Debye-Scherrer and Laue methods in exploring structure of NaCl and Si

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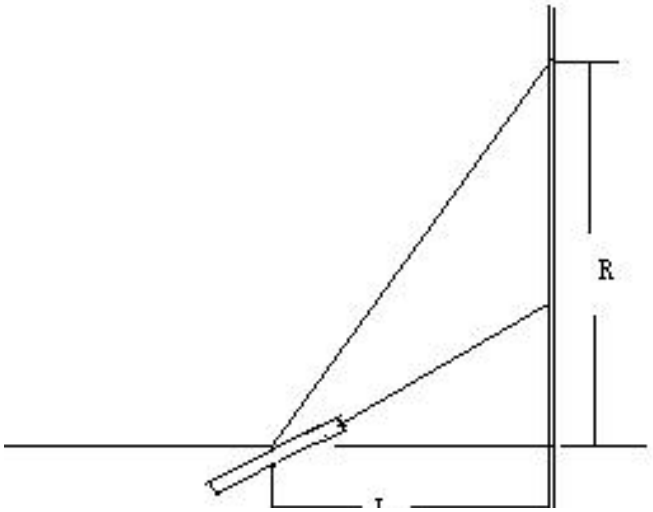
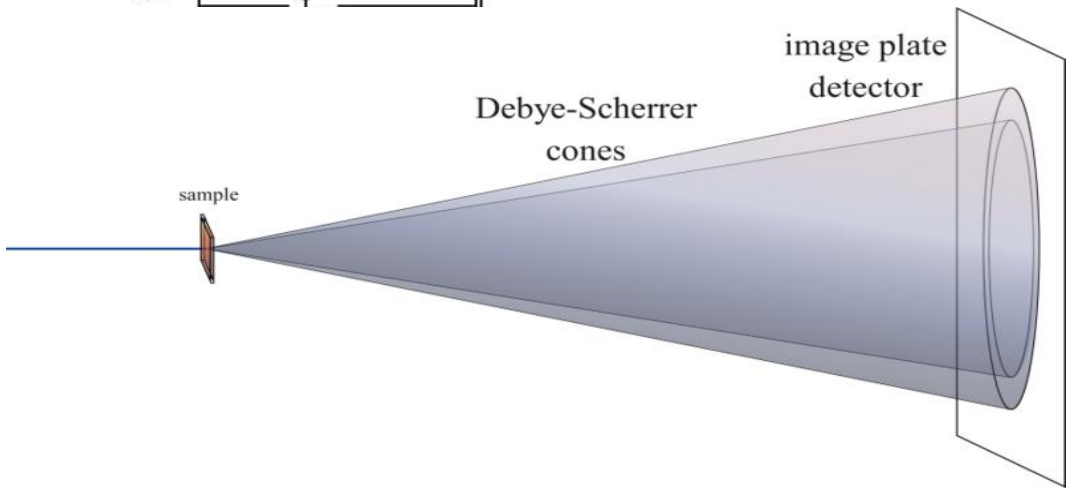
Outline

- Principles
- Results
- Data analysis

Debye-Scherrer methods



Bragg diffraction



Debye ring

Equpiment

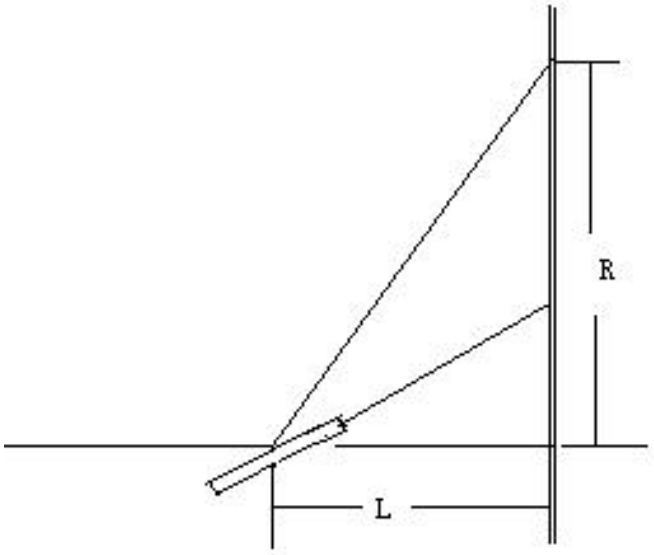
Debye picture of NaCl

Bragg's angle is given by the expression:

