Area detector diffraction: thin films, pole figures, organic semiconducting films

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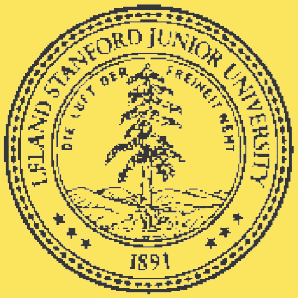

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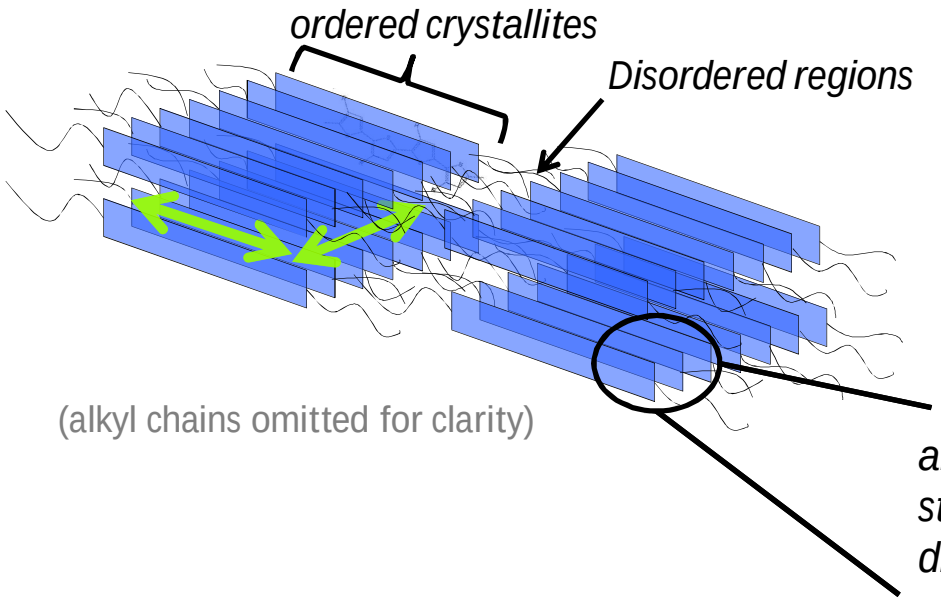
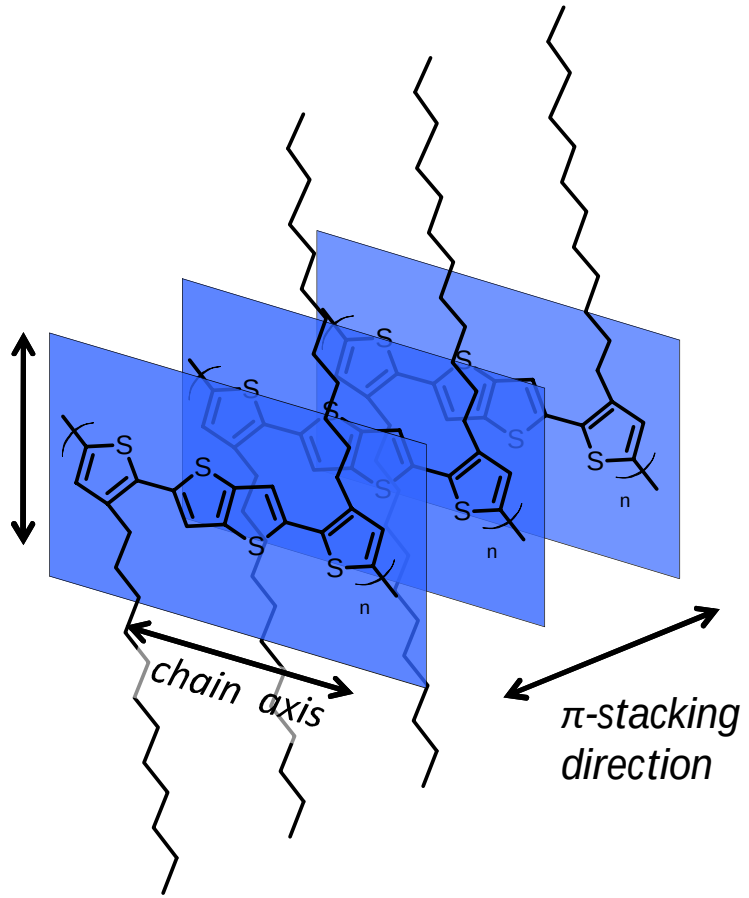
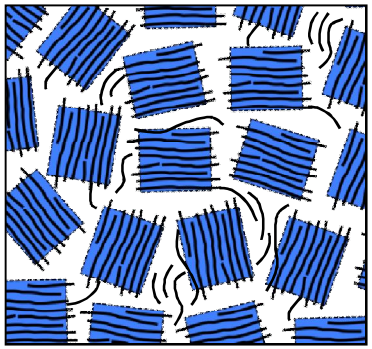
Polymers with π stacking

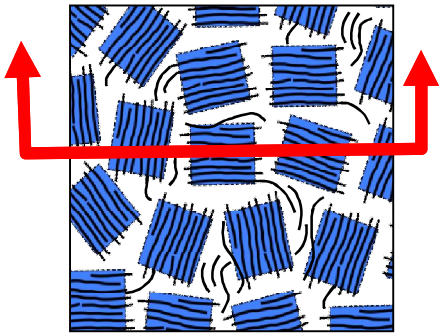




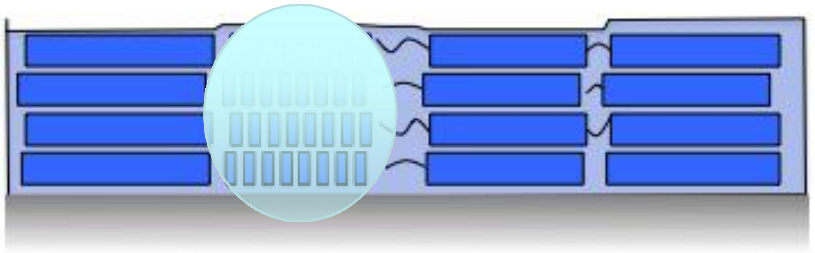
Top View: Isotropic in-plane

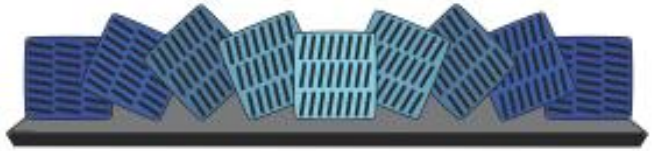


Microstructure at different length scales

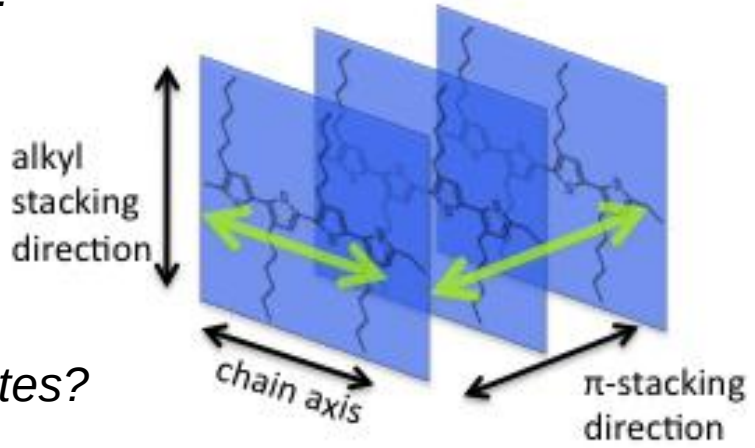


What is the degree of crystallinity (i.e. crystalline fraction) of a polymer film?





