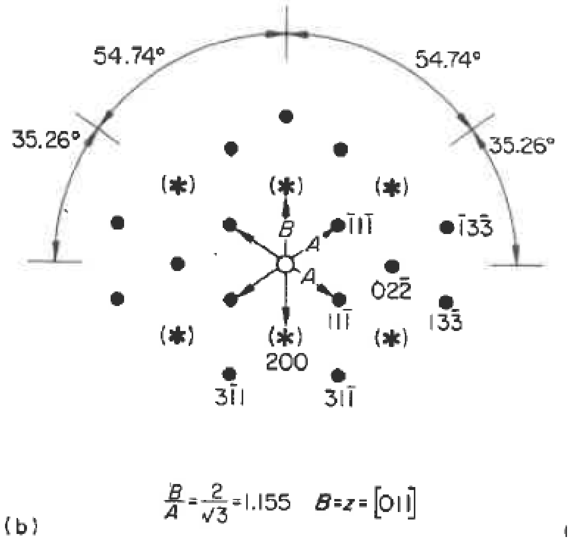
Miller Indices for a cubic cell [2]

Reciprocal Space

- In reciprocal space these individual planes in real space become diffraction spots in 3D space, a.k.a. a reciprocal lattice.
- Distance is now 1/d.
- Furthermore the different patterns are determined by zone axes which is a direction normal to the planes of interest



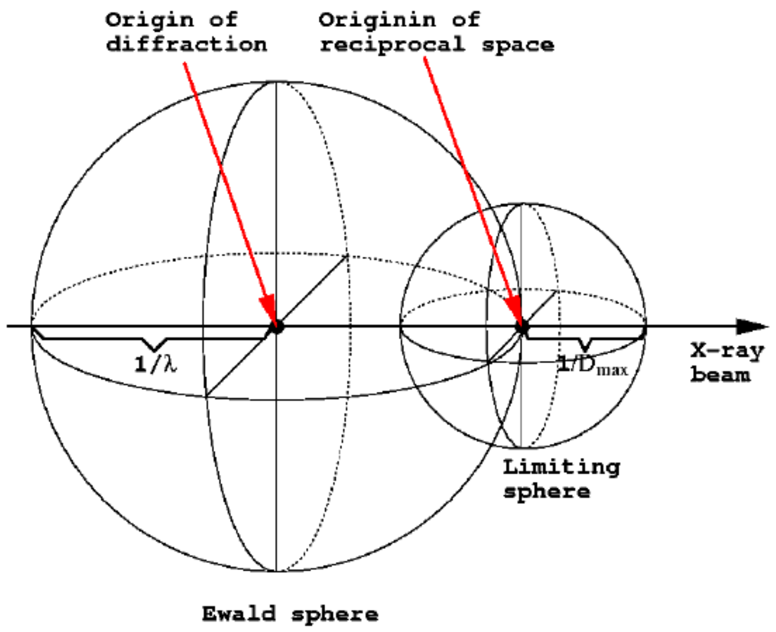
Real SAED pattern along [011]. [4]



[011] Zone Axis in a diamond structure [3]

Ewald Sphere & Laue Conditions

- The Ewald Sphere is an imaginary construct by which when its conditions are met generate an SAED as everywhere it comes in contact on the reciprocal lattice is a diffraction spot
- Laue Conditions determine how far out diffraction spots will occur in a pattern



Interaction of Ewald Sphere and Reciprocal Lattice in 3D space [5]

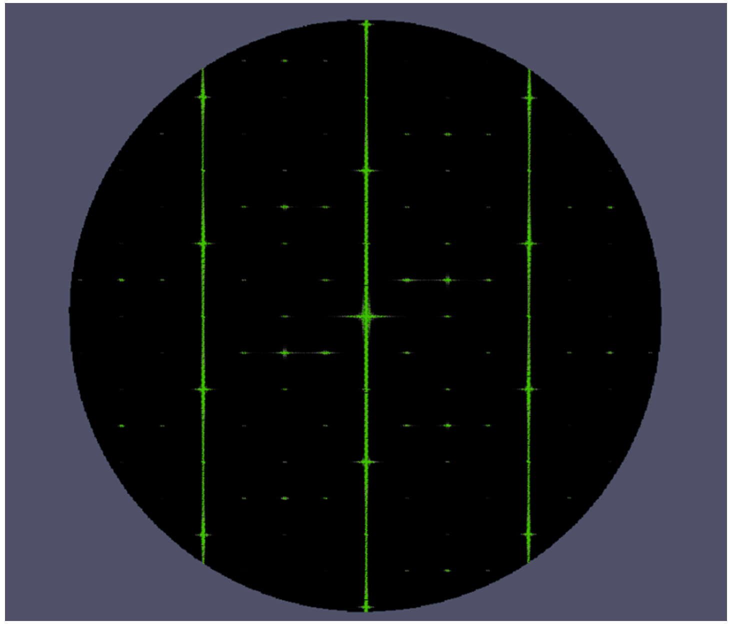
Goal

- Compare a perfect single crystal silicon reciprocal lattice to that of irradiated silicon
- When studying the diffraction patterns is there noticeable peak shifting or broadening in the irradiated samples in the planes of interest
- Quantifying the amount of micro or macro strain occurring in the form of peak broadening or peak shifting

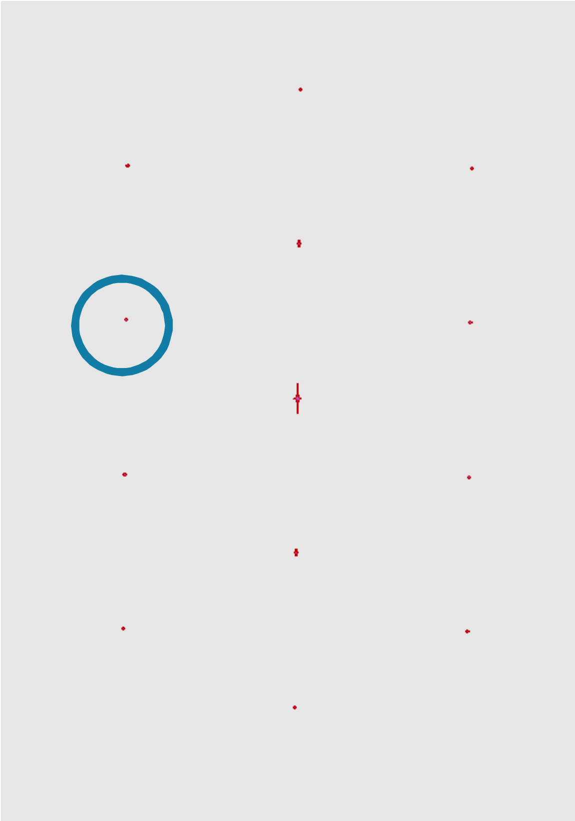
Progress Updates

- Purpose: Validate MD simulation can correctly generate SAED patterns
- Problem: SAED patterns being generated were not aligning with known SAED patterns
- Solution: Threshold intensity to minimum 10,000 to reduce noise yet not cut off signal
  - In addition correctly scale intensity range to show distribution.
    - Value of 10,000 is approximately 0.2% of maximum intensity
      - More thresholding can be done later if necessary in the process
- Outcome: Model SAED of perfect silicon align with Eddington reference patterns
  - Shown by matching 2 distinct angles on each pattern