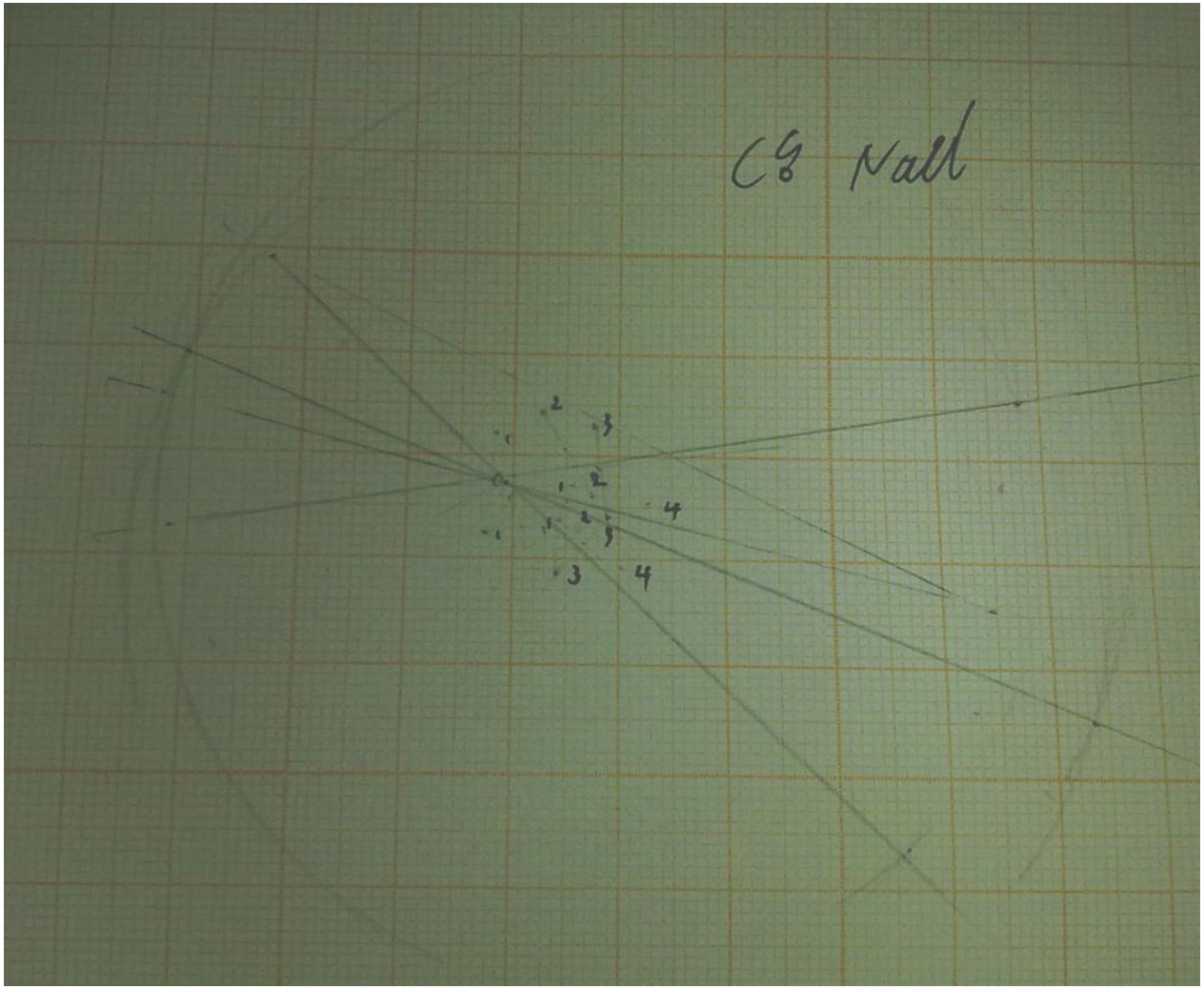
$$\theta = \frac{1}{2}\arctan\frac{R}{L} \cdots\cdots(1) \qquad 2d\sin\theta = \lambda \cdots\cdots(2)$$

