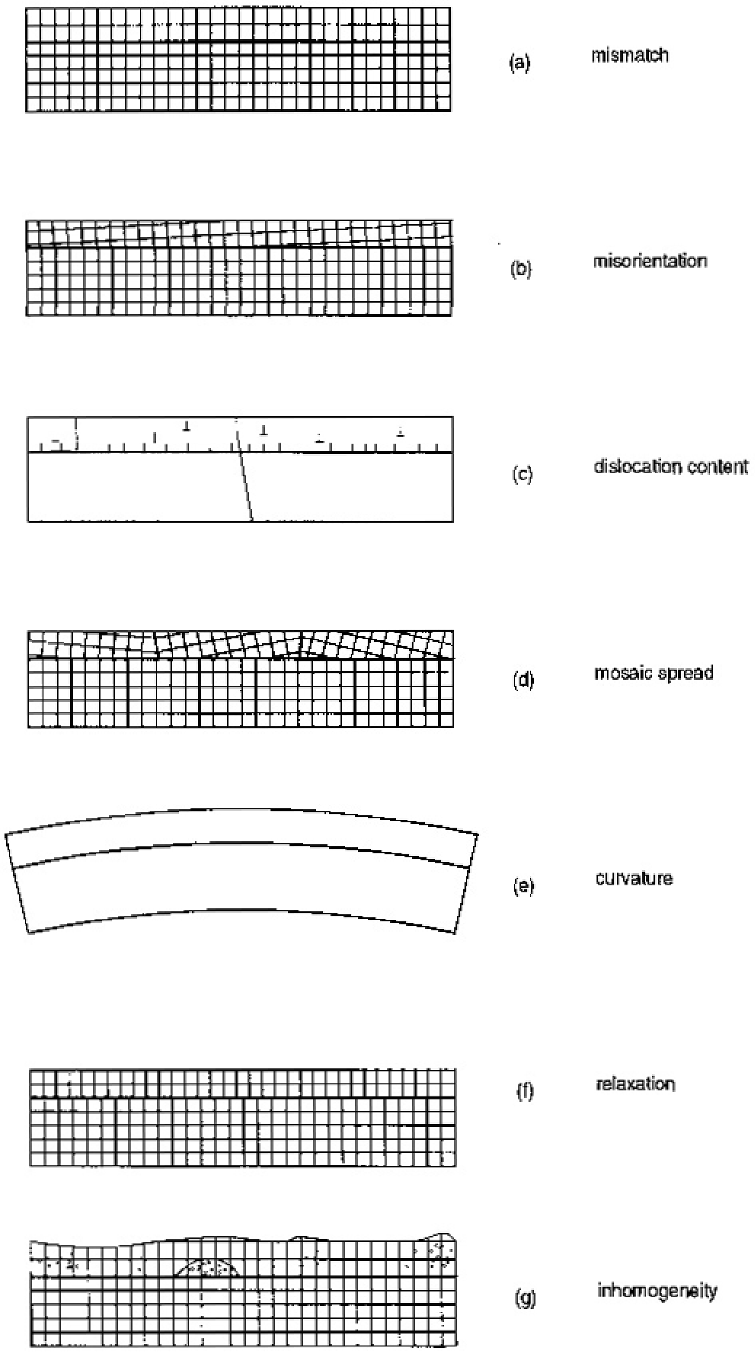
Thin films

(see Bowen & Tanner, High Resolution X-ray Diffractometry and Topography, Chap. 3)

Common epilayer defects

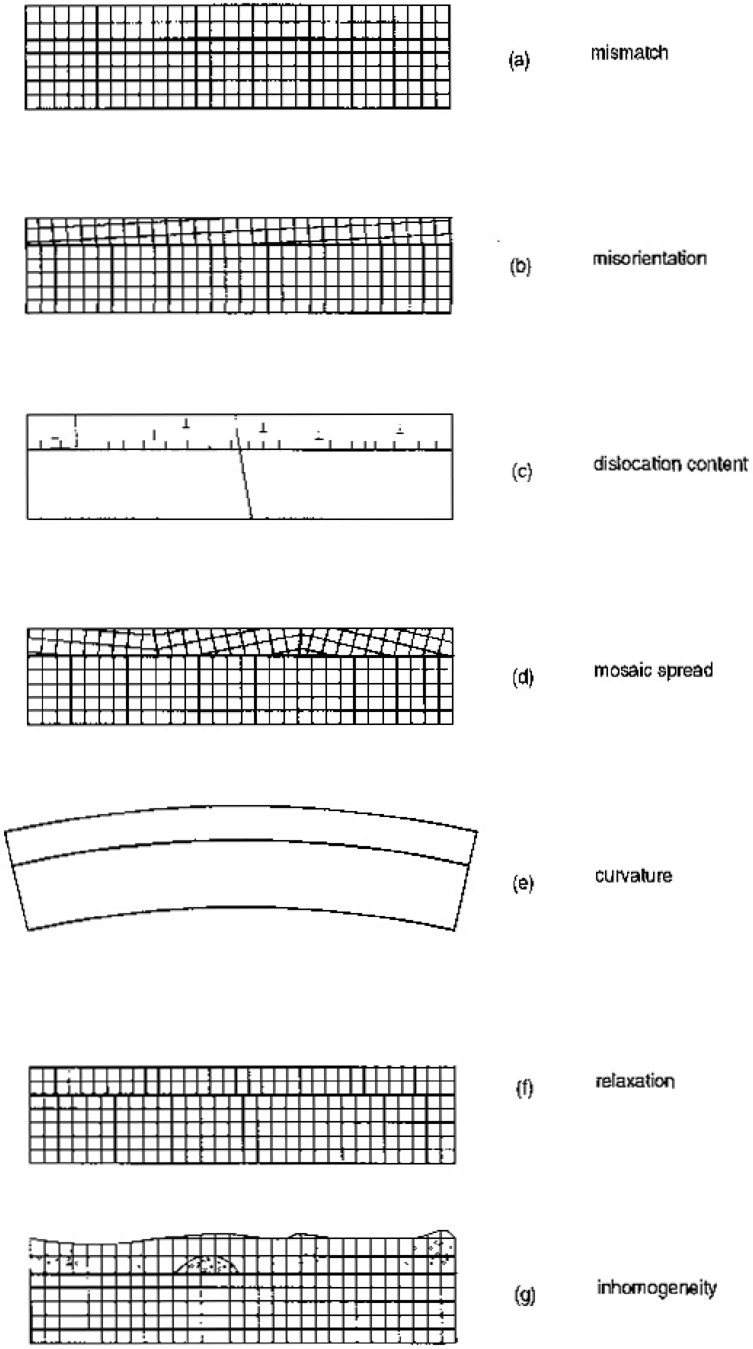


Thin films

(see Bowen & Tanner, High Resolution X-ray Diffractometry and Topography, Chap. 3)