What is the texture of the crystallites?

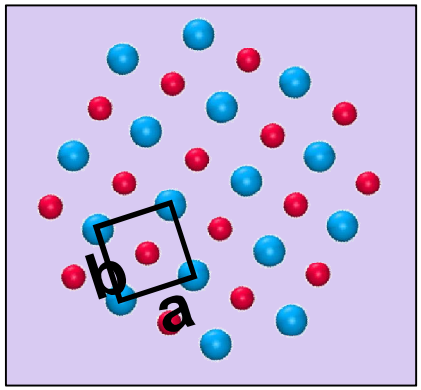


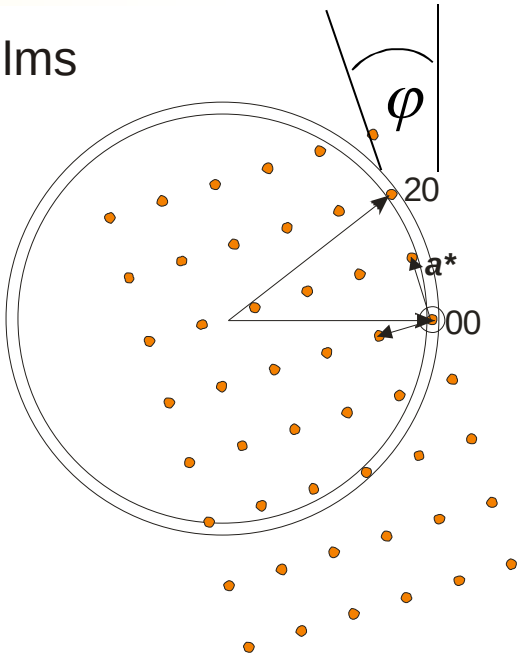
How perfect are the crystallites?

X-ray diffraction: Reciprocal lattice

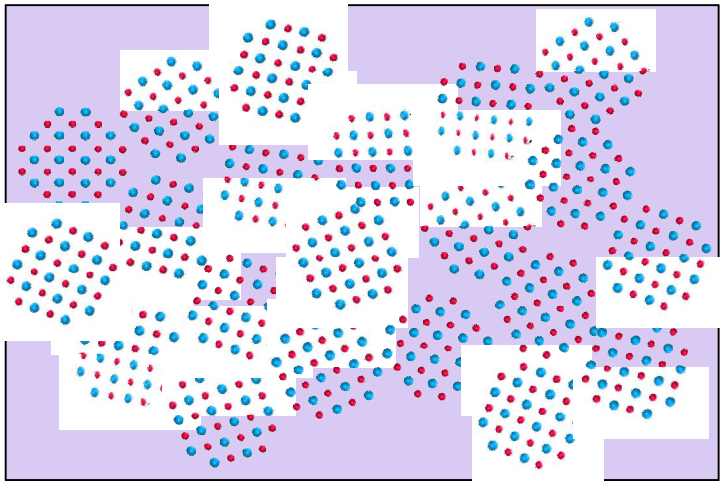
- The advantage in having polycrystalline thin films

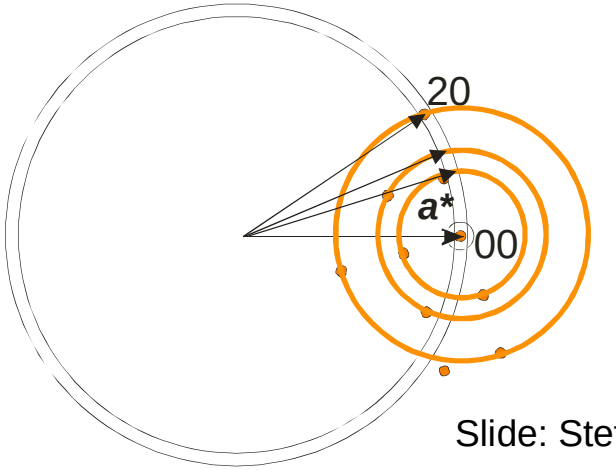
Single domain/crystal





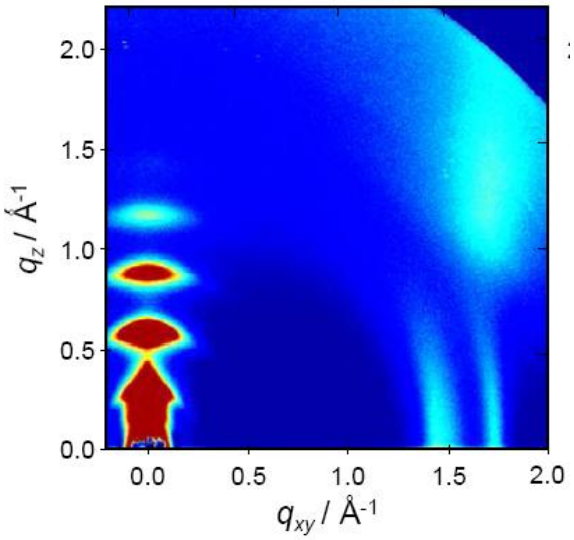
Polycrystalline thin film (here 2D powder)

