

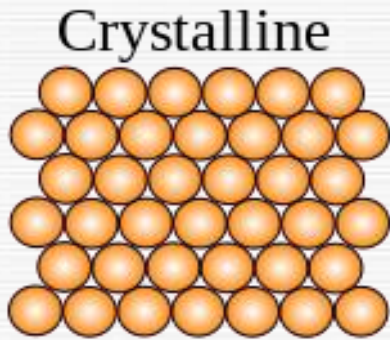
Crystal size from Xrd

Xuanyuan Jiang

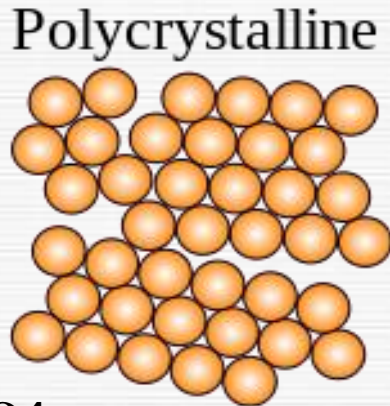
2016-01-20

What is a crystal and crystal size?

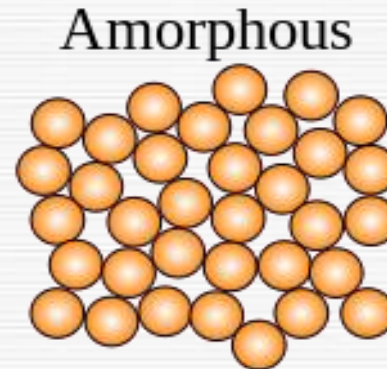
- Periodically arranged atoms.



**RFeO₃, Fe₃O₄, NiCo₂O₄
from PLD**



**Organic film
(CA, 3HPLN, BIPY)
from EvoVac**



**Organics (Alq₃)
metals
(Al, Co, Pd),
oxides (SiO₂)
from EvoVac**

- Single crystal size in polycrystal

Why do we need to find out crystal size?



How to calculate crystal size?