$$d = \frac{a}{\sqrt{h^2 + k^2 + l^2}} \cdots\cdots(3)$$

$$\sin^2\theta = \frac{\lambda^2}{4a^2}(h^2 + k^2 + l^2)$$



Calculating Radius



$radius/mm$	$\theta/°$	$\sin\theta$	$\sin^2\theta$	$\sin^2\theta_1 : \sin^2\theta_i$
5.55	15.51	0.267	0.072	1
7.89	21.53	0.367	0.135	1.875
9.90	26.34	0.444	0.197	2.736
13.63	34.27	0.563	0.317	4.4

$$\sin^2\theta_1 : \sin^2\theta_i = (h^2 + k^2 + l^2) : (h_a{}^2 + k_b{}^2 + l_c{}^2)$$

$$f_{total} = \sum_{n} f_n \exp[-2\pi i(xh + yk + zl)]$$

in face centered cubic lattices, there has

f = 0 if odd and even coexist in h, k and l

f = f+f’ if the indices h, k and l are either all even or odd

This part involving some guess

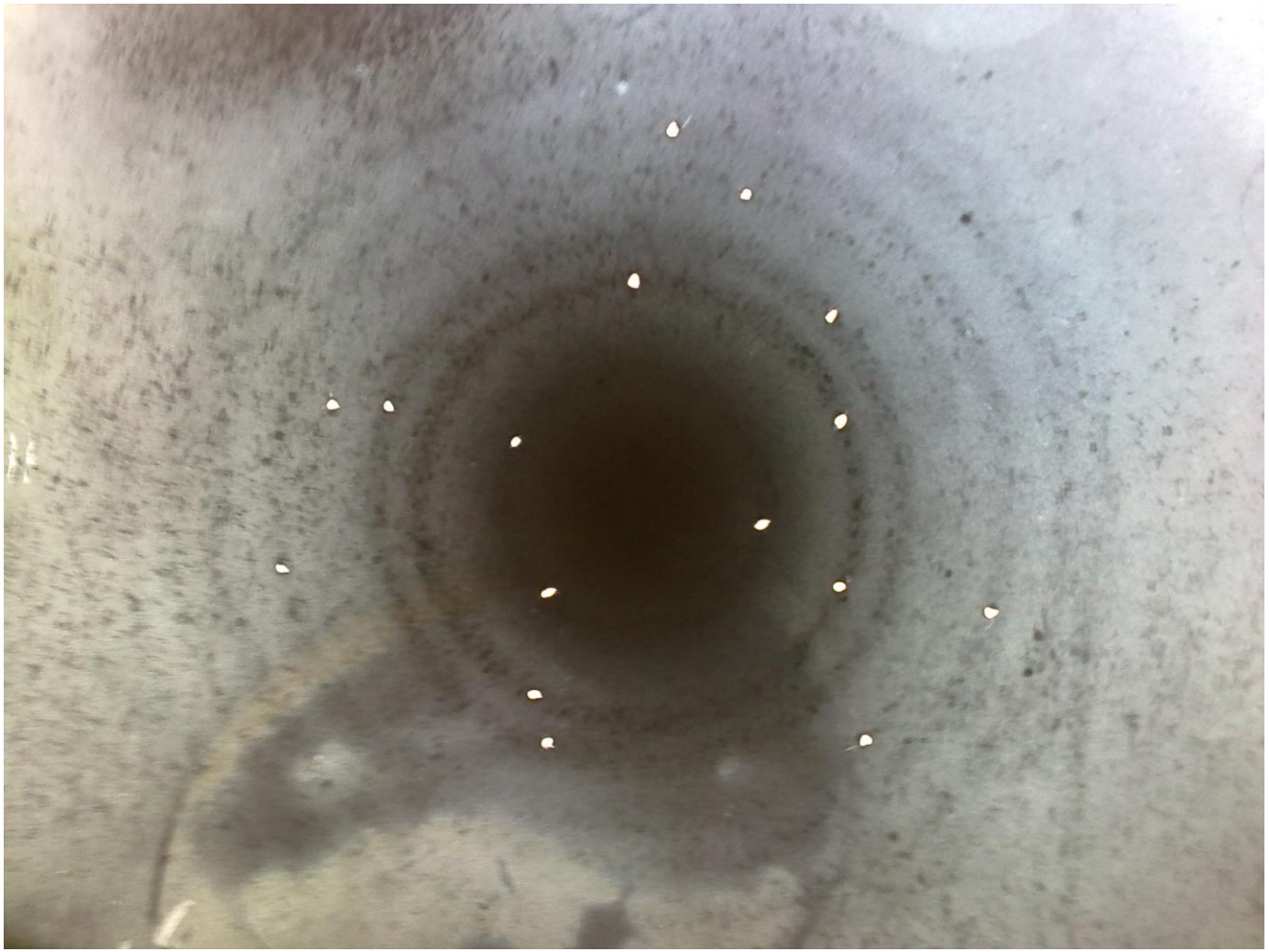
hlk	$\frac{h^2+l^2+k^2}{1+1+1}$	$\frac{h^2+l^2+k^2}{2^2+0+0}$	$\frac{h^2+l^2+k^2}{2^2+2^2+0}$	**Experiment data**
1 1 1	1	-	-	
2 0 0	1.33	1	-	1
2 2 0	2.67	2	1	1.875