Common epilayer defects

Investigate using rocking curves



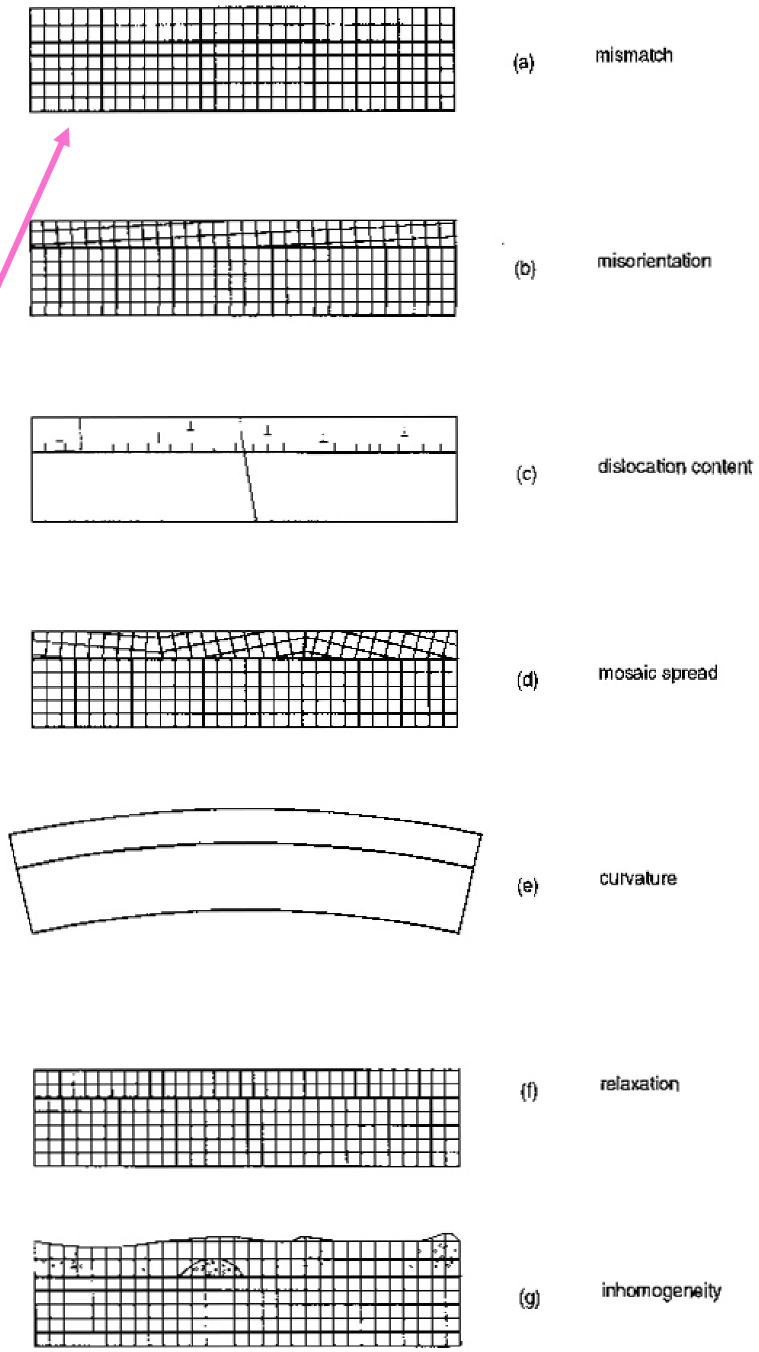
Thin films

(see Bowen & Tanner, High Resolution X-ray Diffractometry and Topography, Chap. 3)