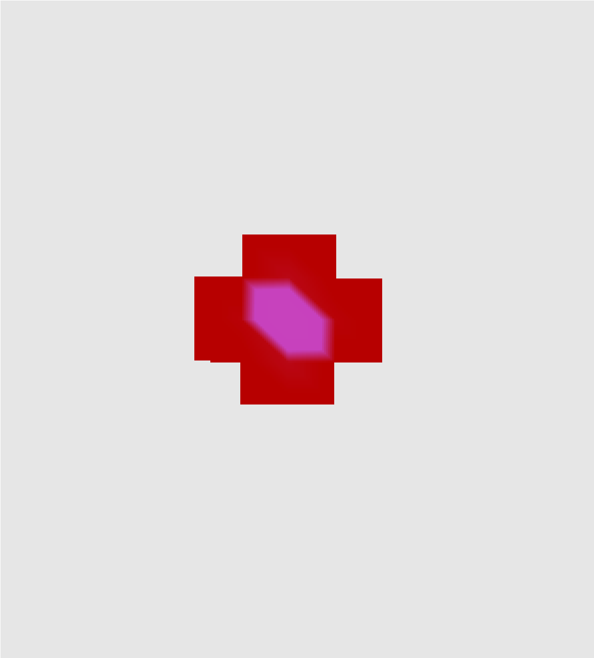
Before → After



[012] Raw Data has a lot of noise

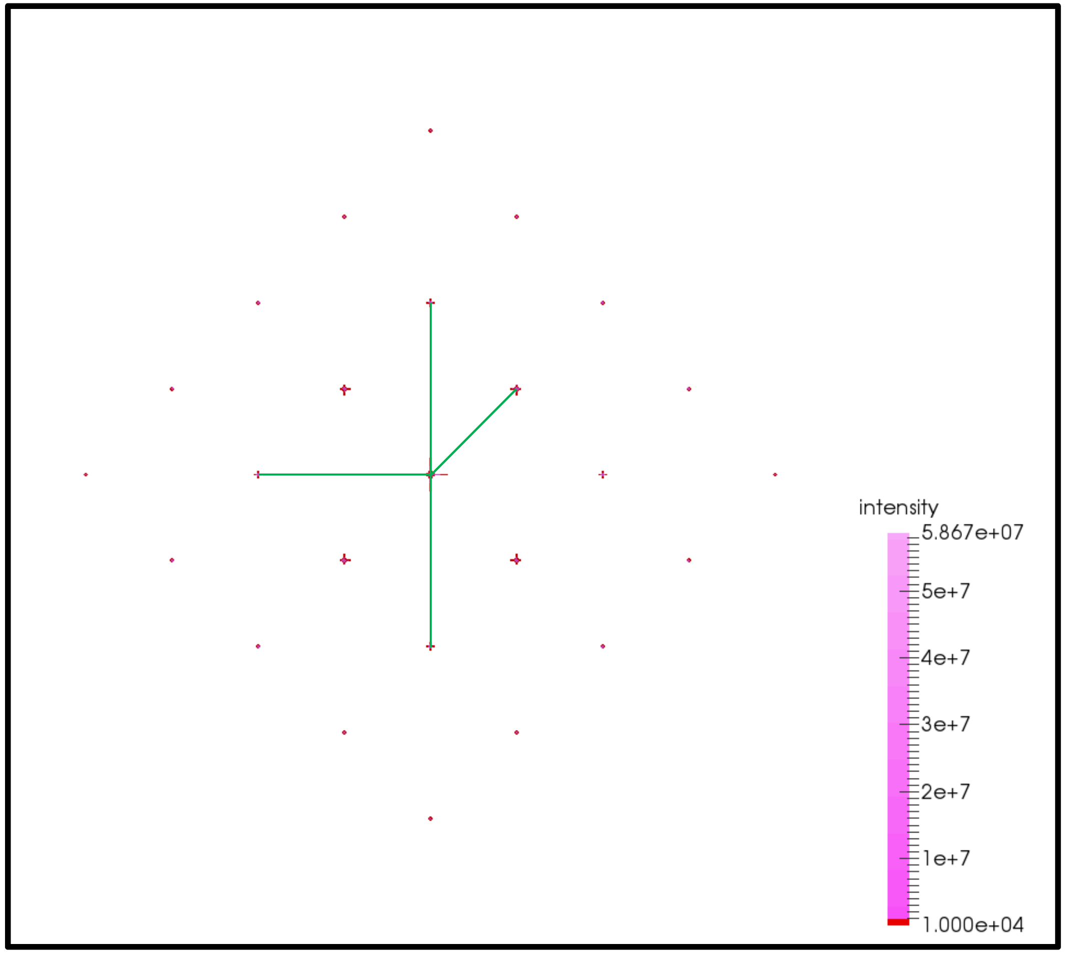


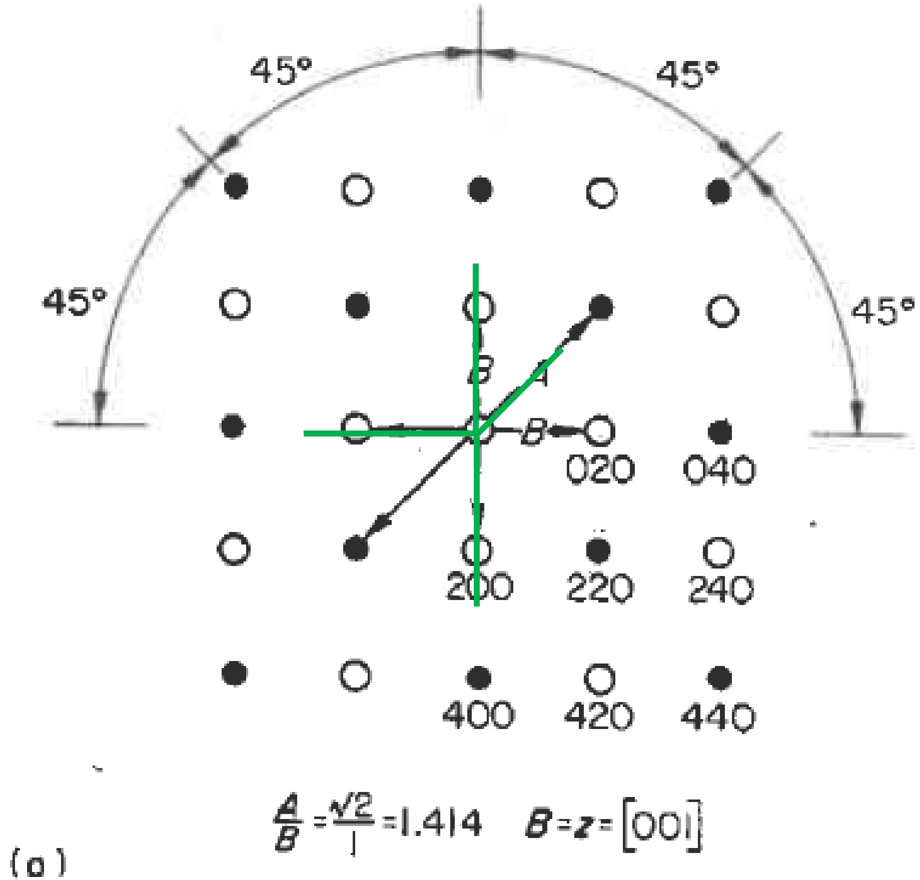
[012] Thresholded at 10k to remove most noise but not signal



<$\bar{2}\bar{4}2$> in [012] Showing distinct diffraction spot surrounded by some noise

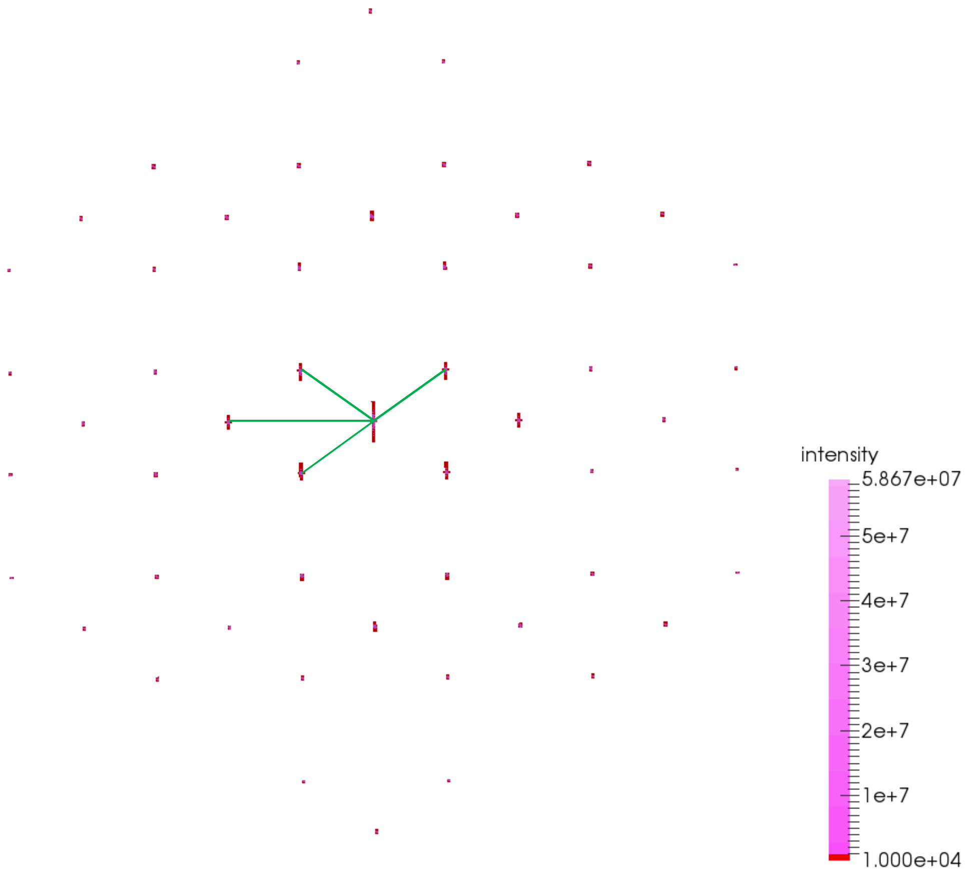
[001]



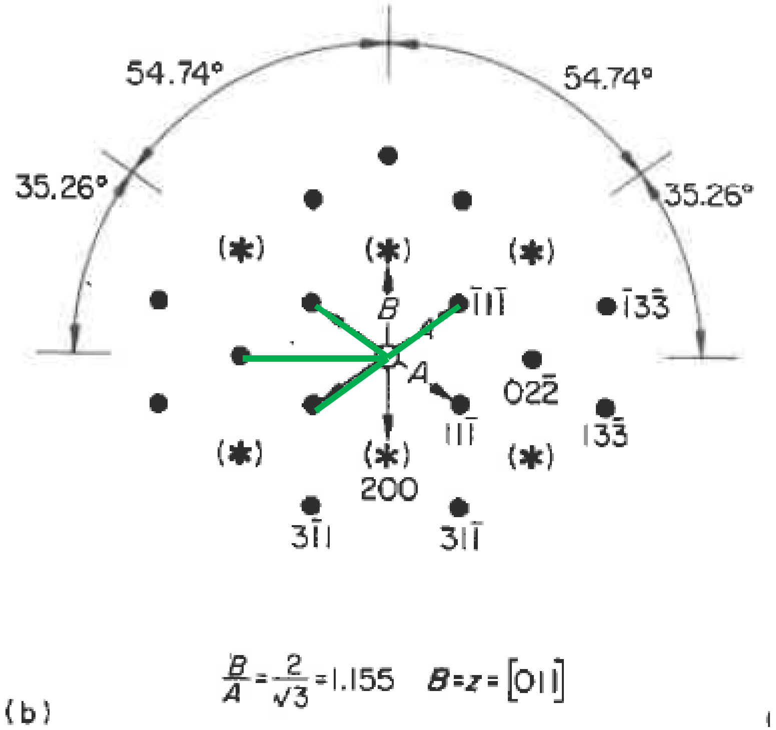


Note: Because of zooming in to see SAED patterns in Paraview. Distances will be off but angles stay true and show that patterns match

[011]