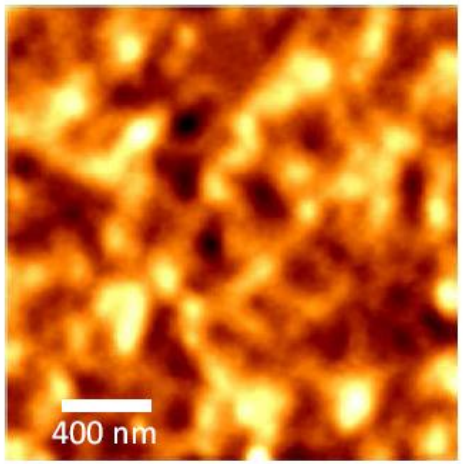




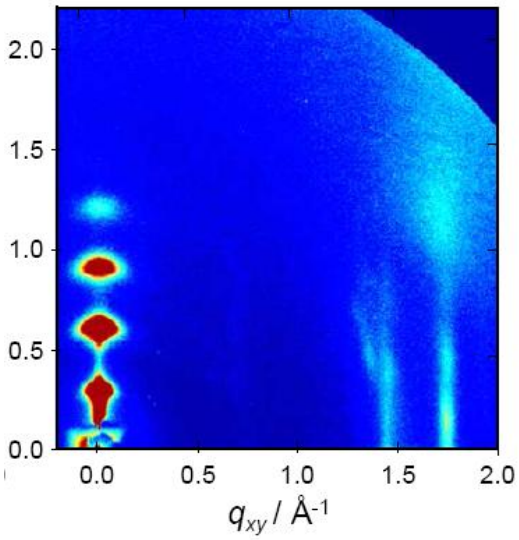
Slide: Stefan Mannsfeld

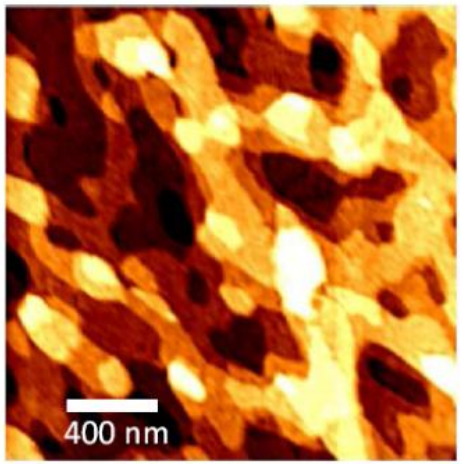
Morphology Change Upon Annealing



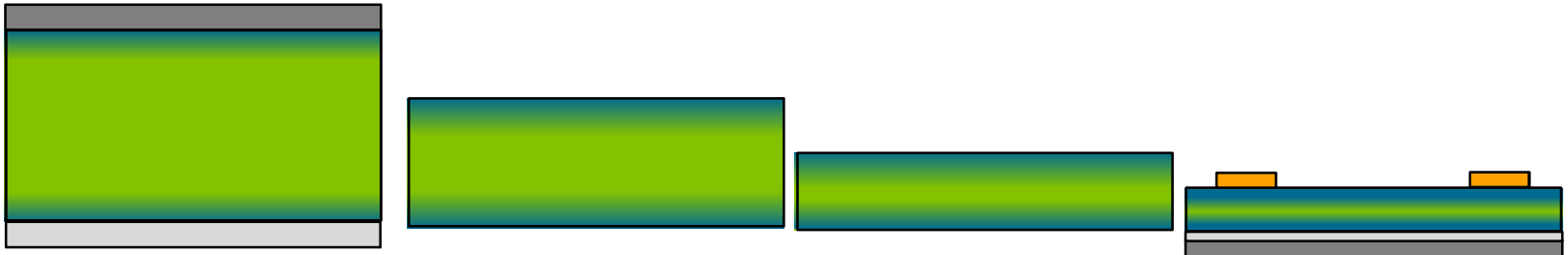


Anneal 180 °





What are the Effects of a Confined Geometry?

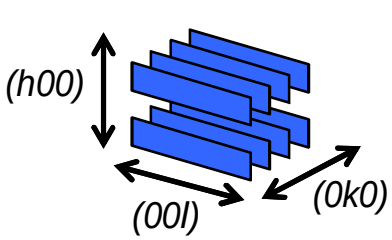


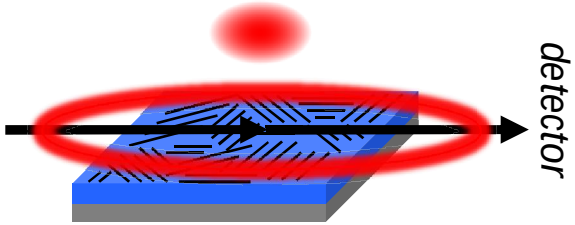
~100 nm
Diode, Solar Cell

<10 nm
Thin Film Transistor
Active Layer

- What happens to microstructure?
  - Crystallinity
  - Texture
- Do the electrical properties of the film change as a function of thickness?
- Are the effects of interfaces and a confined geometry the same for annealed and unannealed films?

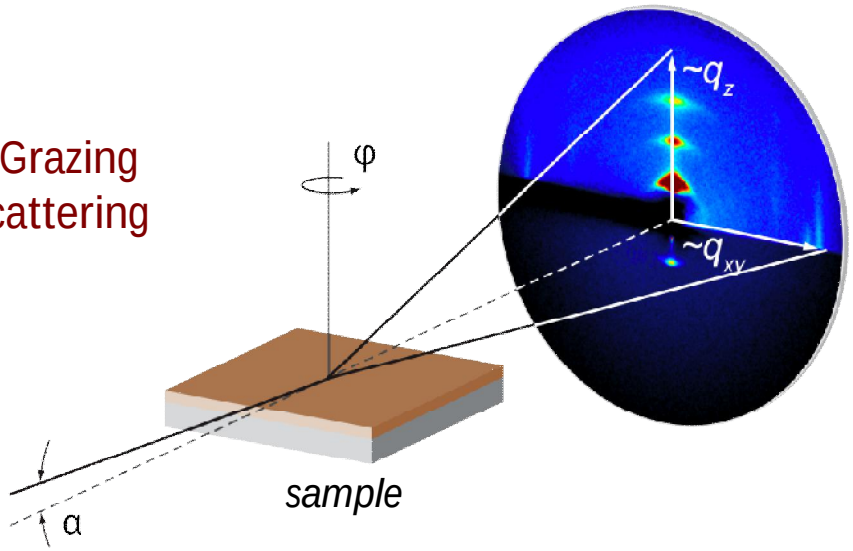
Texture from XRD



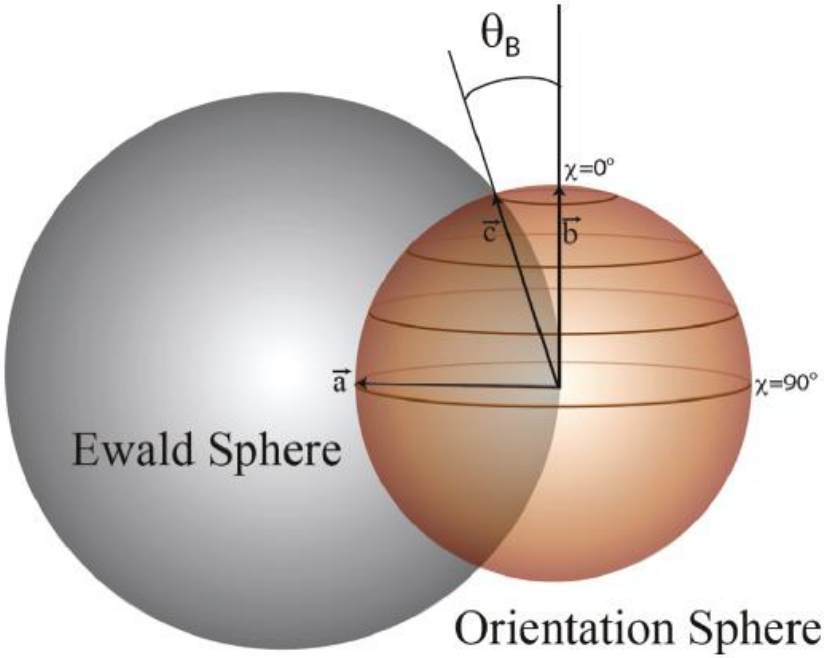


Synchrotron lightsource, SSRL
Energy of 8 keV (BL 2-1, 7-2), 12.7 keV (BL 11-3)
Wavelength of ~1 Å (10^{-10} m)