Common epilayer defects

Investigate using rocking curves

Layer & substrate peaks split rotation invariant

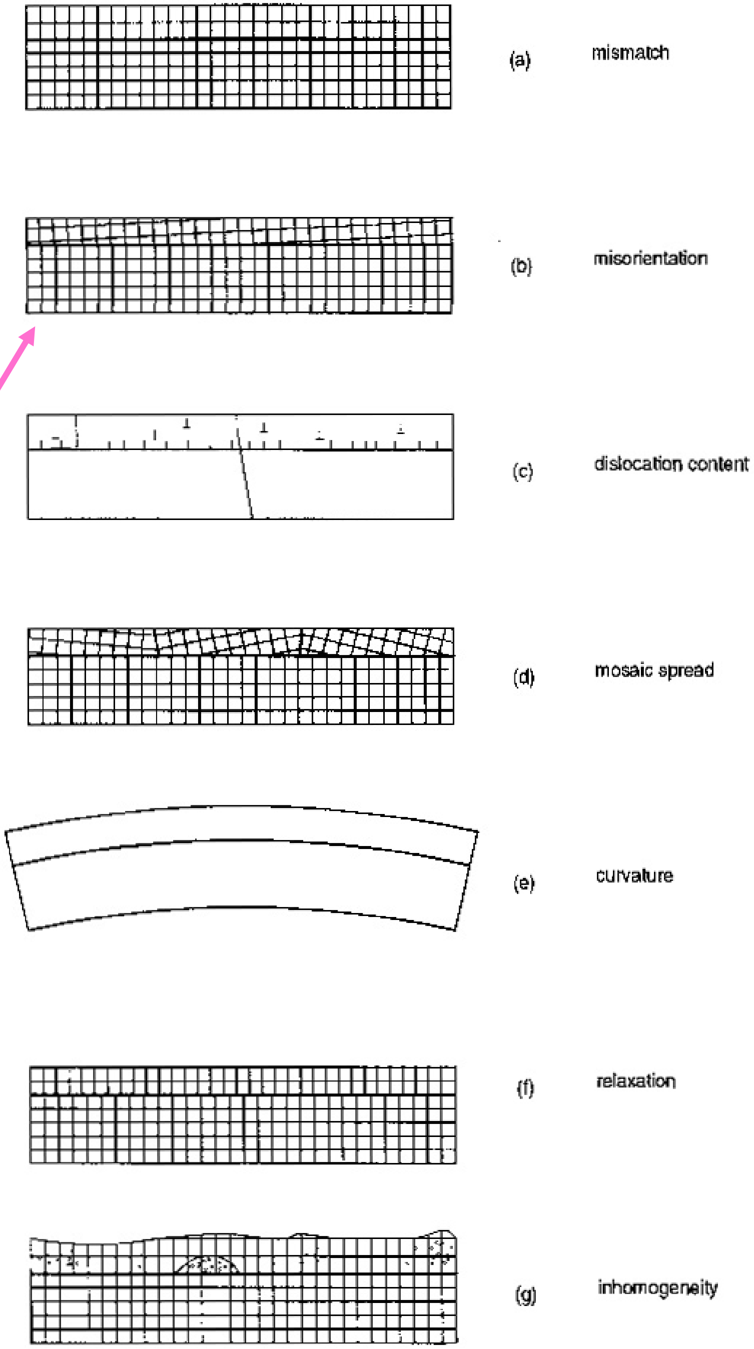


Thin films

Common epilayer defects

Investigate using rocking curves

Layer & substrate peaks split varies w/rotation

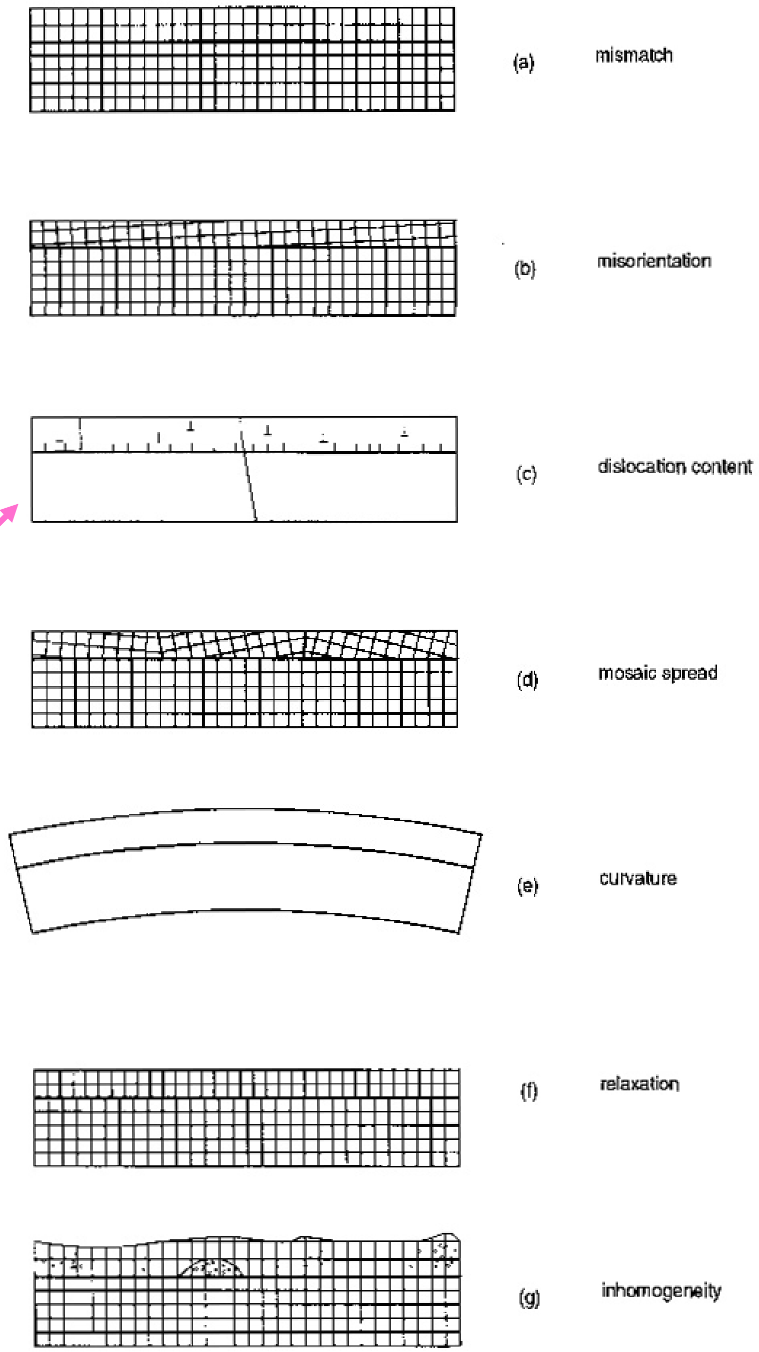


Thin films

Common epilayer defects

Investigate using rocking
curves

Broadens layer peak
- invariant w/ beam size
- peak position invariant
  w/ sample position

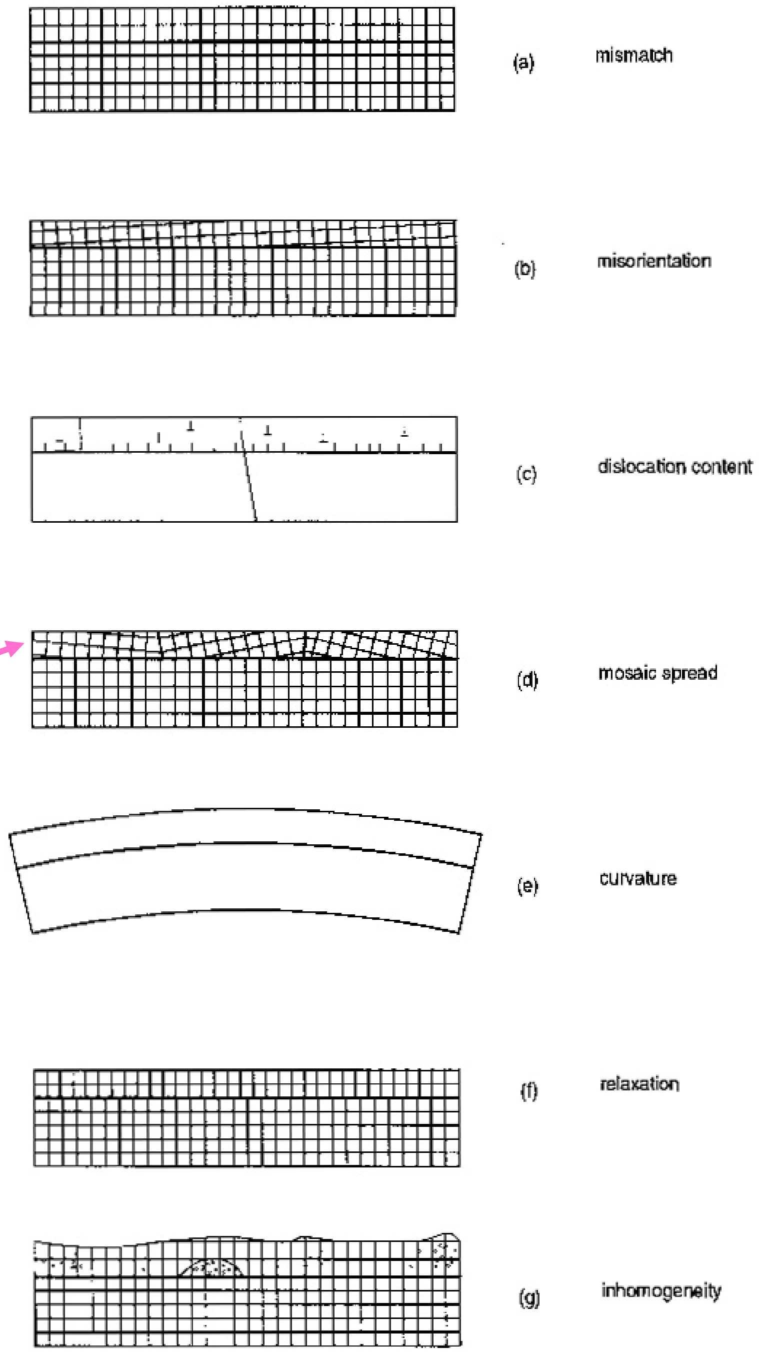


Thin films

Common epilayer defects

Investigate using rocking
curves

Broadens layer peak
may increase w/ beam
size
peak position invariant
w/ sample position