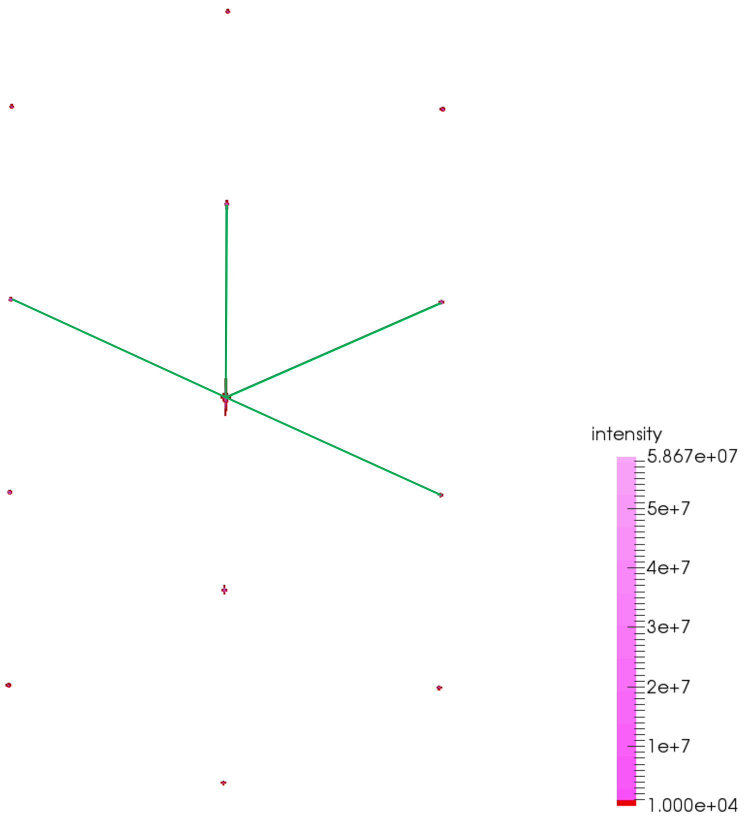


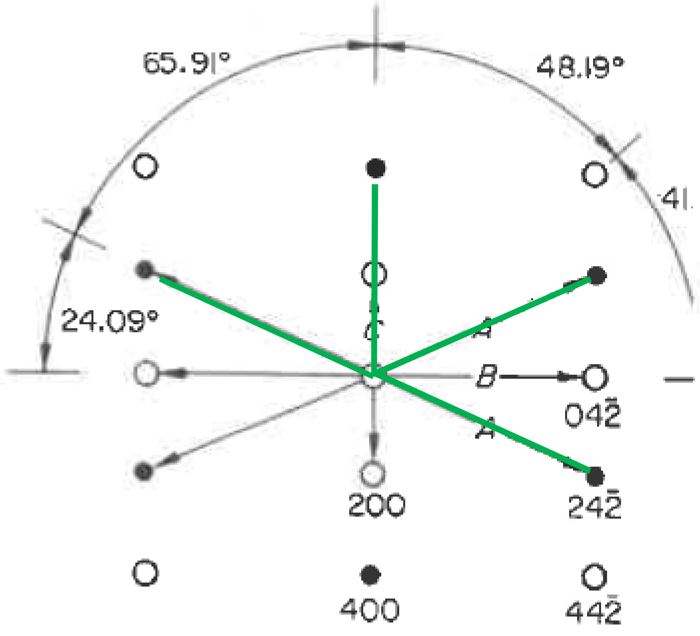
intensity
5.867e+07
5e+7
4e+7
3e+7
2e+7
1e+7
1.000e+04



54.74°
54.74°
35.26°
35.26°
B
A
1̄11̄
1̄33̄
022̄
133̄
111̄
200
31̄1
311̄
(b)
$\frac{B}{A} = \frac{2}{\sqrt{3}} = 1.155$ $B = z = [01\bar{1}]$

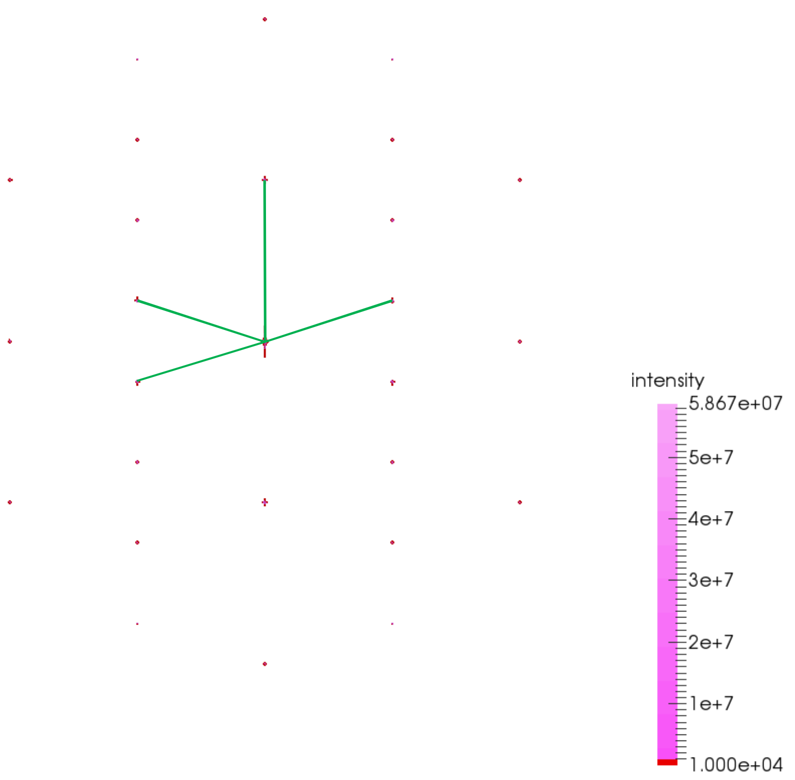
[012]





$\frac{A}{C} = \frac{\sqrt{24}}{\sqrt{4}} = 2.450 \quad \frac{B}{C} = \frac{\sqrt{20}}{\sqrt{4}} = 2.236 \quad B = z = [012]$

[013]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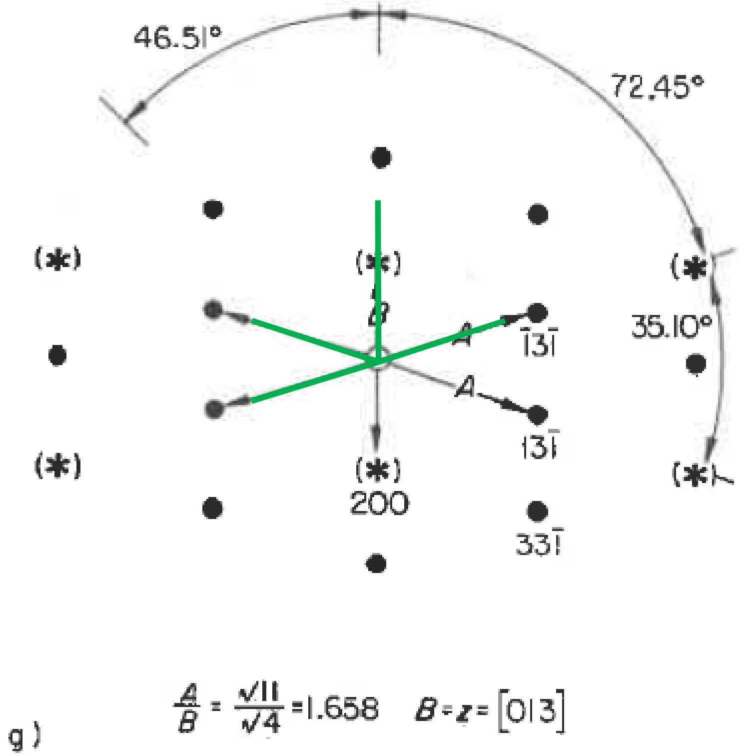
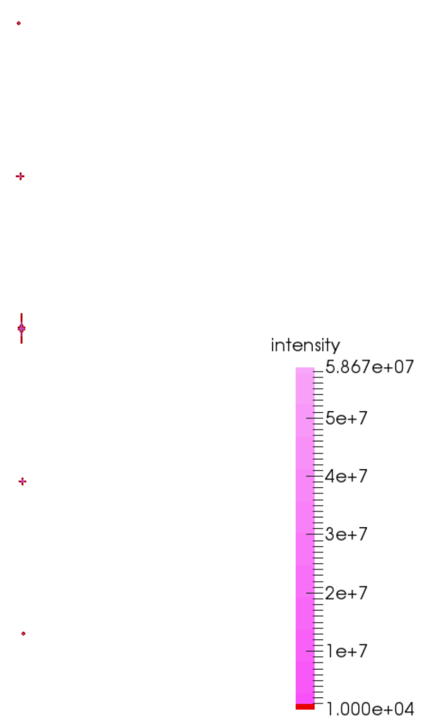
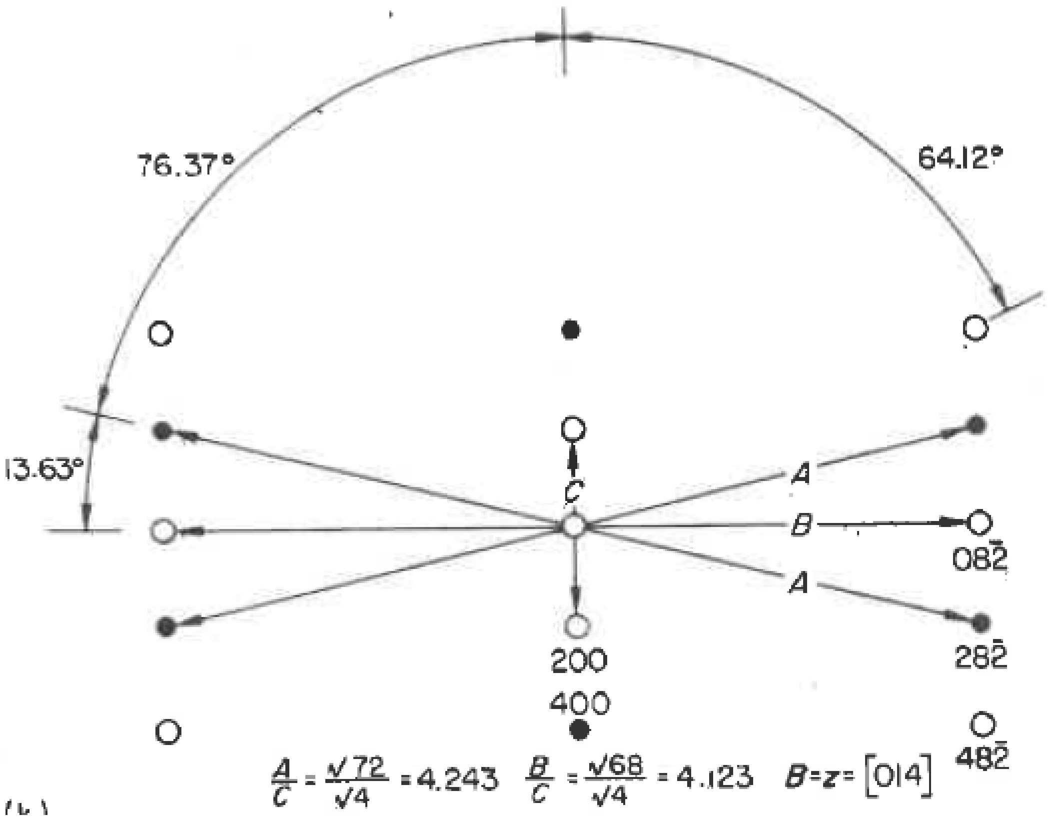
5.867e+07
5e+7
4e+7
3e+7
2e+7
1e+7
1.000e+04