3 1 1	3.67	2.75	1.375	2.736
2 2 2	4	3	1.5	
4 0 0	5.33	4	2	
3 3 1	6.33	4.75	2.375	4.4
4 2 2	8	6	3	
4 4 0	10.67	8	4	

Use h,l,k calculating a

$$a = \frac{\lambda}{2\sin\theta}\sqrt{h^2 + k^2 + l^2}$$

- We get 531pm,542pm, 521.9pm,530pm for a for each four point and get average a for 531.23pm
- Comparing with standard a=564.02pm, we have c%=5.8%

Same for Silicon



Calculating ratio

$radius/mm$	$\theta/°$	$\sin\theta$	$\sin^2\theta$	$\sin^2\theta_1 : \sin^2\theta_i$
5.83	8.5	0.147	0.0218	1
8.34	11.5	0.199	0.0390	1.7
10.82	14.2	0.245	0.0602	2.7
12.44	15.9	0.273	0.0750	3.4
14.50	17.95	0.308	0.0949	4.3

Guess again

hlk	$\frac{h^2+l^2+k^2}{2^2+0+0}$	$\frac{h^2+l^2+k^2}{2^2+2^2+0}$	$\frac{h^2+l^2+k^2}{2^2+2^2+2^2}$	**Experiment data**
2 0 0	1	-	-	
2 2 0	2	1	-	1
2 2 2	3	1.5	1	1.7
4 0 0	4	2	1.33	
4 2 0	5	2.5	1.67	2.7
4 2 2	6	3	2	3.4
4 4 0	8	4	2.67	
4 4 2	9	4.5	3	4.3