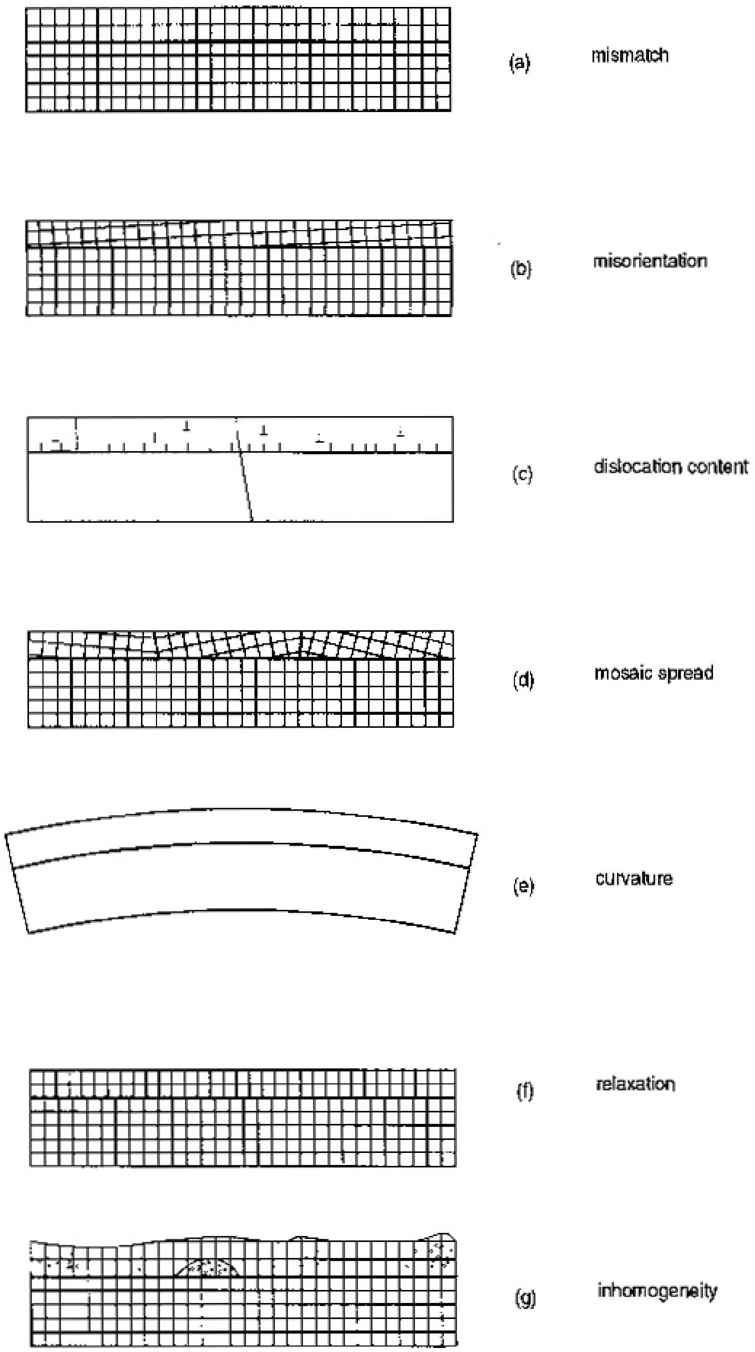


Thin films

Common epilayer defects

Investigate using rocking curves

- Broadens layer peak
  - increases w/ beam size
  - peak position varies
    - w/ sample position

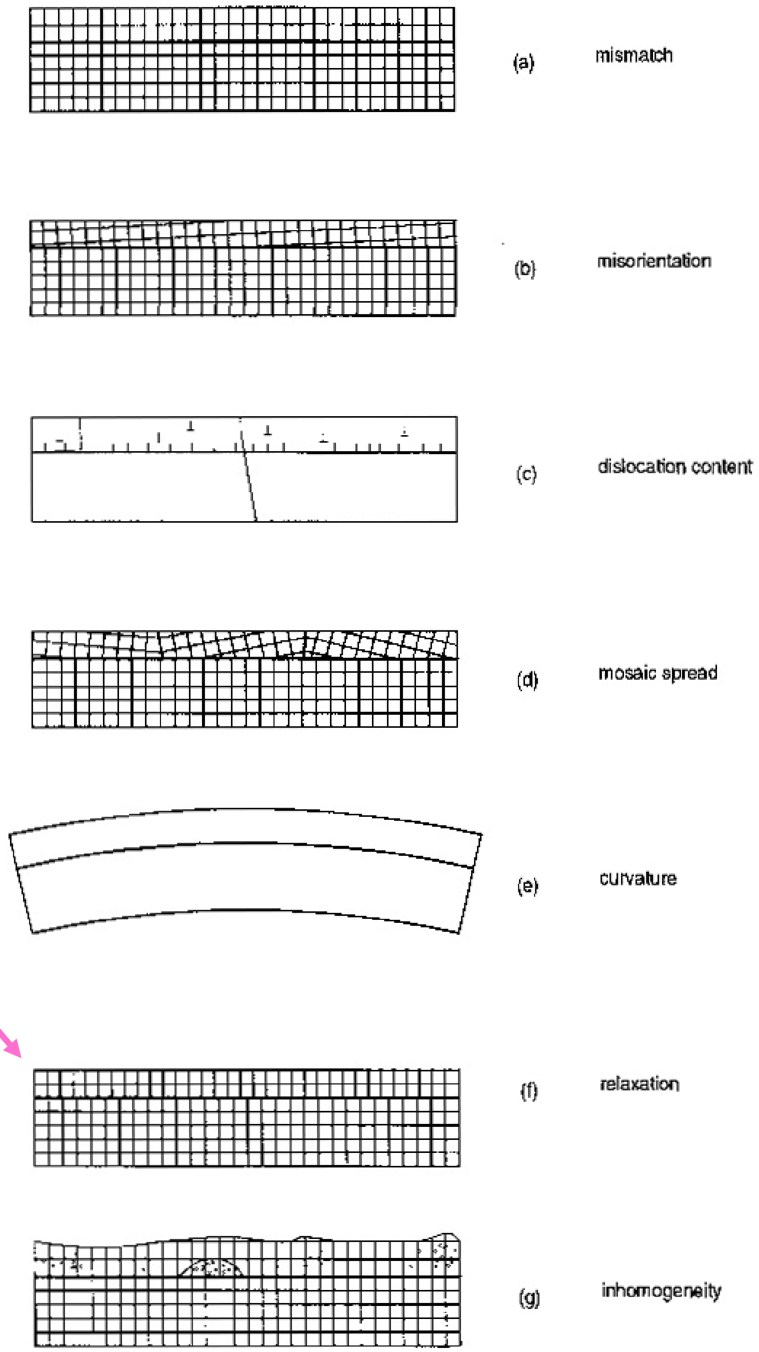


Thin films

Common epilayer defects

Investigate using rocking curves

Layer & substrate peaks split splitting different for symmetric & asymmetric reflections