46.51°
72.45°
35.10°
B
A
A
1̄31̄
131̄
200
331̄
g)
A/B = √11/√4 = 1.658 B = z = [013]

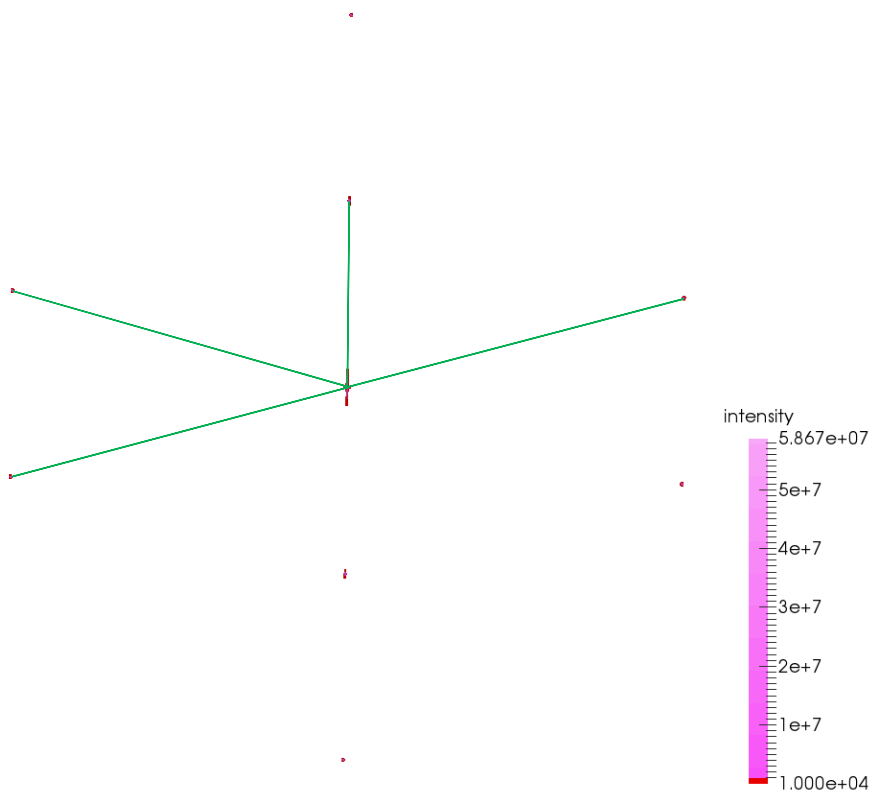
[014]



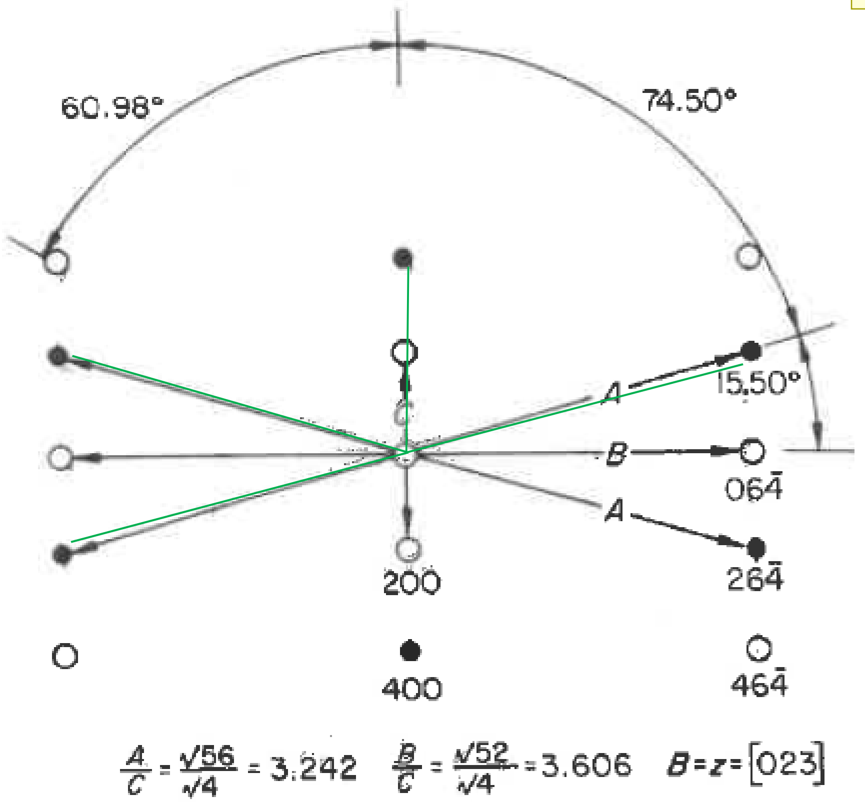


Reason for no exact match is likely due to thresholding value to remove noise and retain signal. No other reference SAED pattern has planes that go out as far as <#8#>

[023]


intensity
5.867e+07
5e+7
4e+7
3e+7
2e+7
1e+7
1.000e+04

FMU1

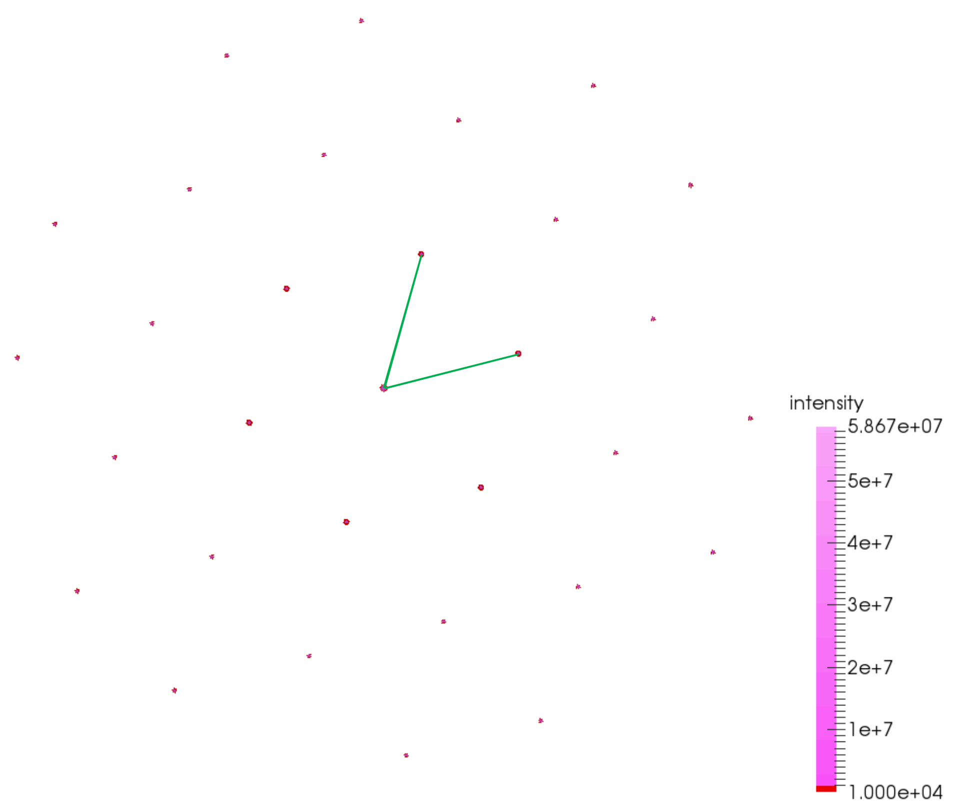

60.98°
74.50°
15.50°
A
B
A
C
064̄
200
264̄
400
464̄
A/C = √56/√4 = 3.242
B/C = √52/√4 = 3.606
B=z=[023]