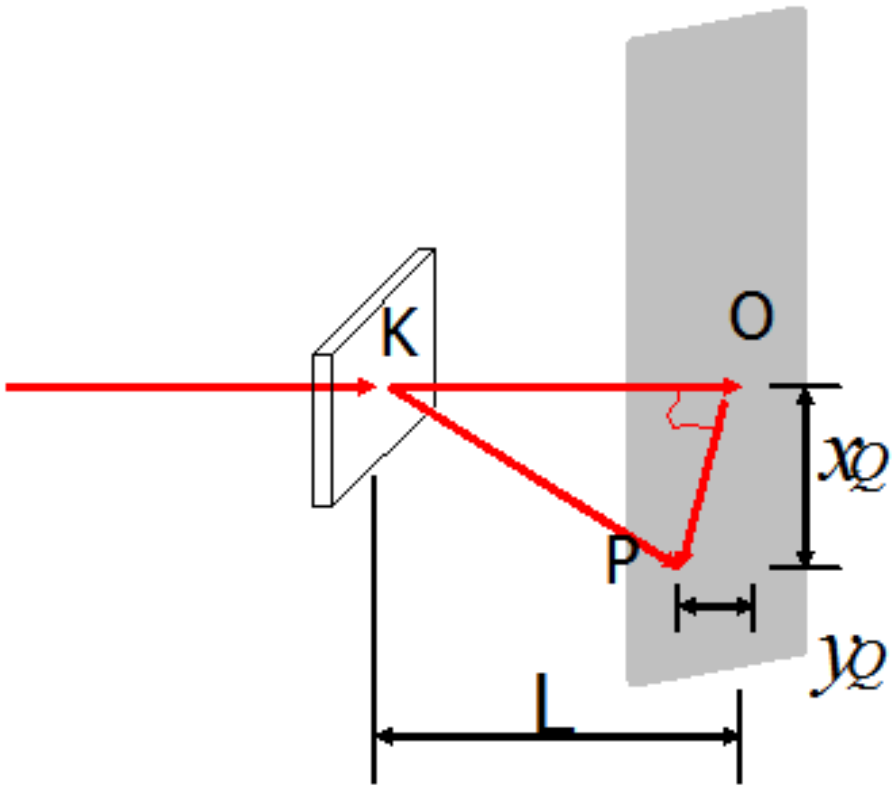
Oops!

- Lattice constant=686.01pm,622.9pm，653.57pm,641.08pm,697.95pm.
- Average=660.32pm,comparing with 543.1pm ,c%=22%.

- If use the first set of calculation

  Average=508.7pm ,c%=6.3%.