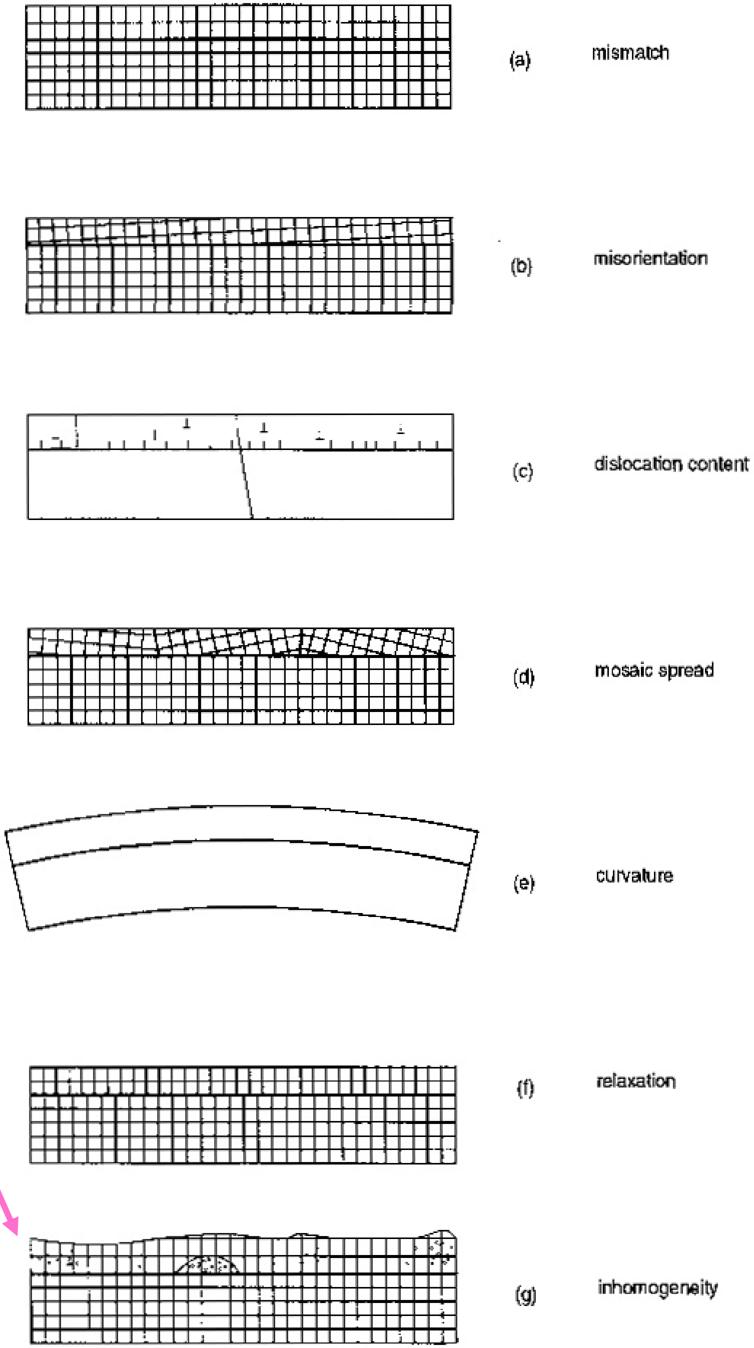


Thin films

Common epilayer defects

Investigate using rocking curves

Various effects vary w/ sample position



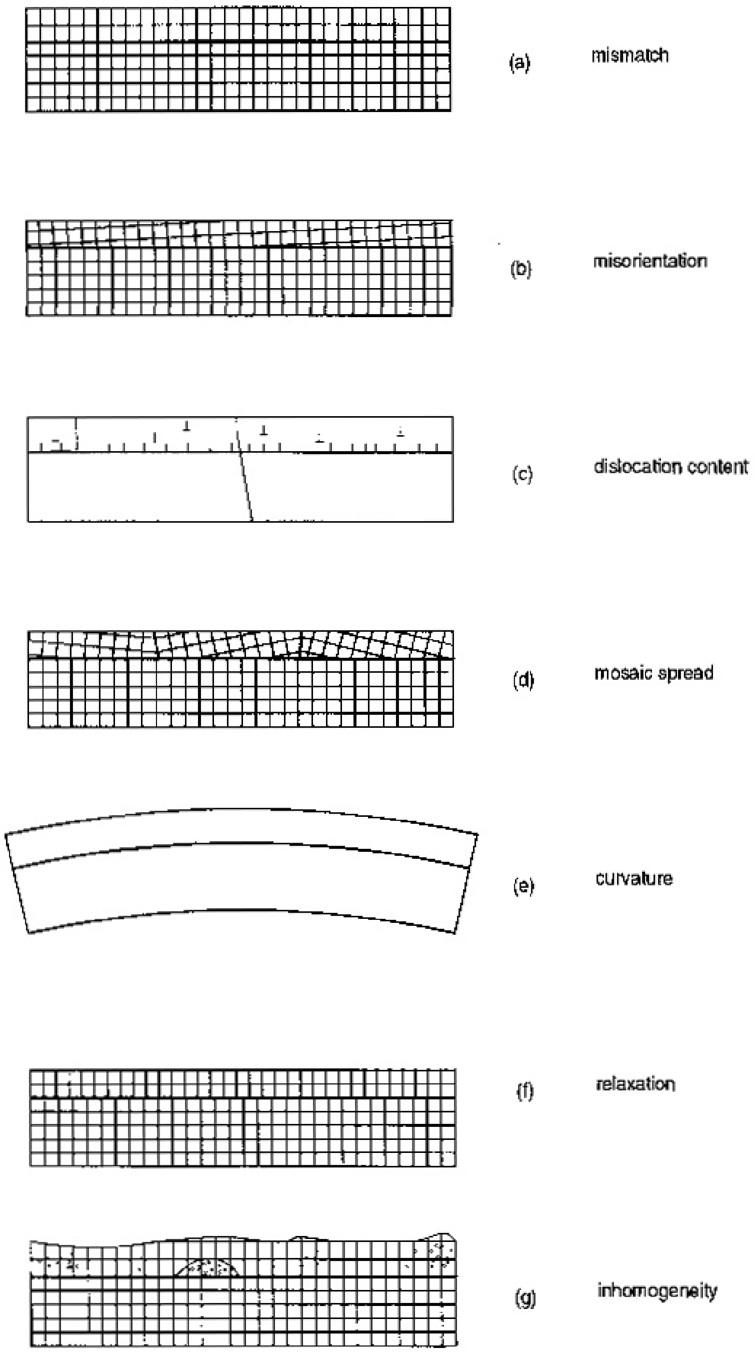
Thin films

Investigate using rocking curves

Film thickness

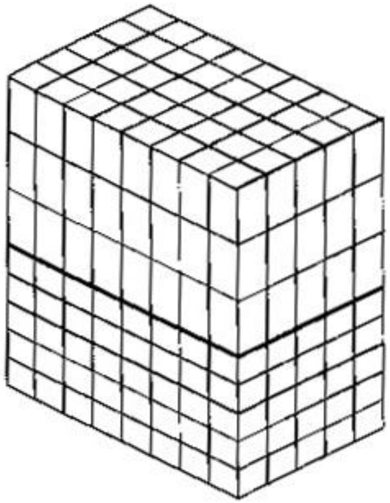
Integrated intensity changes increases w/ thickness