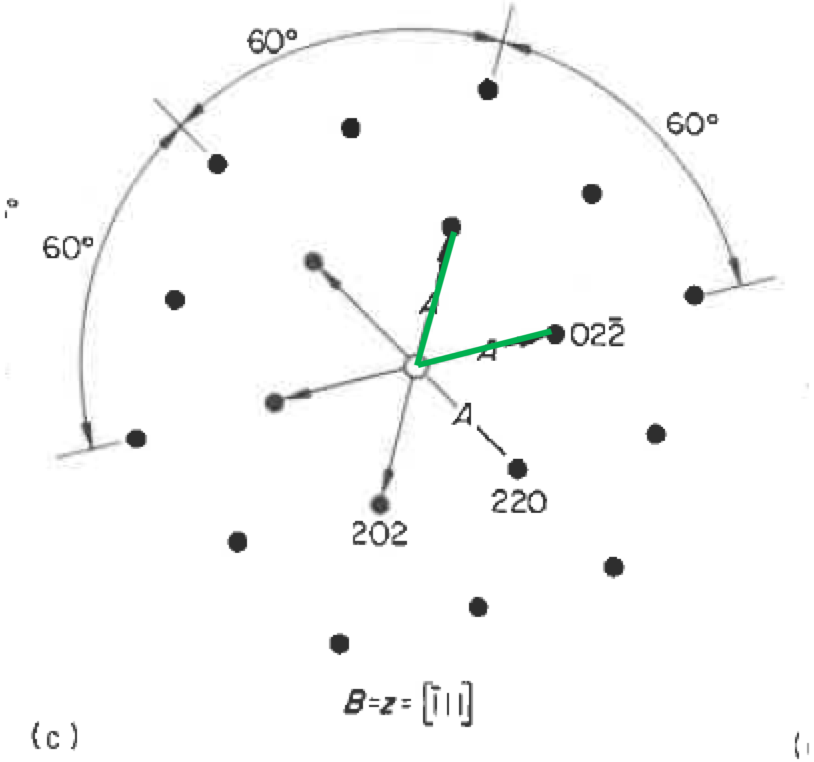
Slide 14

FMU1 check this

Franco, Manuel Uriel, 1/11/2017

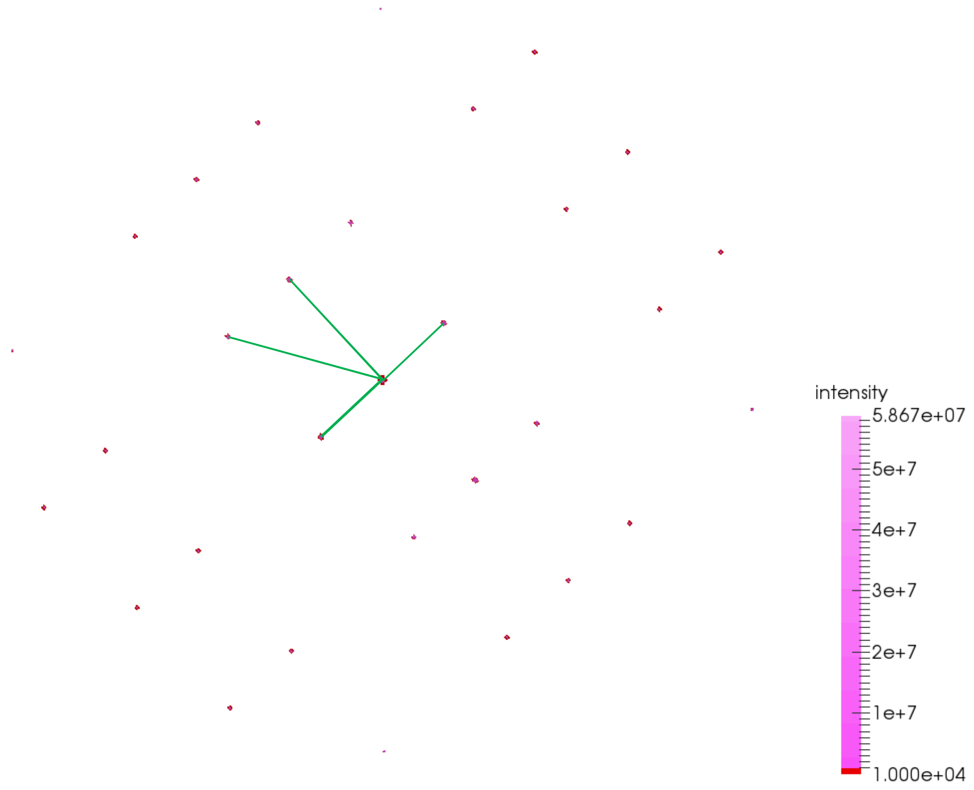
$[\bar{1}11]$



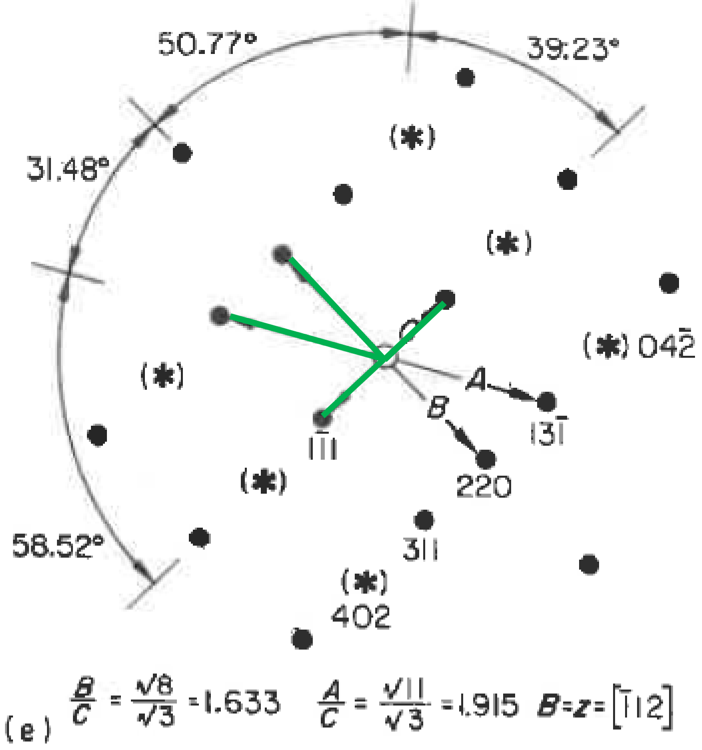


$B = z = [\bar{1}11]$

$[\bar{1}12]$

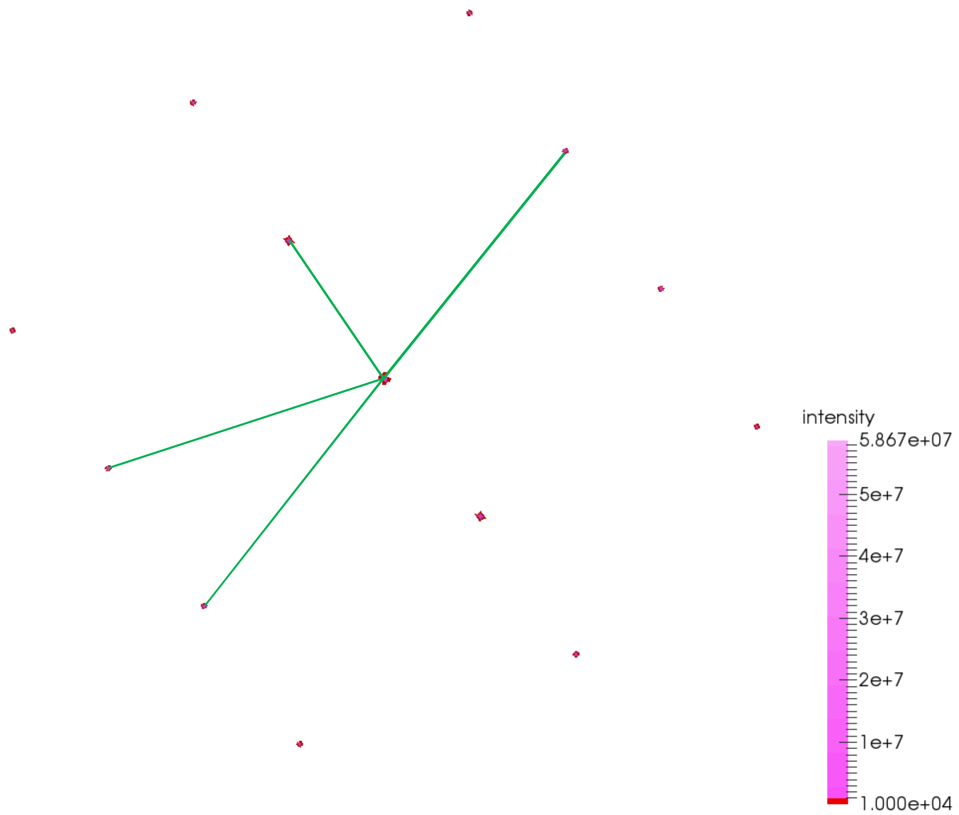


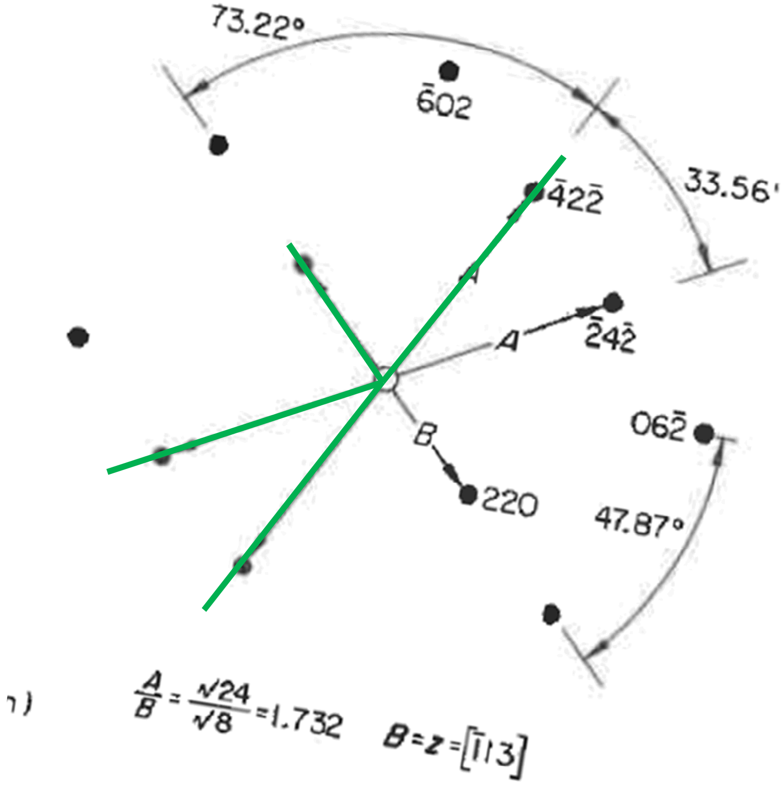
intensity
5.867e+07
5e+7
4e+7
3e+7
2e+7
1e+7
1.000e+04