Two-dimensional Grazing Incidence X-ray Scattering



Ewald Sphere Construction



region of missing intensity

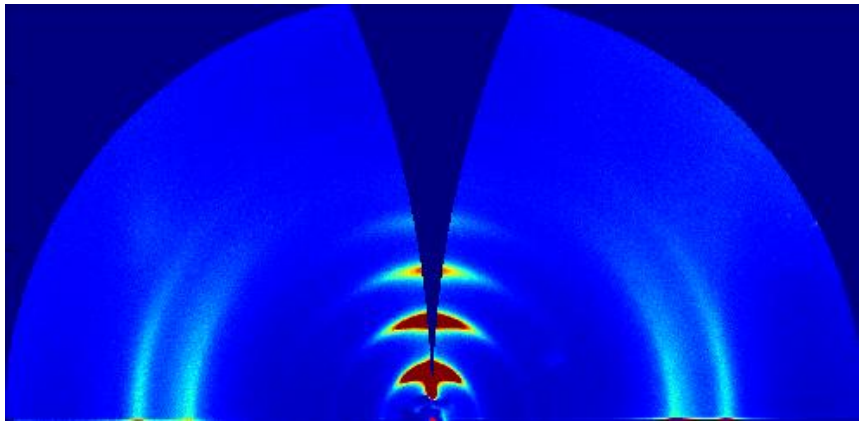
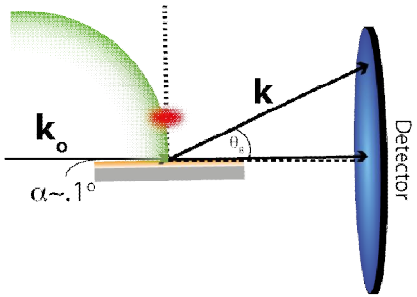
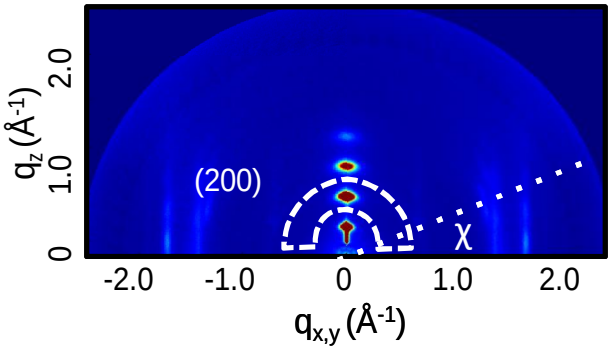


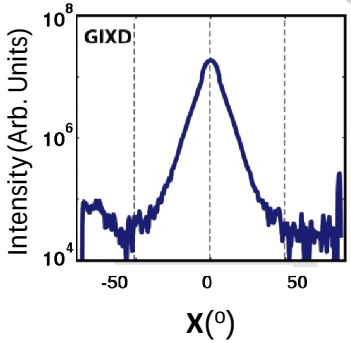
Image: Baker, Langmuir, **26,** 11 (2010)

Constructing Quantitative Pole Figure

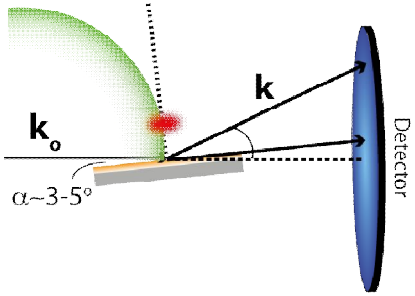
1. GIXD

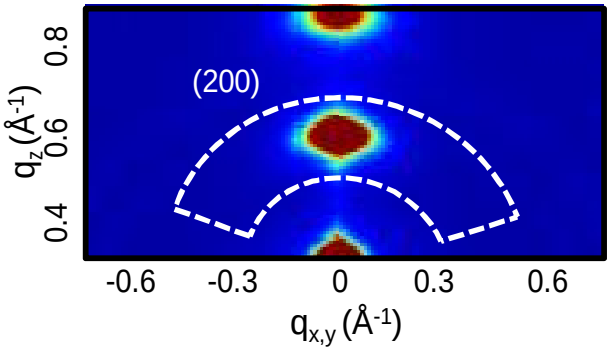


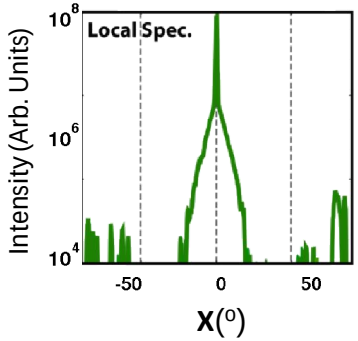




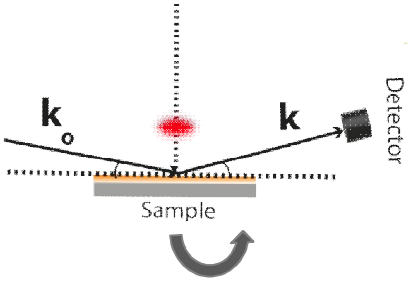
2. Local Spec.