Laue Methods



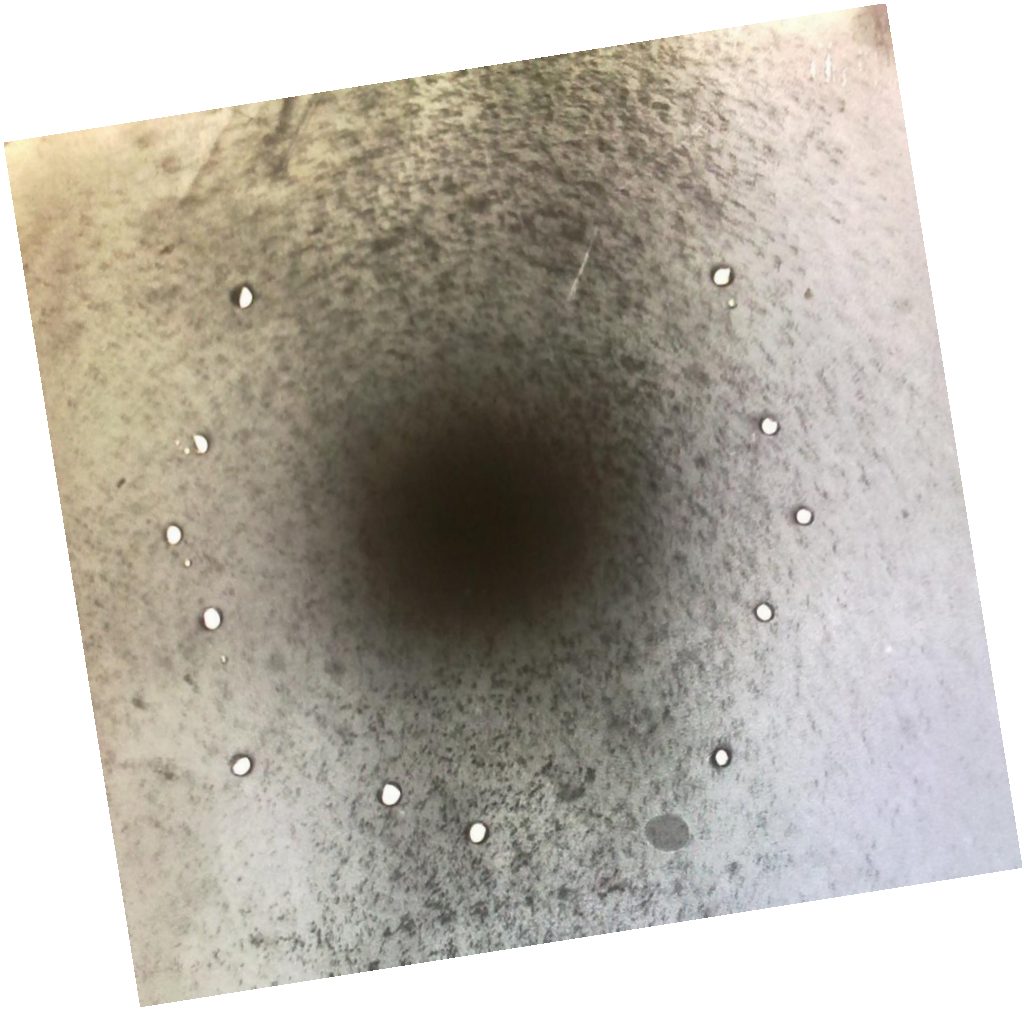
$$\tan\theta = \frac{\sqrt{x_Q^2 + y_Q^2}}{L}$$