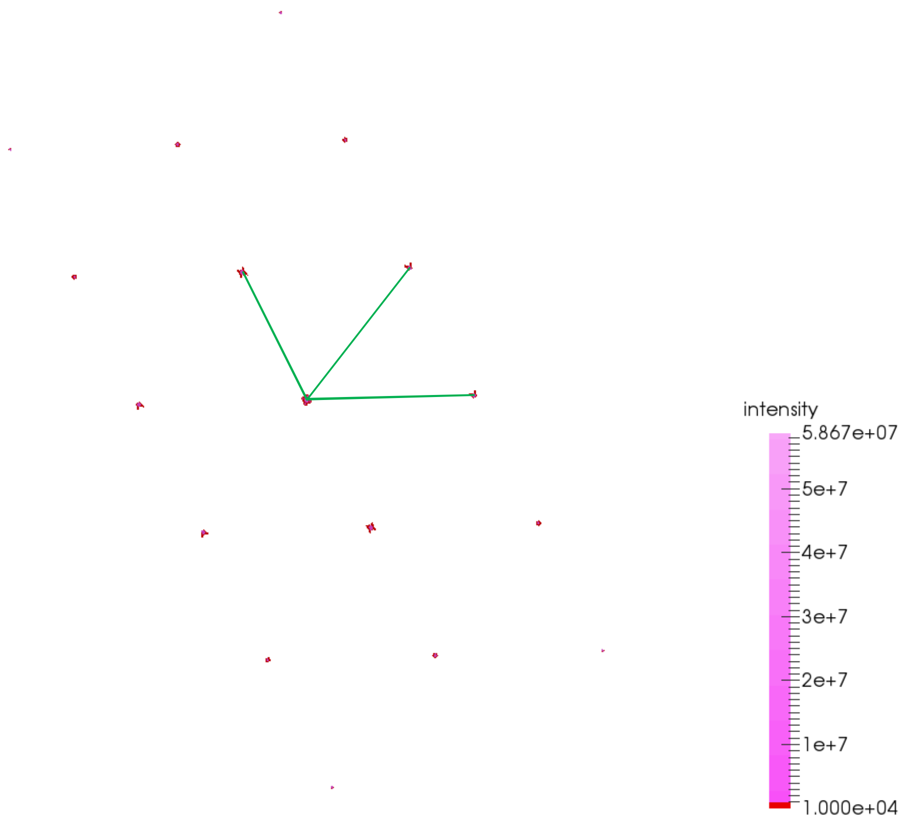
50.77°
39.23°
31.48°
58.52°
(✱)
(✱) 04$\bar{2}$
A
B
C
1$\bar{1}$1
13$\bar{1}$
220
3$\bar{1}$1
402
(e) $\frac{B}{C}=\frac{\sqrt{8}}{\sqrt{3}}=1.633$ $\frac{A}{C}=\frac{\sqrt{11}}{\sqrt{3}}=1.915$ $B=z=[\bar{1}12]$

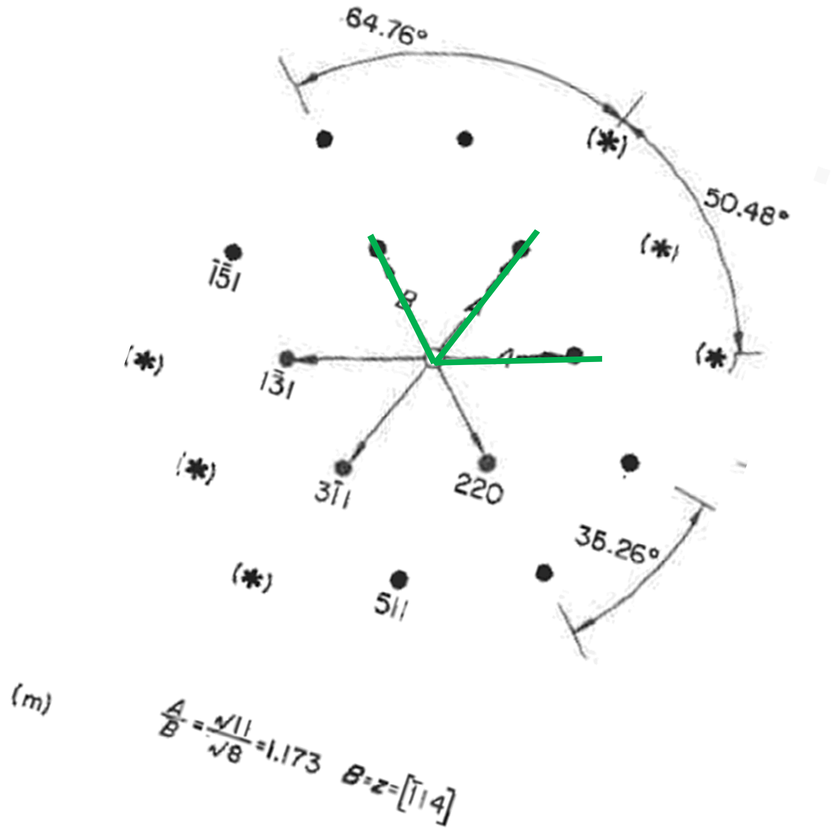
[$\bar{1}$13]


intensity
5.867e+07
5e+7
4e+7
3e+7
2e+7
1e+7
1.000e+04

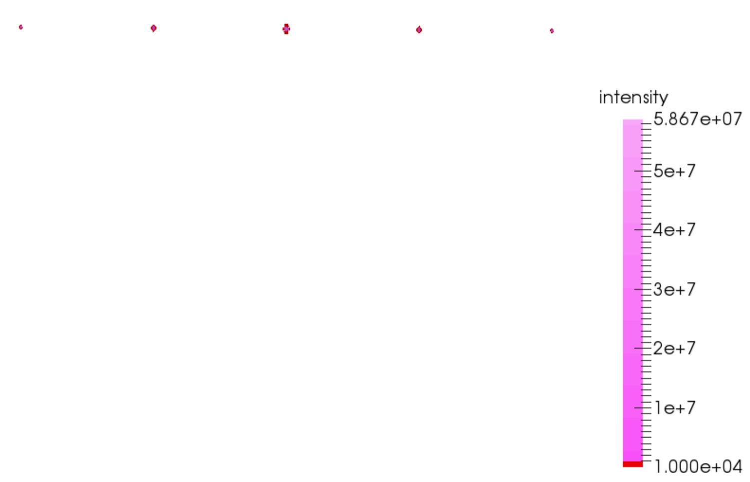

73.22°
$\bar{6}$02
$\bar{4}$2$\bar{2}$
33.56°
A
$\bar{2}$4$\bar{2}$
B
220
06$\bar{2}$
47.87°
$\frac{A}{B} = \frac{\sqrt{24}}{\sqrt{8}} = 1.732$ $B = z = [\bar{1}13]$