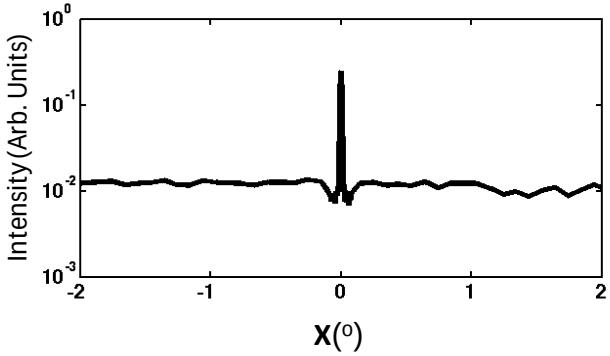


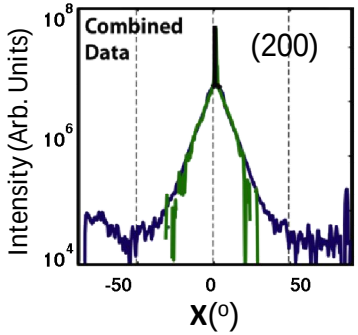


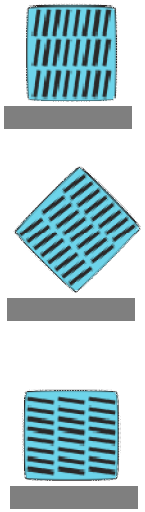


3. High Res. Rocking



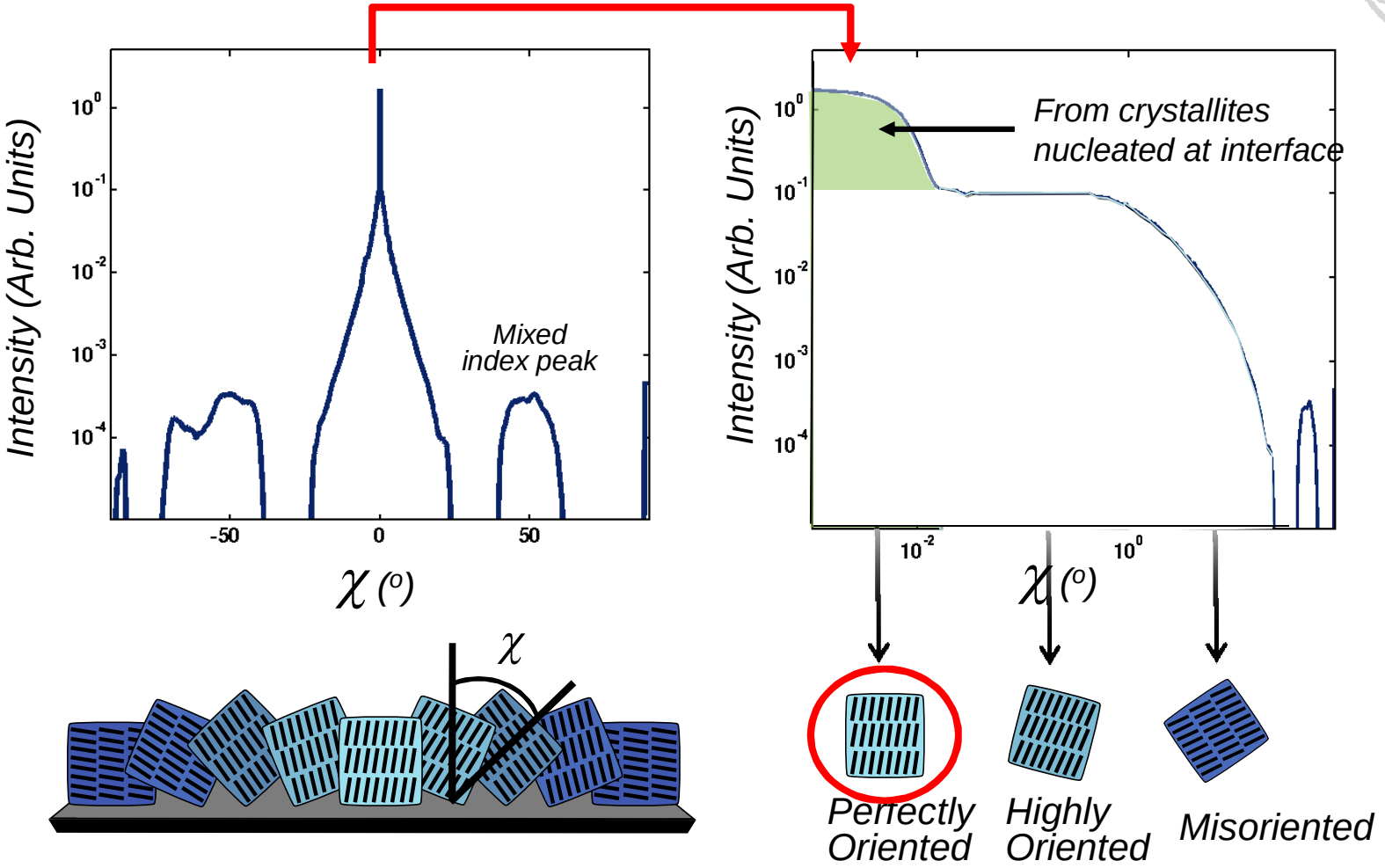






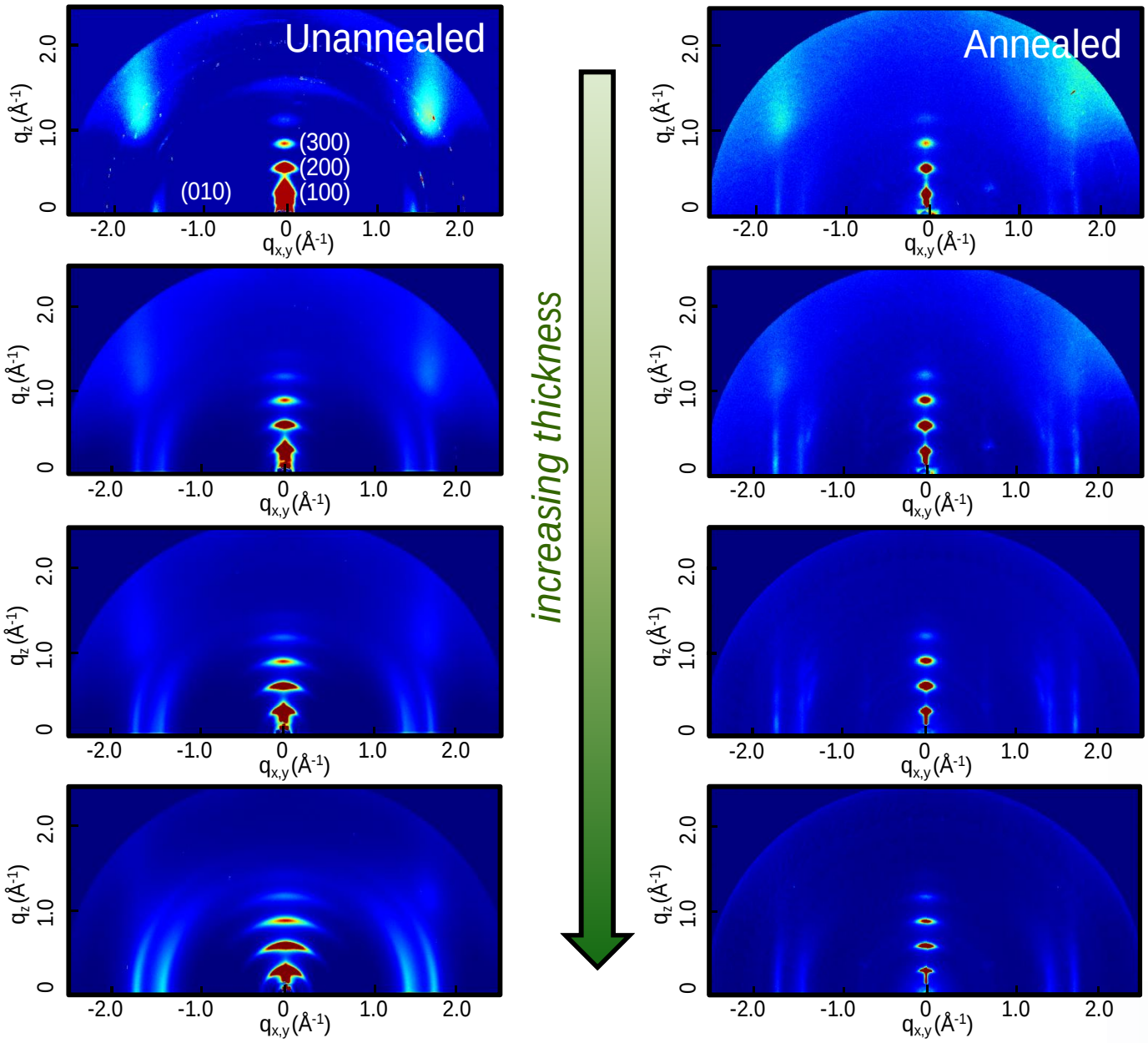
Baker, Jimison, et al. *Langmuir* (2010)

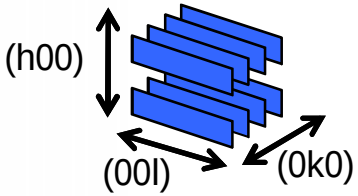
Crystallites nucleated at the interface

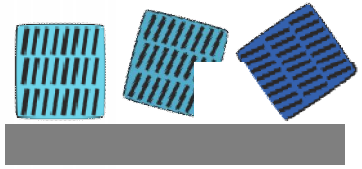


The only way a "perfectly-oriented" population of crystallites can exist is if these crystallites are nucleated on the flat substrate surface.