Interference fringes

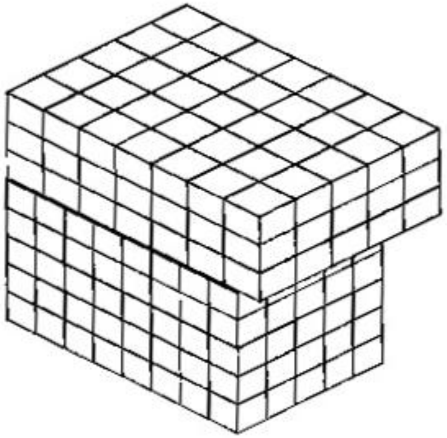


Thin films

Mismatch



constrained



relaxed

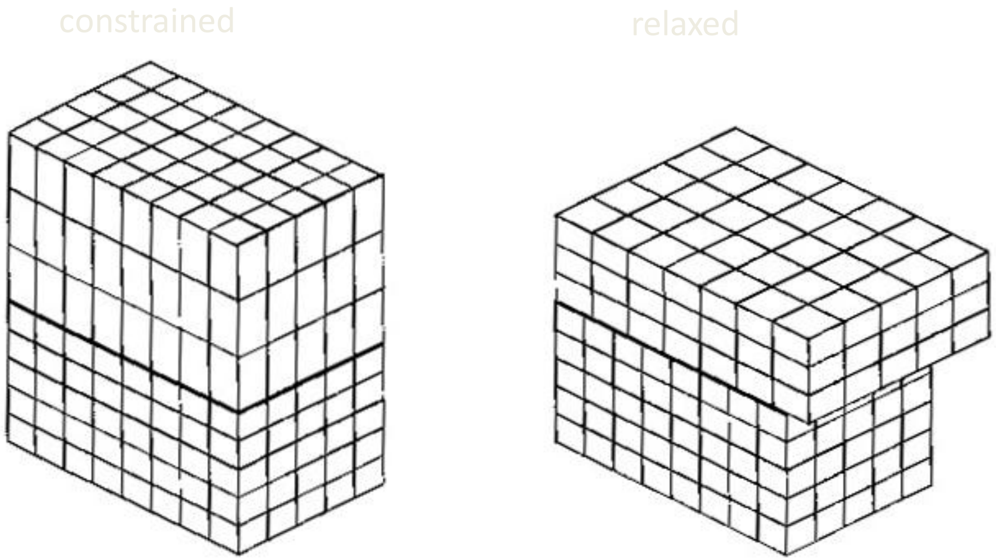
Thin films

Mismatch

Layer & substrate peaks split – rotation invariant

Measure, say, (004) peak separation $\delta\theta$, from which

$$\delta d/d = -\delta\theta \cot\theta = m^* \quad \text{(mismatch)}$$



Thin films

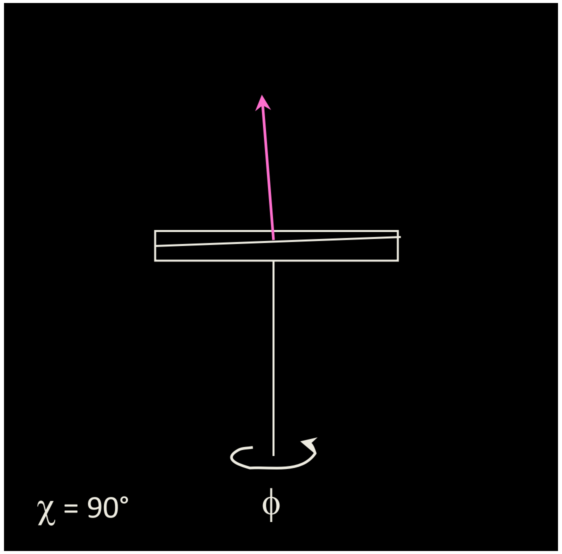
Misorientation

First, determine orientation of substrate

rotate ϕ to bring plane normal into counter plane

do ω scans at this position and at ϕ + 180°

orientation angle = 1/2 difference in two angles



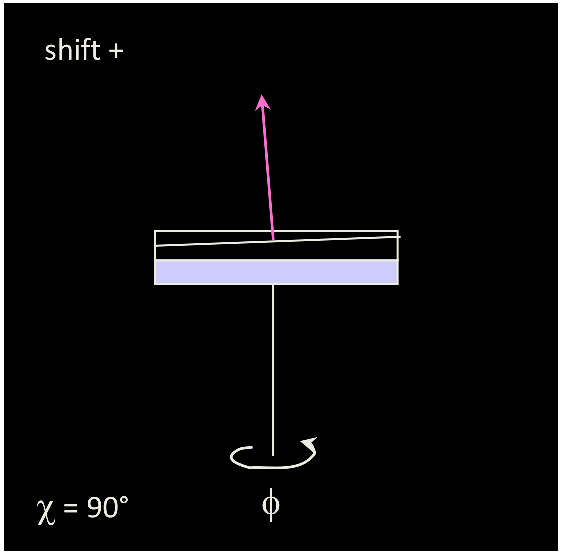
Thin films

Misorientation

First, determine orientation of substrate

Layer tilt (assume small)

layer peak shifts w/ φ
in ω scans



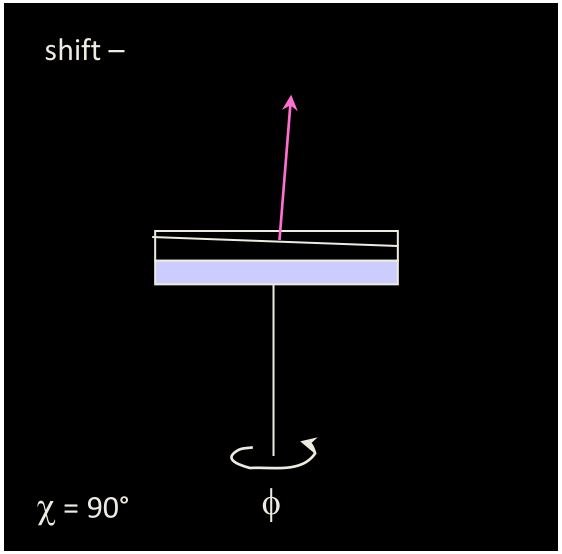
Thin films

Misorientation

First, determine orientation of substrate

Layer tilt (assume small)

layer peak shifts w/ φ
in ω scans



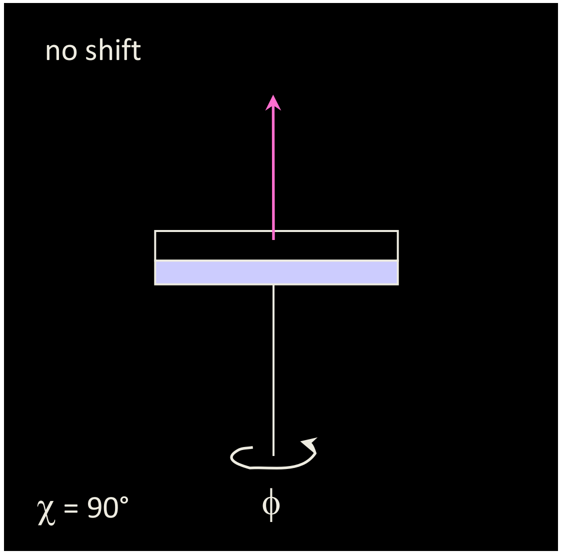
Thin films

Misorientation

First, determine orientation of substrate

Layer tilt (assume small)

layer peak shifts w/ ϕ
in ω scans



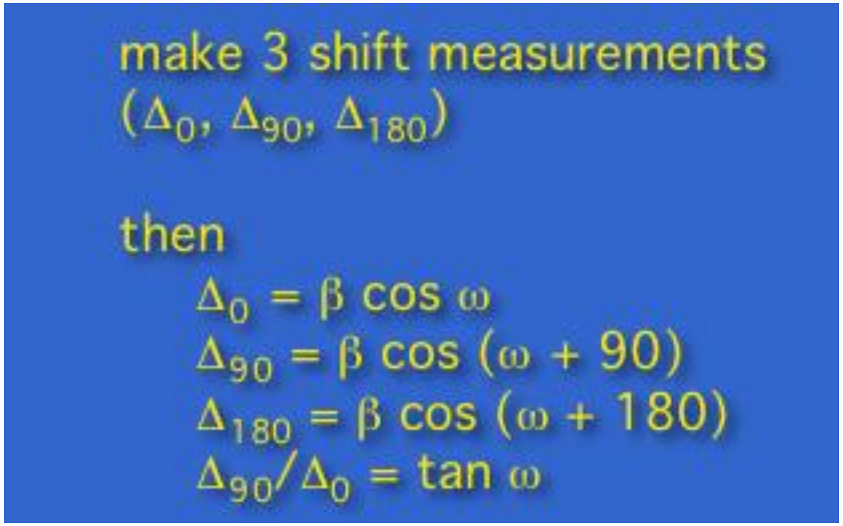
Thin films

Misorientation

First, determine orientation of substrate

Layer tilt (assume small)

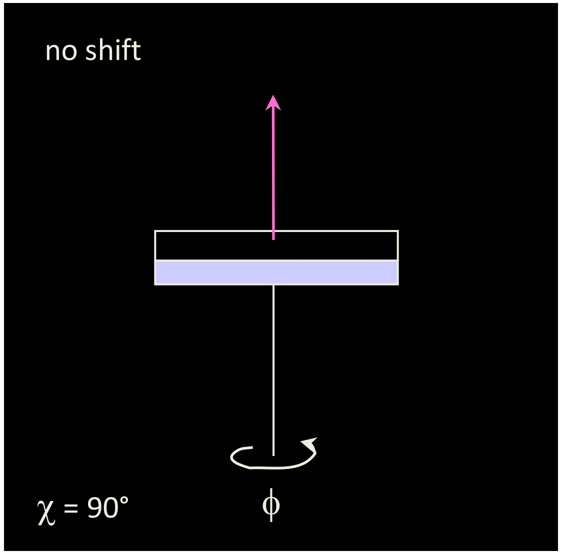
layer peak shifts w/ ϕ
in ω scans



make 3 shift measurements
$(\Delta_0, \Delta_{90}, \Delta_{180})$

then

$$\Delta_0 = \beta \cos \omega$$
$$\Delta_{90} = \beta \cos (\omega + 90)$$
$$\Delta_{180} = \beta \cos (\omega + 180)$$
$$\Delta_{90}/\Delta_0 = \tan \omega$$



Thin films

Dislocations

From:

- high mismatch strain, locally relaxed
- local plastic deformation due to strain
- growth dislocations

Thin films

Dislocations

From:

- high mismatch strain, locally relaxed
- local plastic deformation due to strain
- growth dislocations