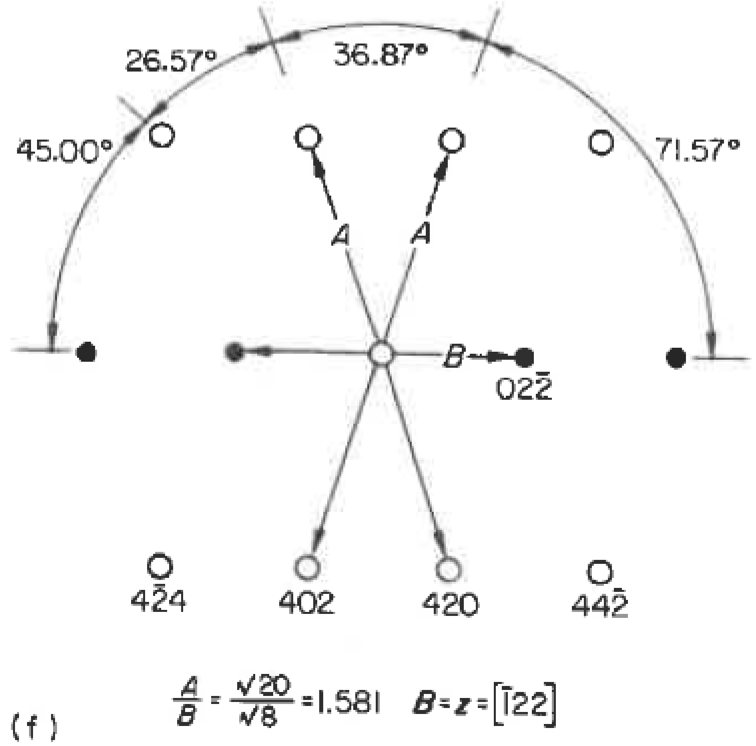
$[\bar{1}14]$


intensity
5.867e+07
5e+7
4e+7
3e+7
2e+7
1e+7
1.000e+04

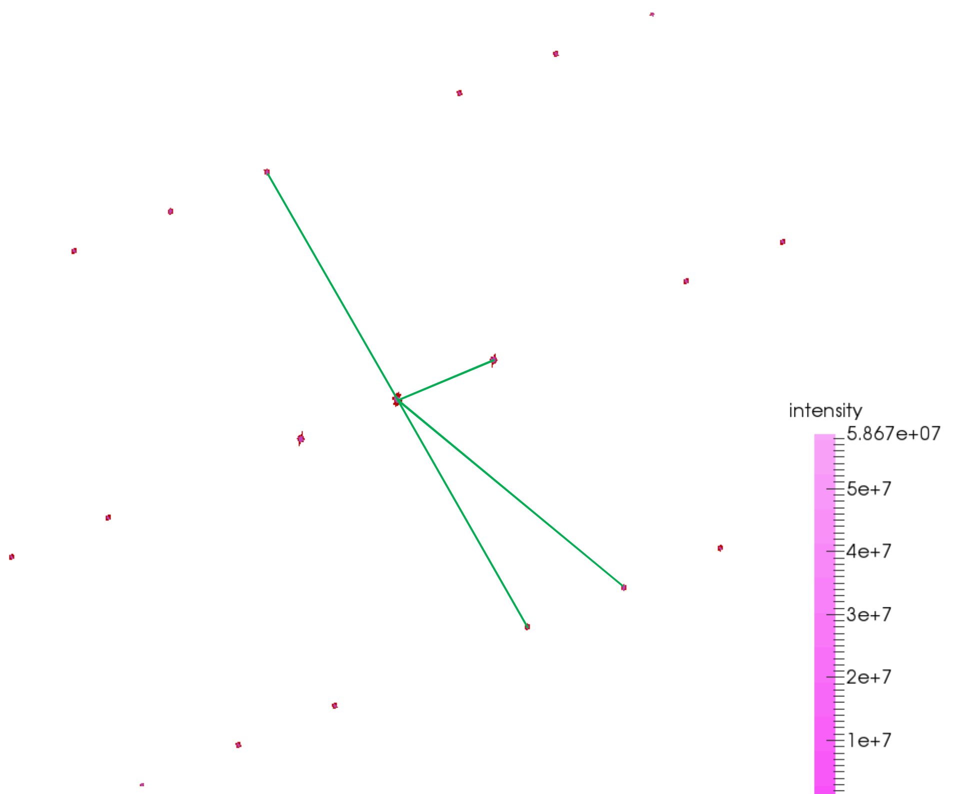

64.76°
50.48°
35.26°
(✱)
$\bar{1}\bar{5}1$
$1\bar{3}1$
$3\bar{1}1$
220
511
(m)
$\frac{A}{B} = \frac{\sqrt{11}}{\sqrt{8}} = 1.173$ $B = z = [\bar{1}14]$

[$\bar{1}22$]

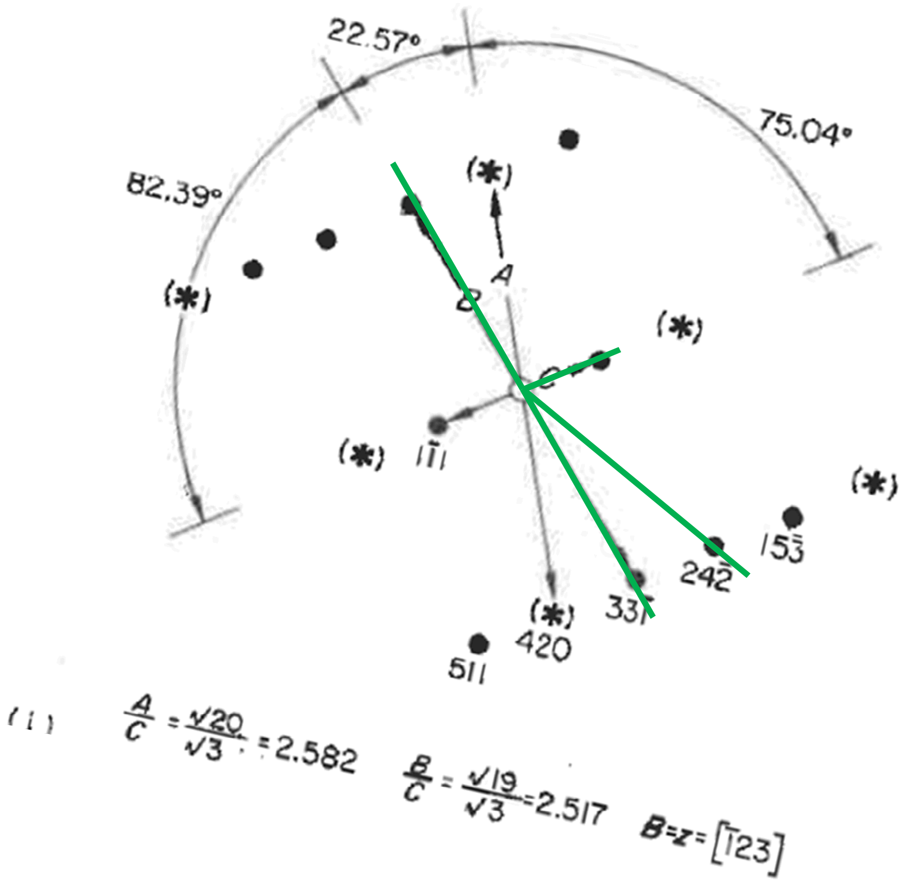

intensity
5.867e+07
5e+7
4e+7
3e+7
2e+7
1e+7
1.000e+04


26.57°
36.87°
45.00°
71.57°
A
A
B
02$\bar{2}$
4$\bar{2}$4
402
420
44$\bar{2}$
(f)
$\frac{A}{B} = \frac{\sqrt{20}}{\sqrt{8}} = 1.581$ $B = z = [\bar{1}22]$

$[\bar{1}23]$

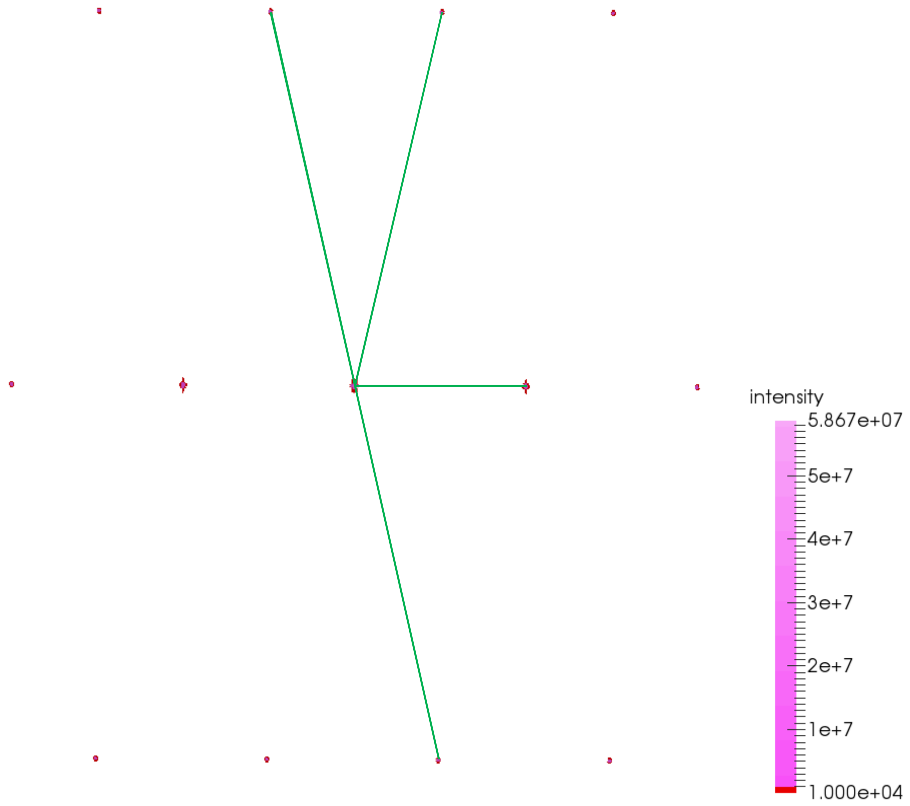


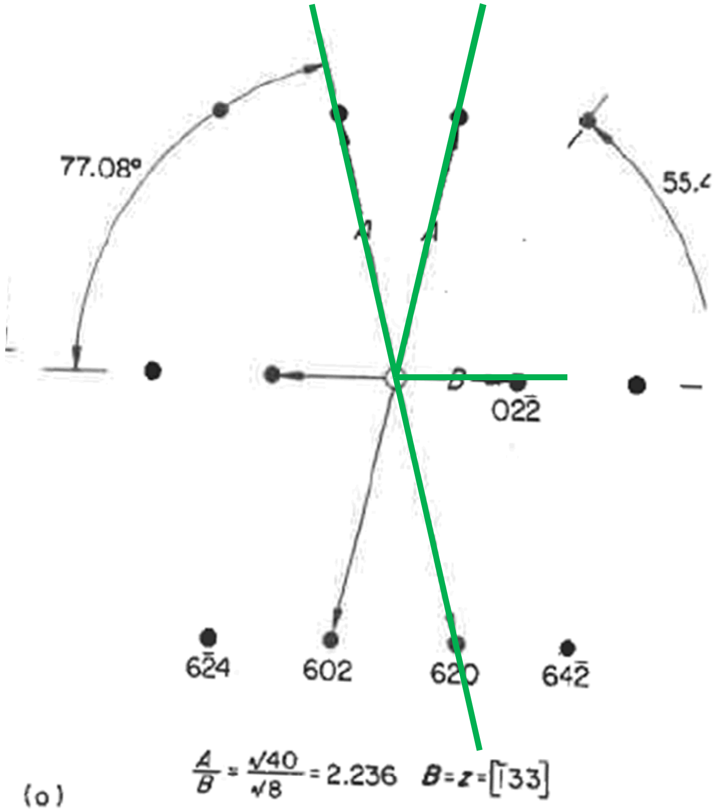
intensity
5.867e+07
5e+7
4e+7
3e+7
2e+7
1e+7
1.000e+04