2D GIXD Reveals Film Texture

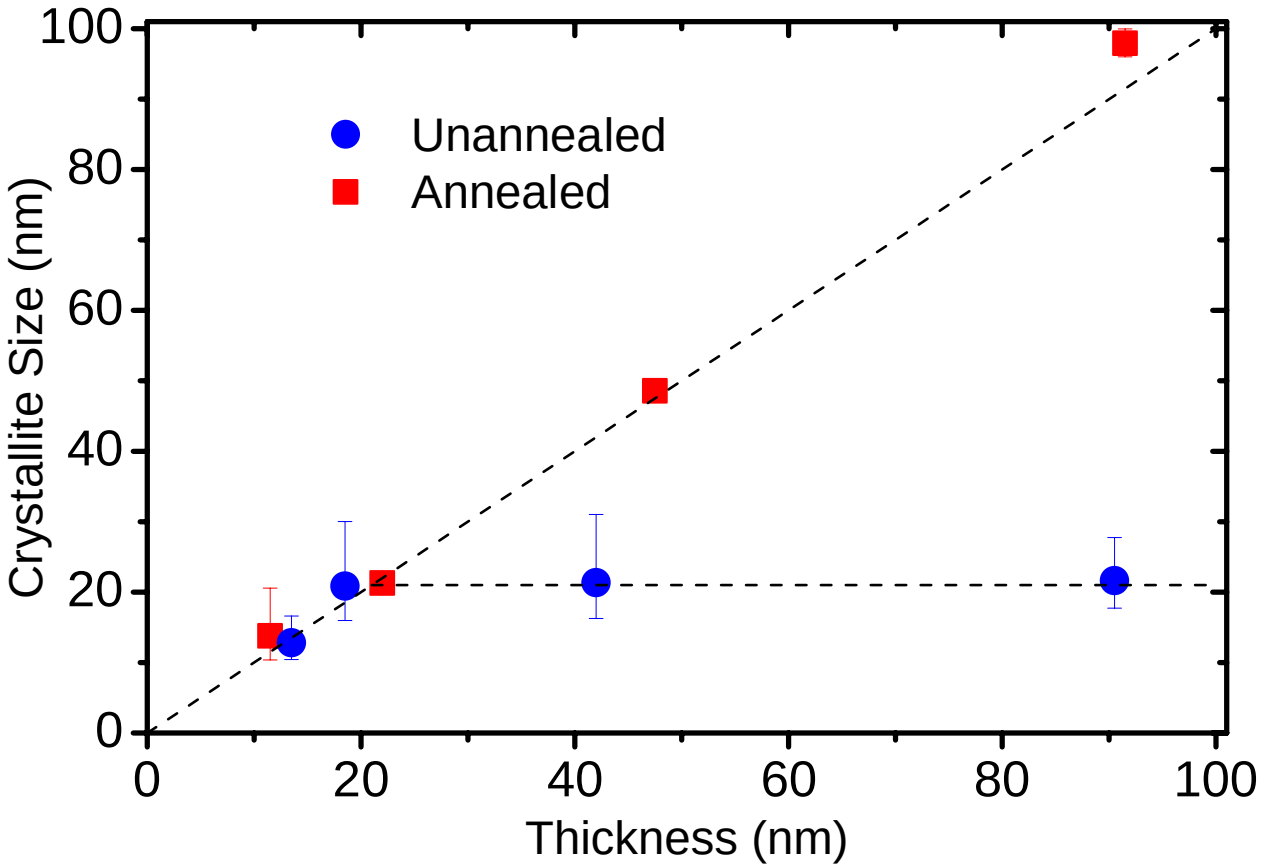




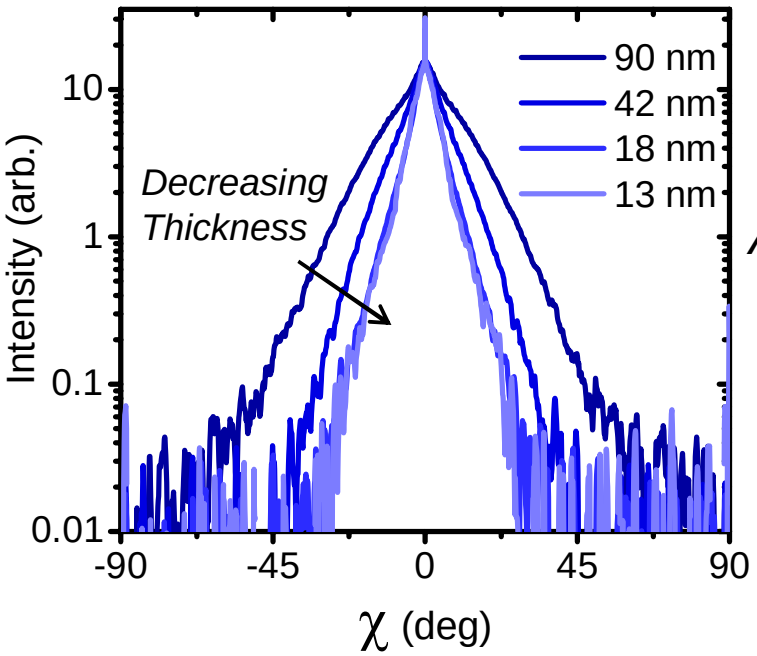


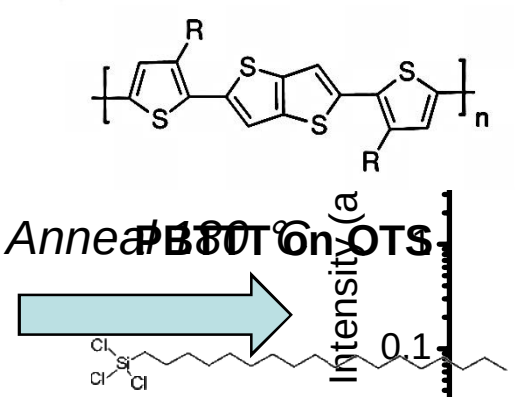
Crystallites Have Characteristic Thickness

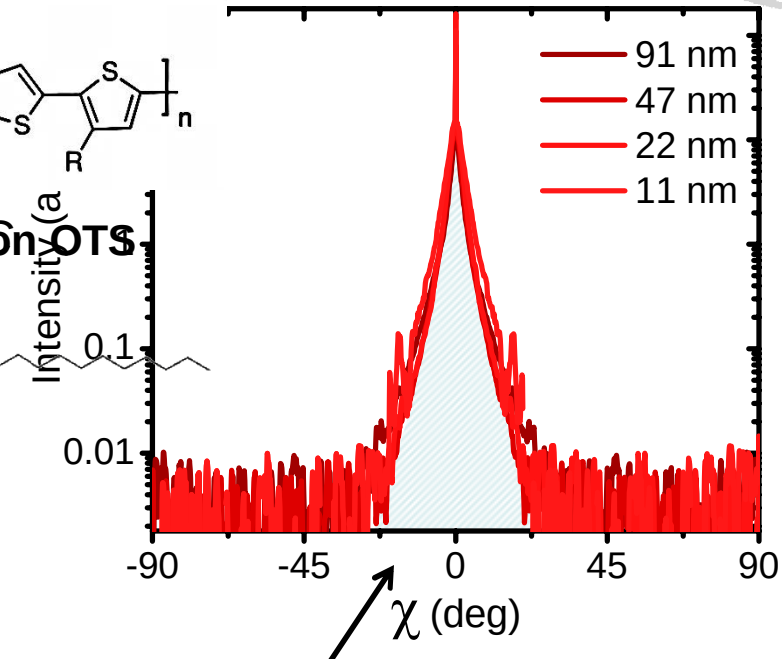
- Crystallites have characteristic size but grow through film upon annealing