Estimate dislocation density ρ from broadening β (radians) & Burgers vector b (cm):

$$\rho = \beta^2/9b^2$$

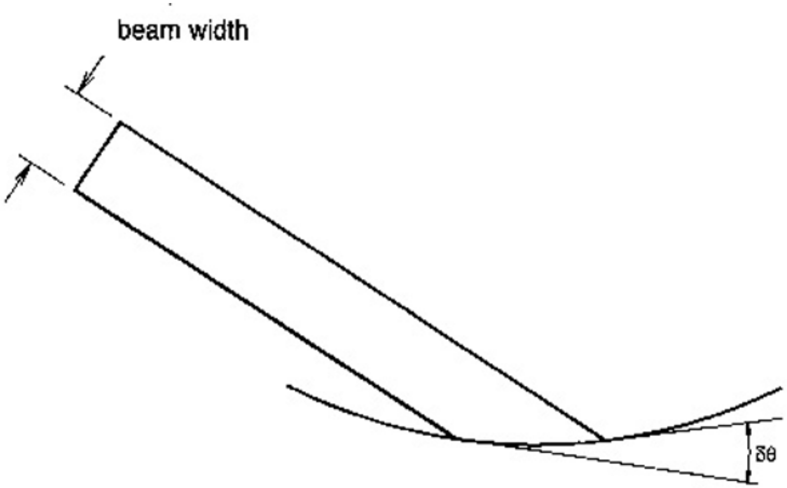
Thin films

Curvature

R = radius of curvature, s = beam diameter

angular broadening = s/R = $\delta\theta$

beam	radius	broadening
5 mm	100 m	10"

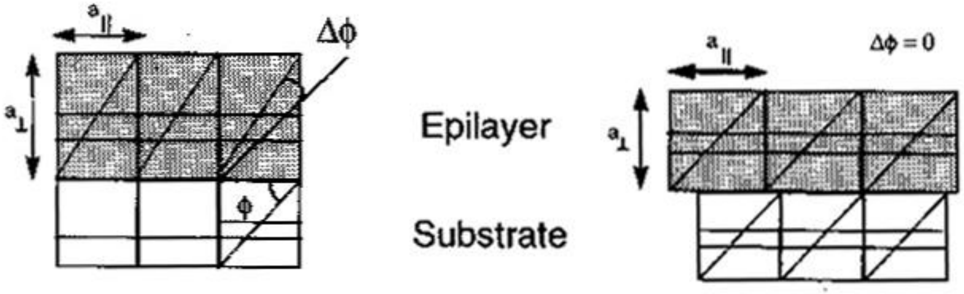


Thin films

Relaxation

Need to measure misfit parallel to interface

Both mismatch & misorientation change on relaxation



Fully Strained

(a)

Fully Relaxed

(b)

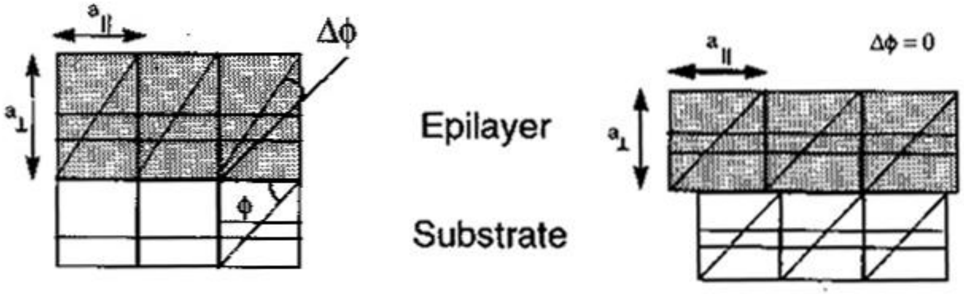
Interplanar spacings change with mismatch distortion & relaxation – changes splittings

Thin films

Relaxation

Need to measure misfit parallel to interface

Both mismatch & misorientation change on relaxation



Fully Strained

(a)

Fully Relaxed

(b)

So, also need misfit perpendicular to interface

Then, % relaxation is

$$R = \frac{a_l - a_s}{a_l^R - a_s} \times 100$$

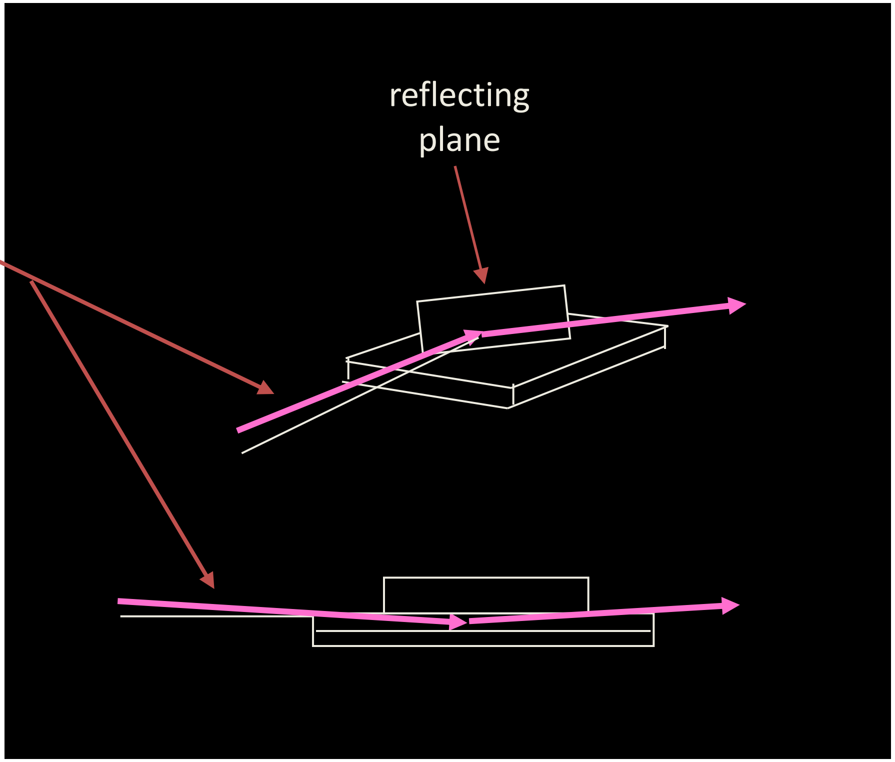
Thin films

Relaxation

Grazing incidence

Incidence angle usually very low….~1-2°

Limits penetration of specimen



Thin films

Relaxation

Grazing incidence

- Incidence angle usually very low….~1-2°

- Limits penetration of specimen

Penetration depth – G(x) = fraction of total diffracted intensity from layer x cm thick compared to infinitely thick specimen

$$G(x) = 1 - \exp\left(\frac{-2\mu\rho x}{\sin\theta}\right) = \frac{\text{intensity from a layer x cm thick}}{\text{intensity from an infinitely thick sample}}$$

Thin films

Relaxation

Grazing incidence

- Incidence angle usually very low.....~1-2°

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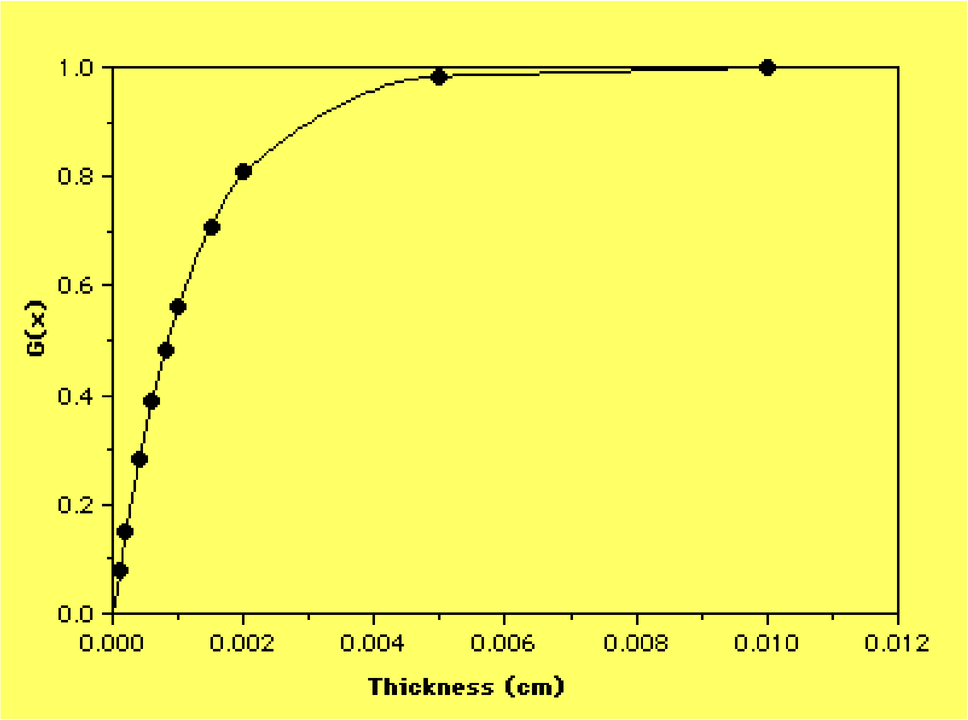