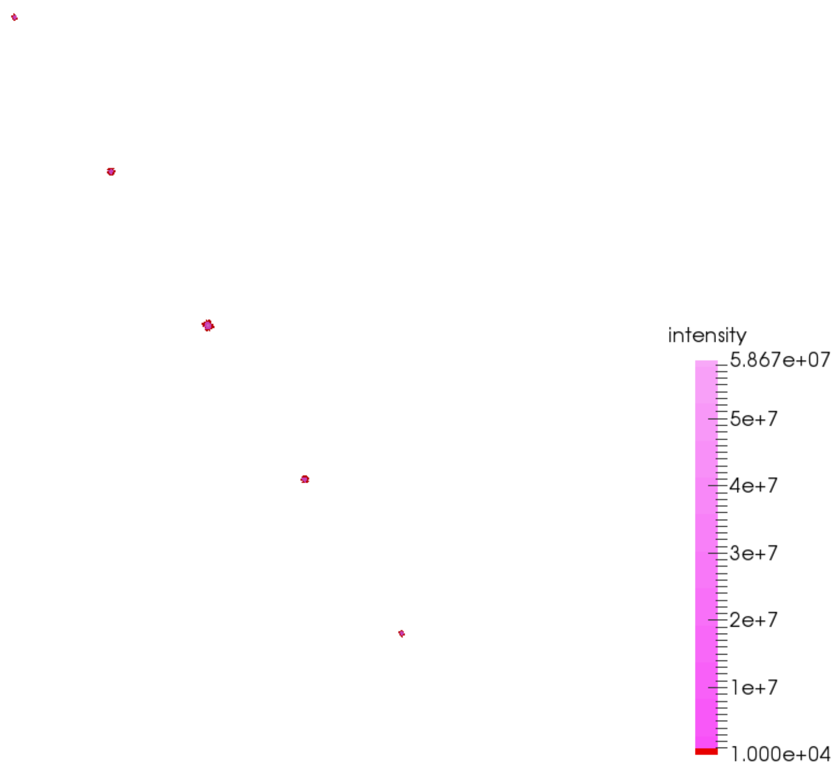
22.57°
75.04°
82.39°
A
B
C
(*)
1$\bar{1}$1
153
242
331
420
511
(i)
$\frac{A}{C} = \frac{\sqrt{20}}{\sqrt{3}} = 2.582$
$\frac{B}{C} = \frac{\sqrt{19}}{\sqrt{3}} = 2.517$
$B = z = [\bar{1}23]$

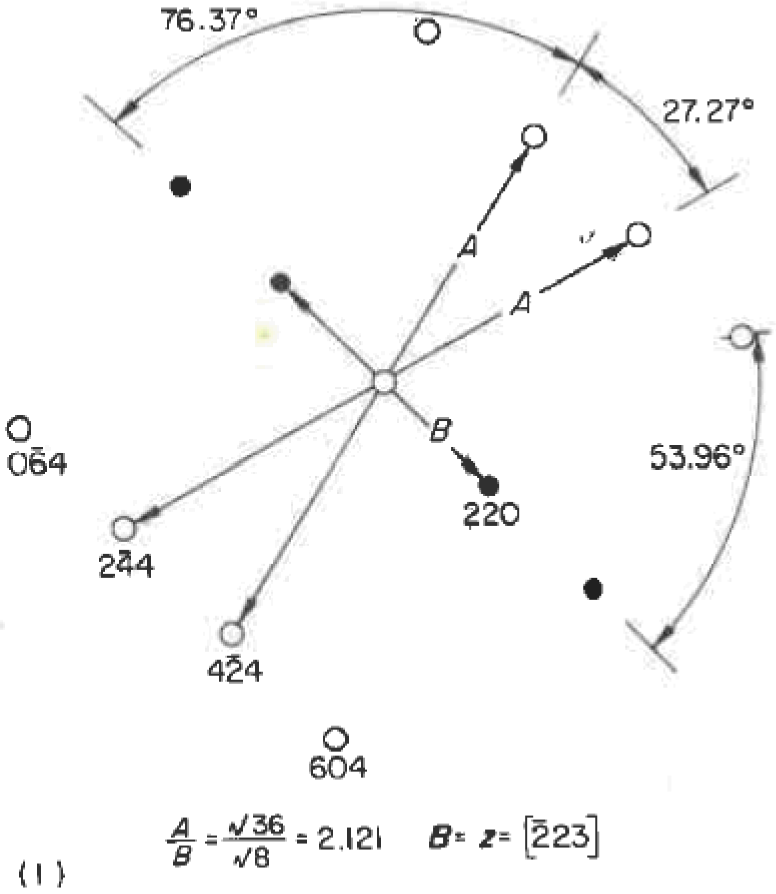
$[\bar{1}33]$


intensity
5.867e+07
5e+7
4e+7
3e+7
2e+7
1e+7
1.000e+04

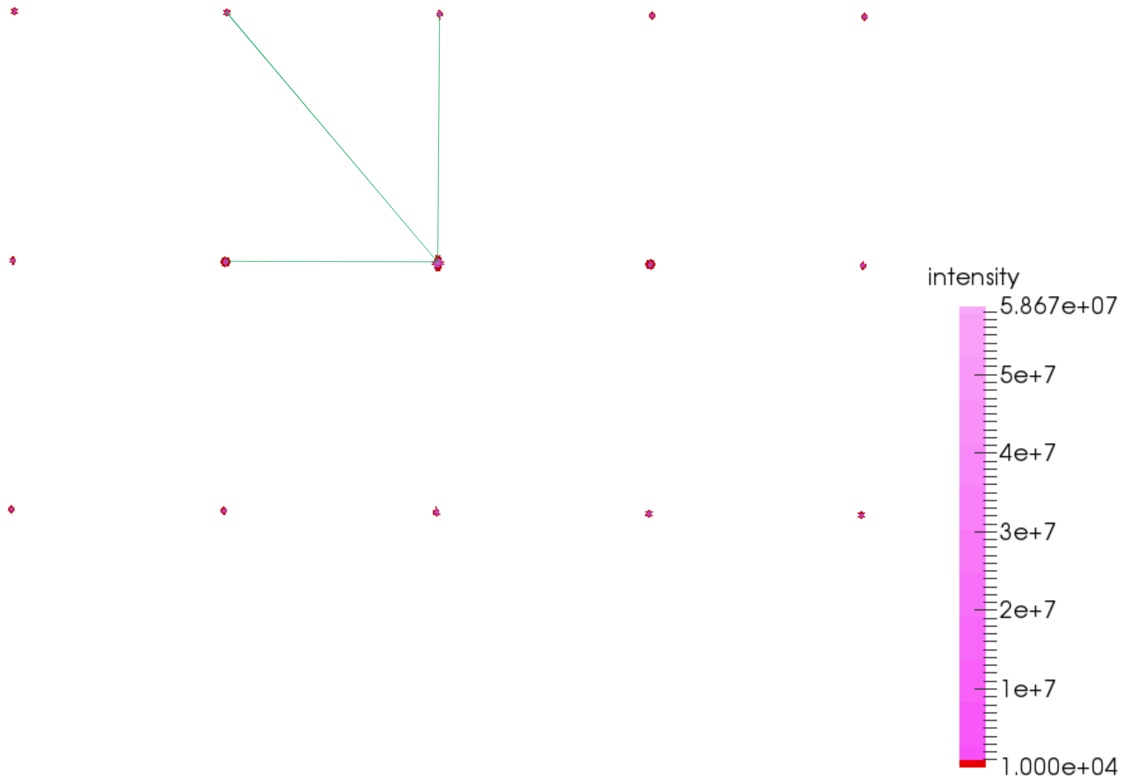

77.08°
55.4
02$\bar{2}$
6$\bar{2}$4
602
620
64$\bar{2}$
(o)
$\frac{A}{B} = \frac{\sqrt{40}}{\sqrt{8}} = 2.236$ $B = z = [\bar{1}33]$

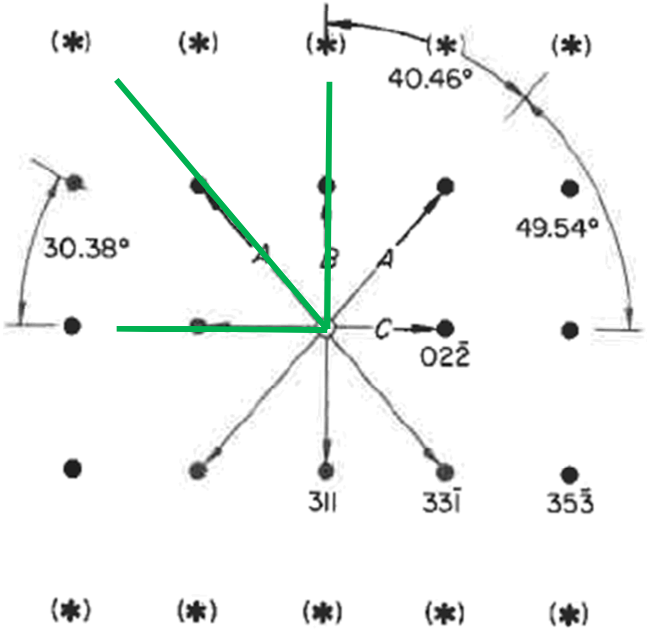
$[\bar{2}23]$


intensity
5.867e+07
5e+7
4e+7
3e+7
2e+7
1e+7
1.000e+04


76.37°
27.27°
53.96°
A
A
B
0$\bar{6}$4
2$\bar{4}$4
4$\bar{2}$4
220
604
$\frac{A}{B} = \frac{\sqrt{36}}{\sqrt{8}} = 2.121$
B = z = $[\bar{2}23]$
(1)

$[\bar{2}33]$





(n) $\frac{A}{C} = \frac{\sqrt{19}}{\sqrt{8}} = 1.541$ $\frac{B}{C} = \frac{\sqrt{11}}{\sqrt{8}} = 1.173$ $B = z = [\bar{2}33]$

Next Steps

- Generate algorithm or scripts to quickly identify center of diffraction points on an SAED pattern corresponding to known d-spacings and planes.
  - Using ParaView isolate a volume of space surrounding a diffraction sphere using the identified center points
    - Take difference of (Damaged – Perfect) Diffraction Sphere to identify peak shifting or peak broadening phenomena
      - Generate algorithm to make 2 separate difference pole plots (one for broadening and one for shifting) to identify planes of interest that would drive future experimental work from the modeling data

References

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   http://hazeslab.med.ualberta.ca/tutorials/data_collection/ewald/ewald-sphere.html
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