Texture Changes with Thickness







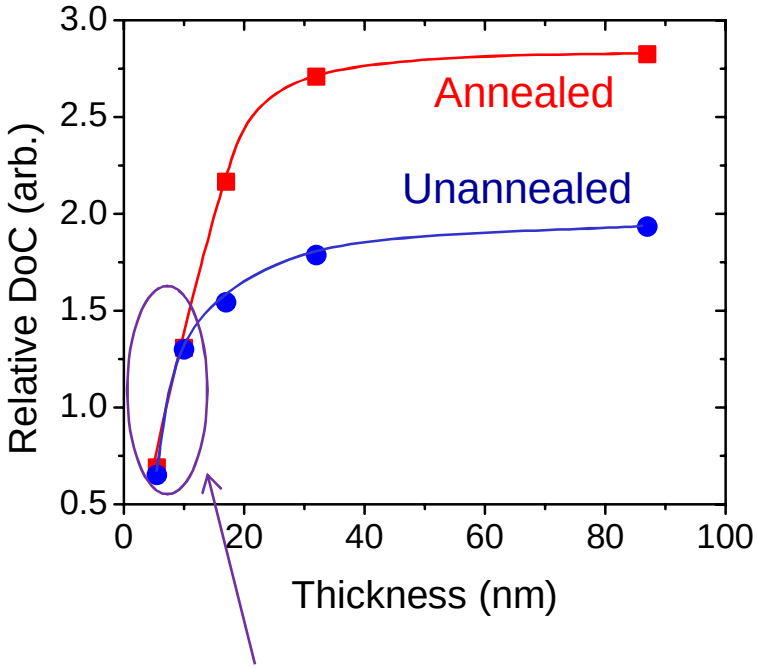
PBTTT on OTS

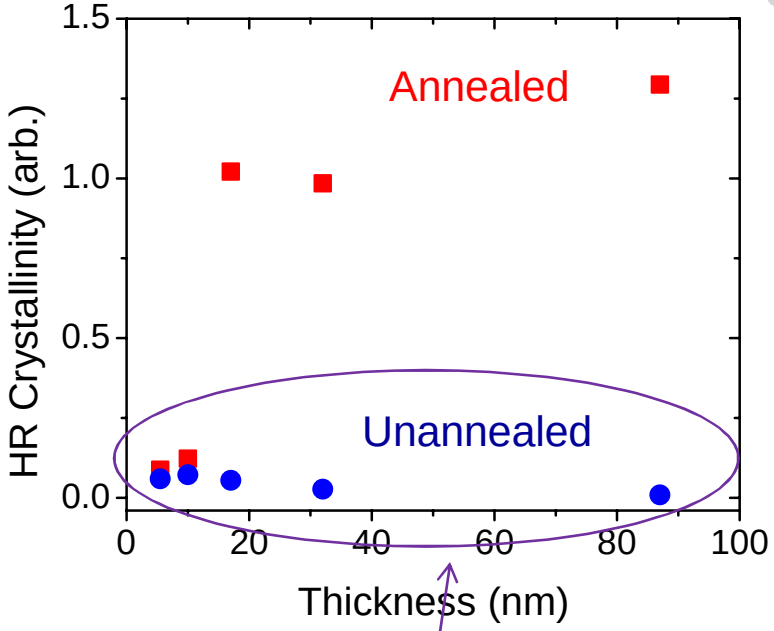
- Crystallite angular distribution tightens with decreasing thickness for unan

$$DoC \propto \Delta\beta\Delta\theta[I_{peak} - I_{base}] + 2\pi \int_0^{\pi/2} \sin(\chi) I(\chi) d\chi$$

- No thickness dependence for annealed films

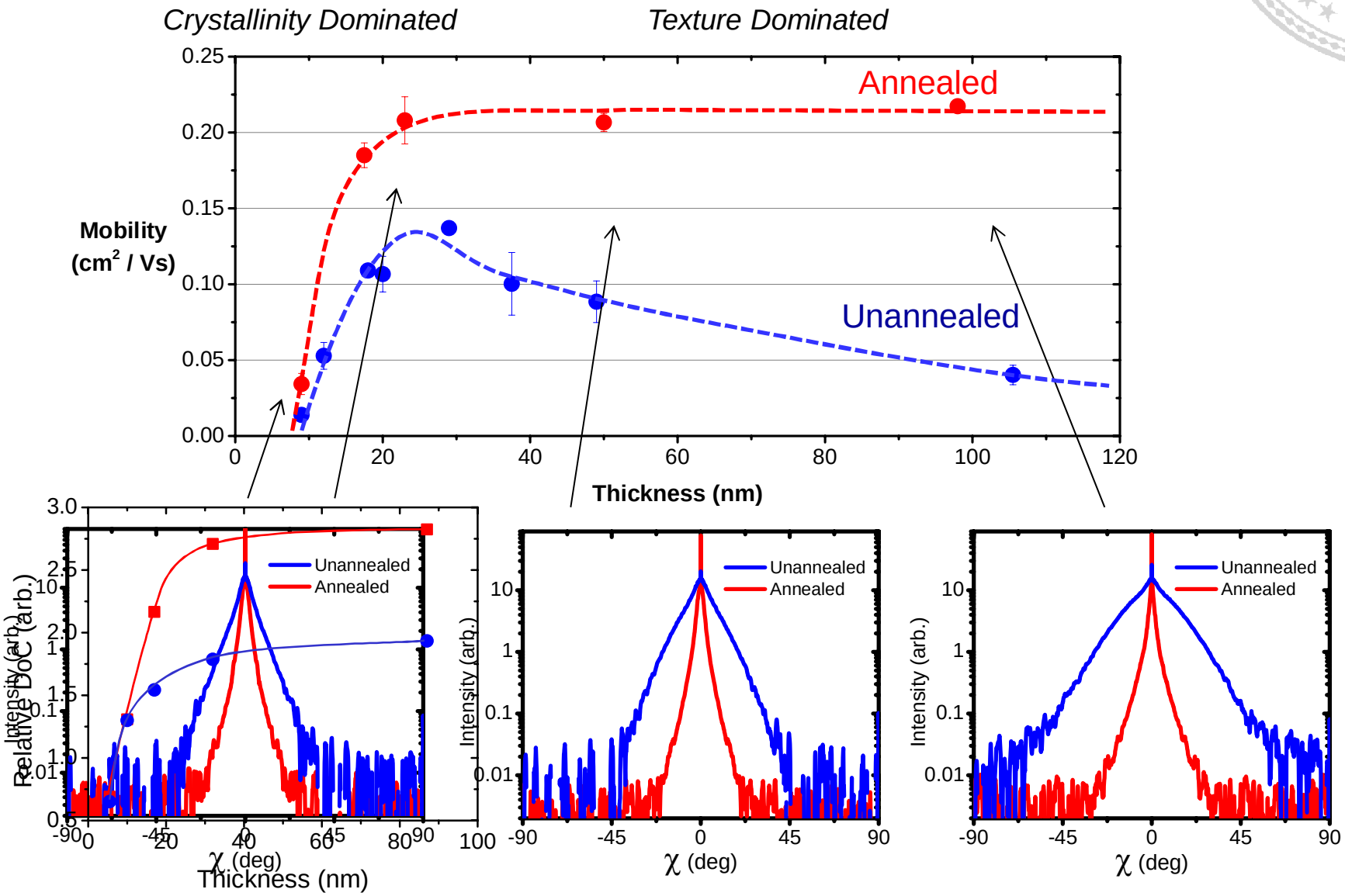
Crystallinity Varies with Thickness





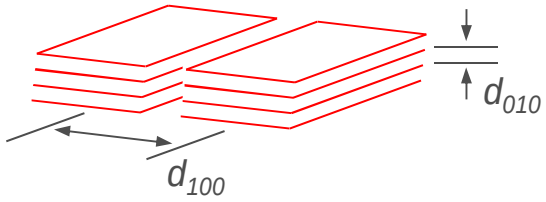
- Crystallinity for thinnest films is diminished
- Crystallinity increases upon annealing
- Few highly oriented crystallites for unannealed and ultrathin films