- From Xrd peak position and peak width

Scherrer equation

$$\tau = \frac{K\lambda}{\Delta(2\theta)\cos\theta}$$

- Due to

$$S(q) = \frac{1}{N} \frac{\sin^2(Nqa/2)}{\sin^2(qa/2)} \sim N$$

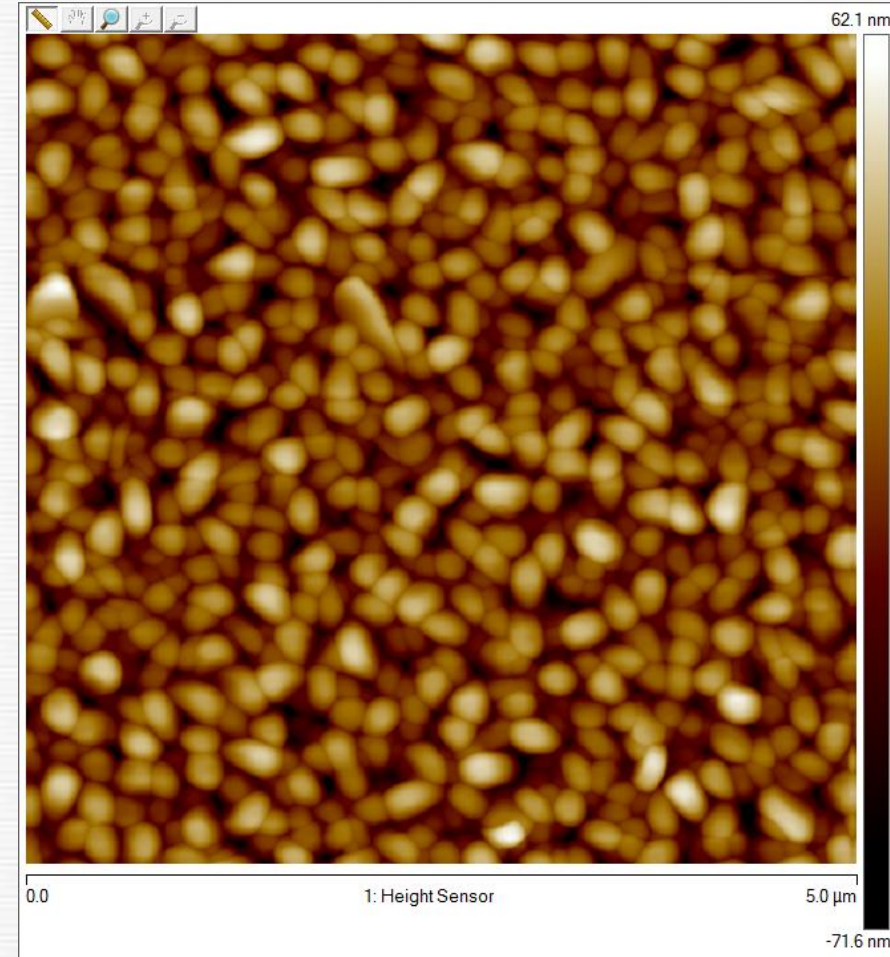
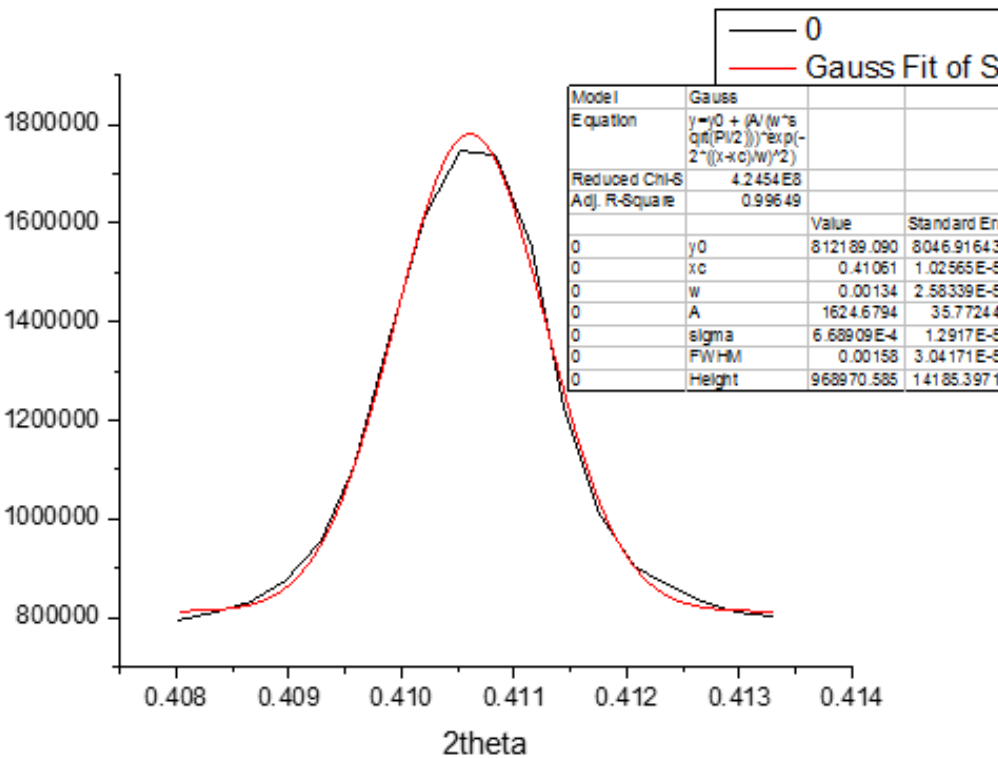
Take $S(q+\Delta q) = N/2$

$$\rightarrow \tau = Na = \frac{5.56}{\Delta q}$$

Plus $q = (4\pi/\lambda)\sin\theta$

$$\rightarrow \tau = \frac{K\lambda}{\Delta(2\theta)\cos\theta}$$

Example: CA 200nm RT growth film



$$\tau = \frac{K\lambda}{\Delta(2\theta)\cos\theta}$$

$$= \frac{0.9 * 1.033}{0.00134 * \cos(0.2053)}$$

$$= 70.8\text{nm}$$

From AFM, smallest crystal is ~80nm, average crystal size ~170nm.