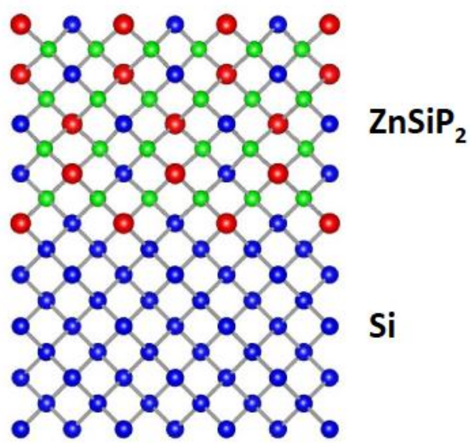
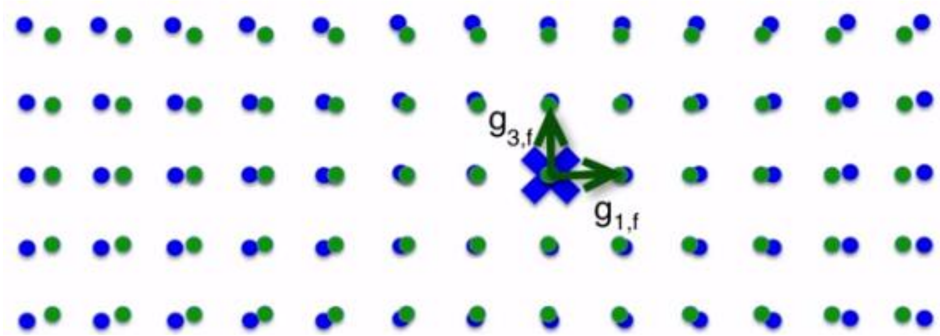
Topic 4-3: Omega Rocking Curves

Summary: We begin by discussing epitaxial thin films as a superposition of the film and substrate lattice and measure an intensity spectrum of a perfect film with an ω-2θ scan. We then discover that, in reality, the film with be tilted off the substrate normal. We use an ω rocking curve to measure the amount of out-of-plane alignment of the film.

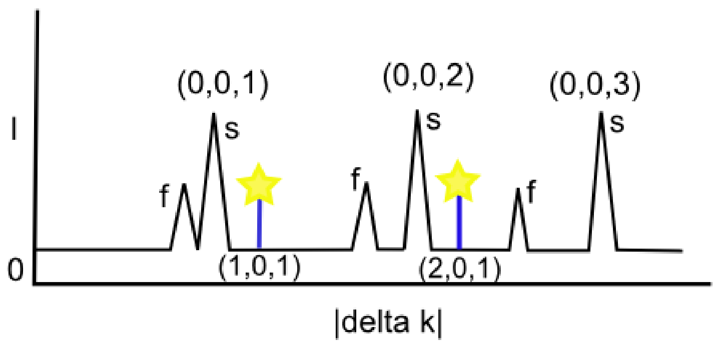
- Looking at thin film diffraction
- Epitaxial thin films- crystallographic relationship between the film and the substrate the film is grown on
  - An example is growing AlAs on GaAs.
  - Another example: $ZnSiP_2$ on Si:



  - The lattice constants may not be an exact match, but the film is oriented with the substrate
- Epitaxial thin films require less than 1% mismatch of the lattice in the substrate and film
- Any more than that and the stress will likely lead to strain – eg dislocations, defects, or even a failure to grow epitaxially
- In reciprocal space, if the film is sufficiently thin, the incoming wave will interact with the substrate and the film at the same time
- We can then create a reciprocal space made of a superposition of the film and the substrates reciprocal lattices
- Because we assume the film has a slightly bigger lattice in real space it has a smaller lattice in reciprocal space (shown in green)

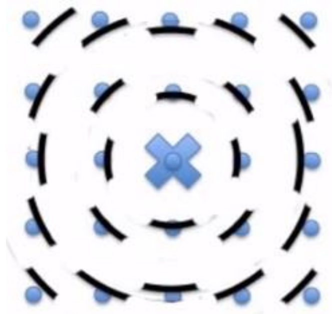


- As we move out from the origin the spacing between the film (green) and substrate (blue) lattice points get bigger
- When we do an ω-2θ scan we will see 2 peaks at each reflection, the smaller first peak being the film and the second, larger peak being the substrate (provided the film is thin, and most of the X-rays penetrate into the substrate)
- The space will increase between these two for larger Δk reflections
- This has been for the 'perfect' alignment of the film and substrate
- If there were a powder on the substrate we would get concentric rings in reciprocal space and extra peaks in the intensity. For example, the figure below shows a 001-oriented film grown on a 001 oriented substrate. The delta k vector moves up from the origin in the above figure along g3. However, if we had a polycrystalline (randomly oriented) film, we see additional reflections from (101) and (201).

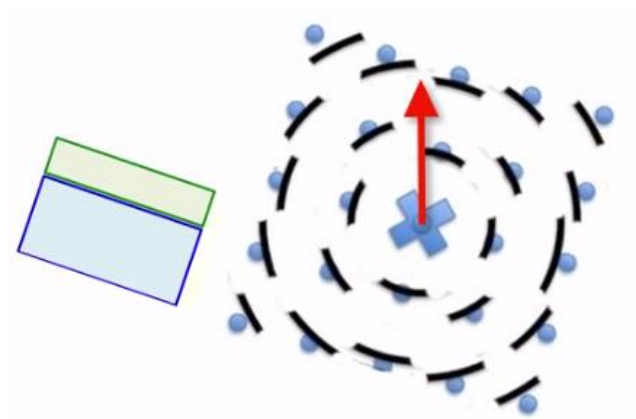


If the film is a cubic crystal, where would the (1,1,1) reflection be?

- In reality, a partially epitaxial film will have some grains correctly oriented and some slightly tilted
- In that case our reciprocal space would have dots for the substrate lattice (since it's 'perfect') and short arcs for the film lattice (not so perfect)
- **Technical goal:** Determine the extent to which the film is tilted off the substrate normal.



- Have to set up Δk so it hits one of the sample arcs
- Fix the source and the detector so Δk never changes
- We then tilt our sample about ω



- As the sample tilts we drag our reciprocal lattice through the fixed k vector, leading to a peak of finite width (recall before we would have had a delta-function [well, in perfect physics-land])
- We use the full width half maximum (FWHM) of the peak to get a measure of the amount of out of plane orientation, that is to say the amount of tilt in the film
- A good film has a FWHM <<1 degree.
- This type of scan gives no in-plane orientation information

Questions to Ponder

1. Draw reciprocal space for a tetragonal film growth on a cubic substrate with good epitaxy.

2. If we do an ω-rocking curve on the (0,1) reflection how will the FWHM average compare to the (0,2) reflection? Think about units to help formulate your response.