Crystallite Distribution Affects Mobility

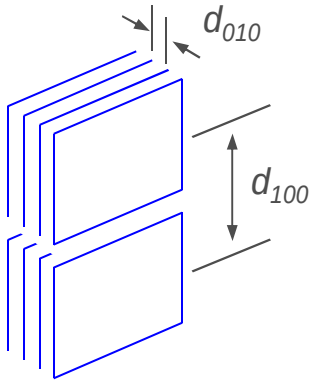


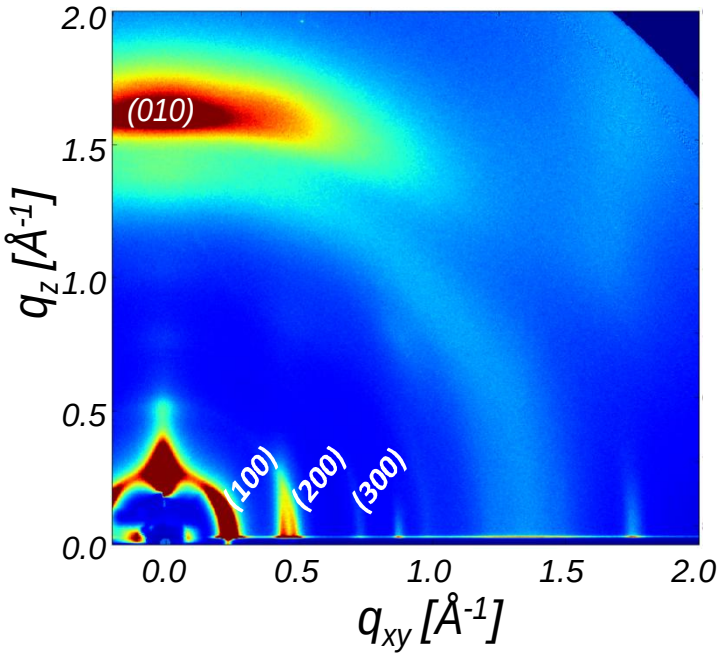
Drastic control of texture by melt annealing

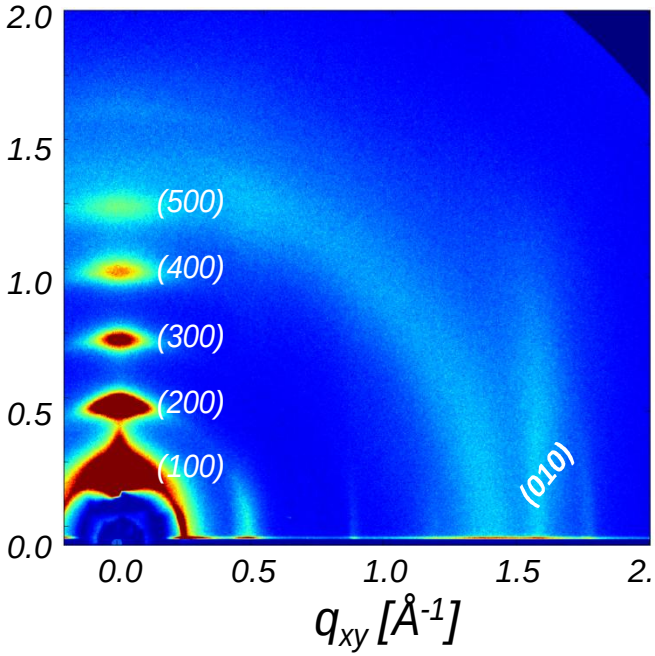
Annealed 150°C



Melt Annealed 300°C (+slow cool)







60% reduction in e$^-$ only diode current

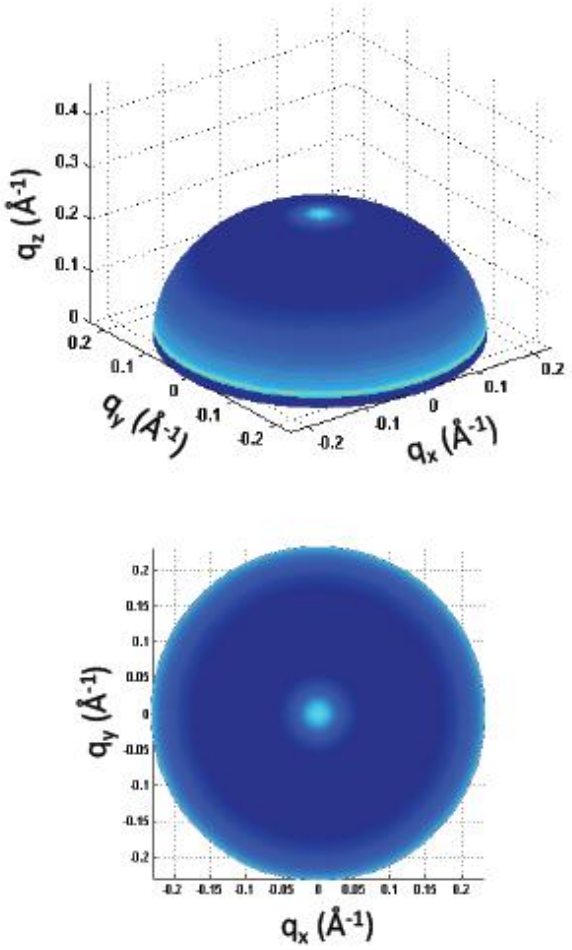
Twice as crystalline

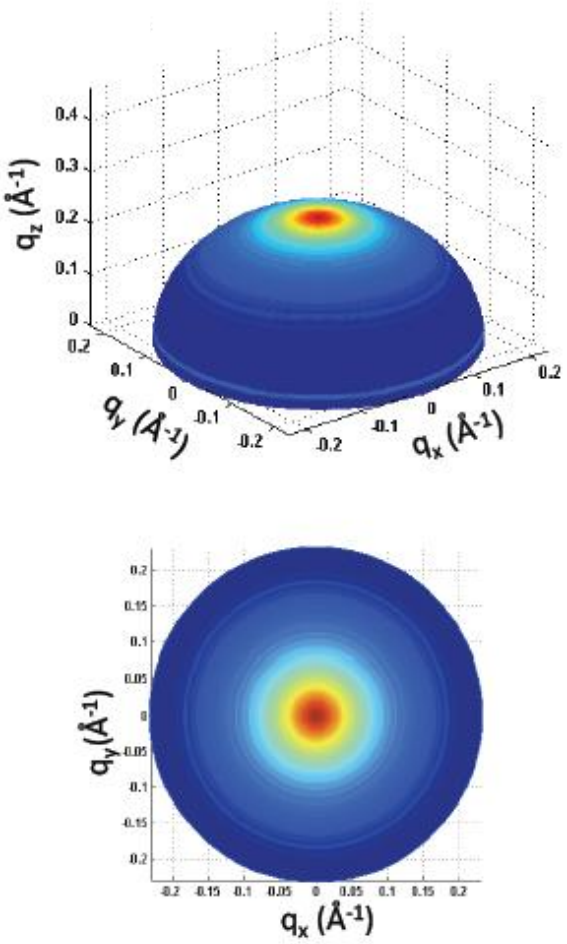
J. Rivnay, et al., Macromolecules (2011).

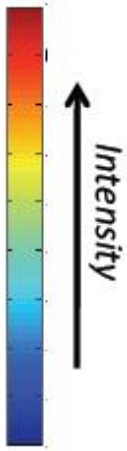
Three Dimensional Pole Figure

Annealed 150℃

Melt Annealed 300℃ (+slow cool)








Thank You!