$$\tan\theta = \frac{z_Q}{\sqrt{x_Q^2 + y_Q^2}}$$

$$z_Q = \sqrt{x_Q^2 + y_Q^2 + L^2} - L$$

$$h : k : l = x_Q : y_Q : z_Q$$

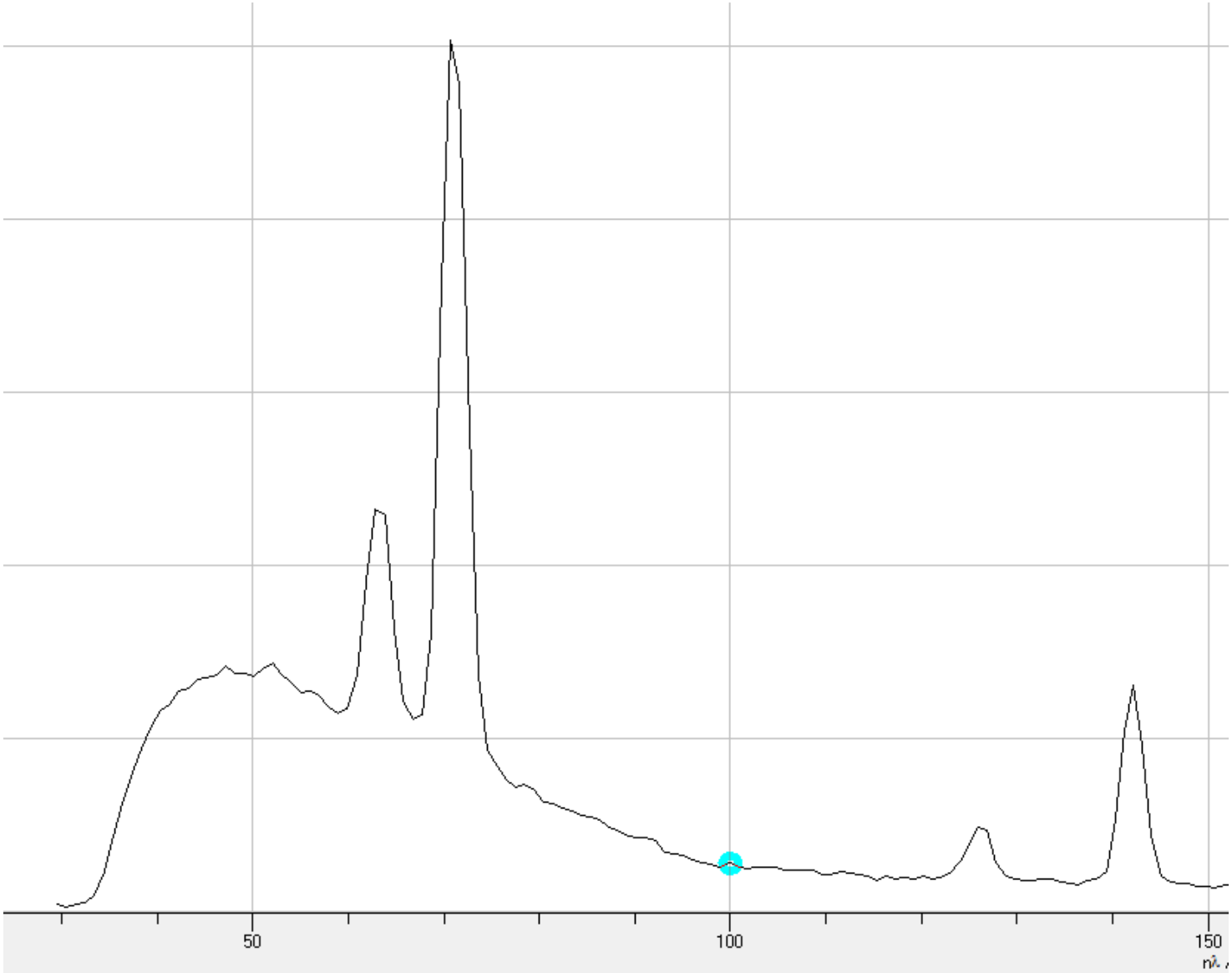
Laue picture for NaCl



Calculating λ

$(x, y)/mm$	$x_Q : y_Q : z_Q$	$h:k:l$	$\theta/°$	λ/pm
-12.5,12.5	-12.5:12.5:6.9	-4,4,2	21.32	68.35pm
-12.5,-12.5	-12.5:-12.5:6.9	-4,-4,2	21.32	…
12.5:-12.5	12.5:-12.5:6.9	4,-4,2	21.32	…
12.5,12.5	12.5:12.5:6.9	4,4,2	21.32	…
14,4.5	14:4.5:4.8	6,2,2(3,1,1)	18.08	52.83(105.66)
14,-4.5	14:-4.5:4.8	6,-2,2(3,-1,1)	18.08	…
…	…	…	…	…
…	…	…	…	…
0,-15.5	0:-15.5:5.3	0,-6,2	18.43	56.39pm

XRD for NaCl



Conclusion

XRD is a good way to sound evidence of the wave property of the x-ray, yet not so convincing tools to determine the lattice structure.

Debye method is more convenient than Laue method. It’s cheap in samples and has low requirement for x-ray source.

Disadvantage in experiment involves the overexposure in the central area, and the method to read the radius can also bring about inaccuracy.

Finally, it’s good to combine the theory studied in the Solid State Physics with experiment and solve some problems.

Thanks my partner Wu Hao

Pro.Yu and Pro.Le for supporting.

Thanks for attention!