Penetration depth – G(x) = fraction of total diffracted intensity from layer x cm thick compared to infinitely thick specimen

$$G(x) = 1 - \exp\left(\frac{-2\mu\rho x}{\sin\theta}\right) = \frac{\text{intensity from a layer x cm thick}}{\text{intensity from an infinitely thick sample}}$$

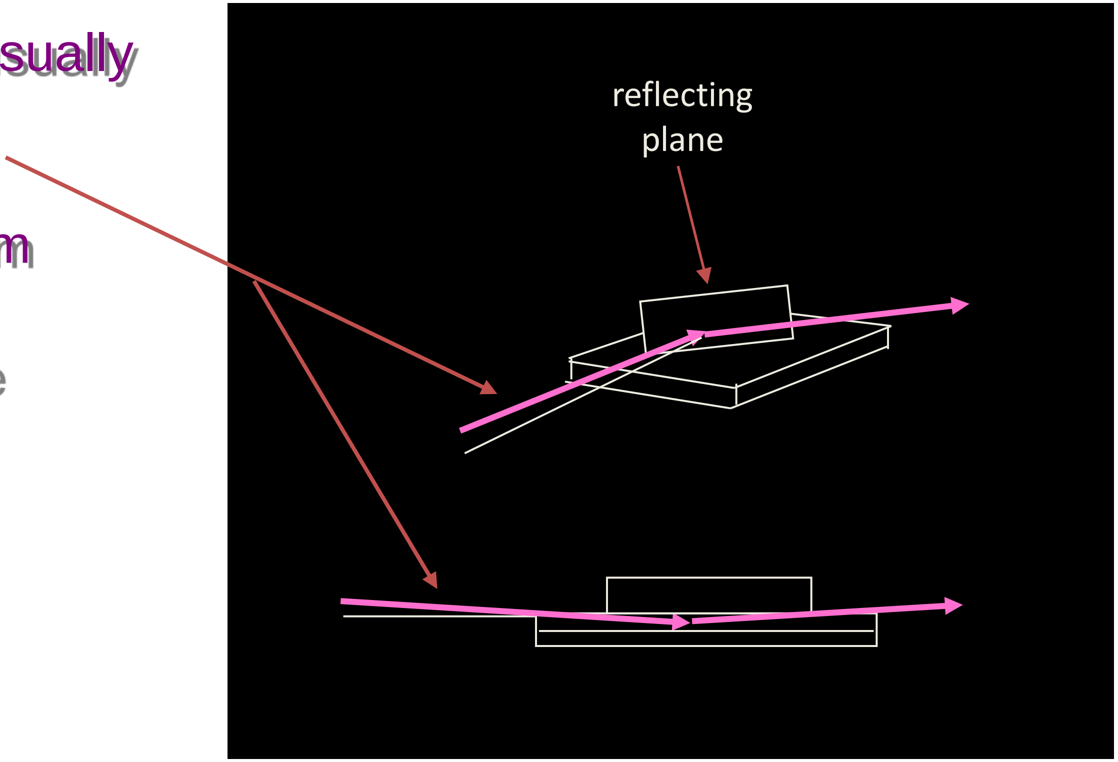
Thin films

Relaxation

Grazing incidence

Incidence angle usually very low…..~1-2°

Reflection not from planes parallel to specimen surface

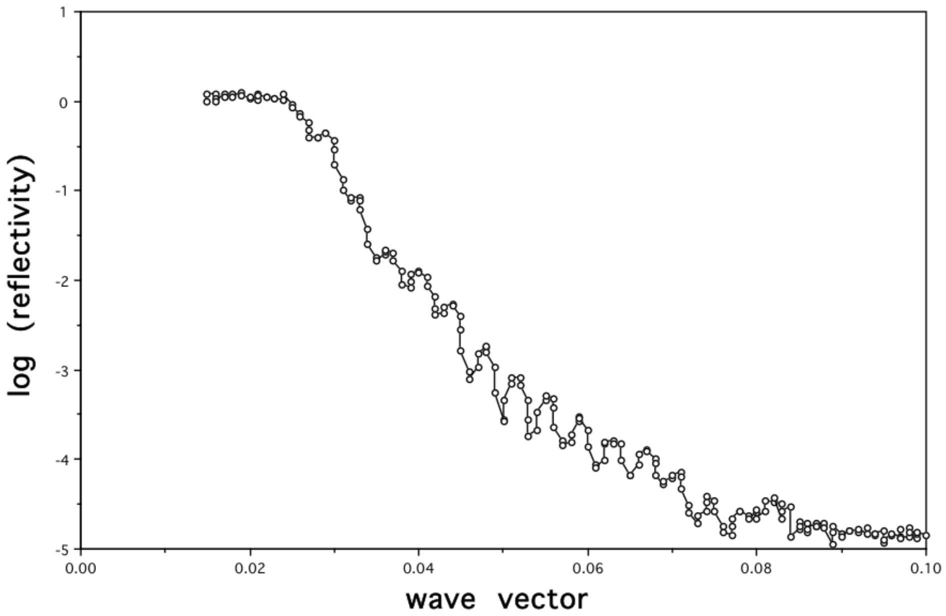


Thin films

Relaxation

Grazing incidence

If incidence angle ~0.1-5° & intensity measured in symmetric geometry (incident angle = reflected angle), get reflectivity curve

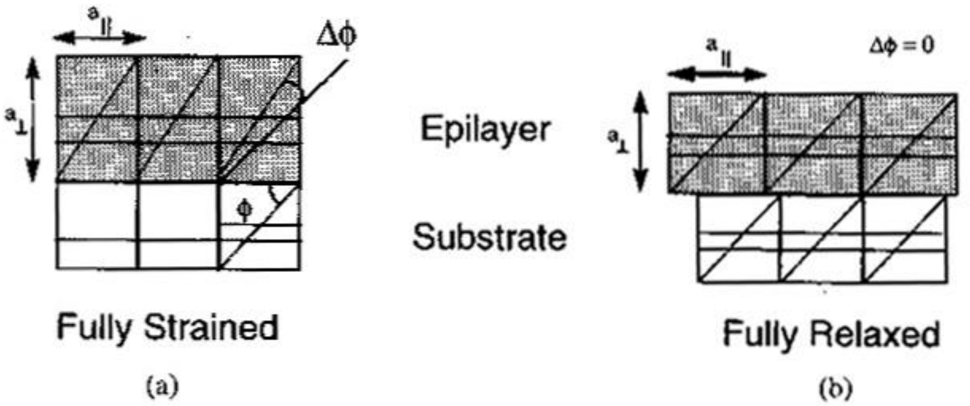


Thin films

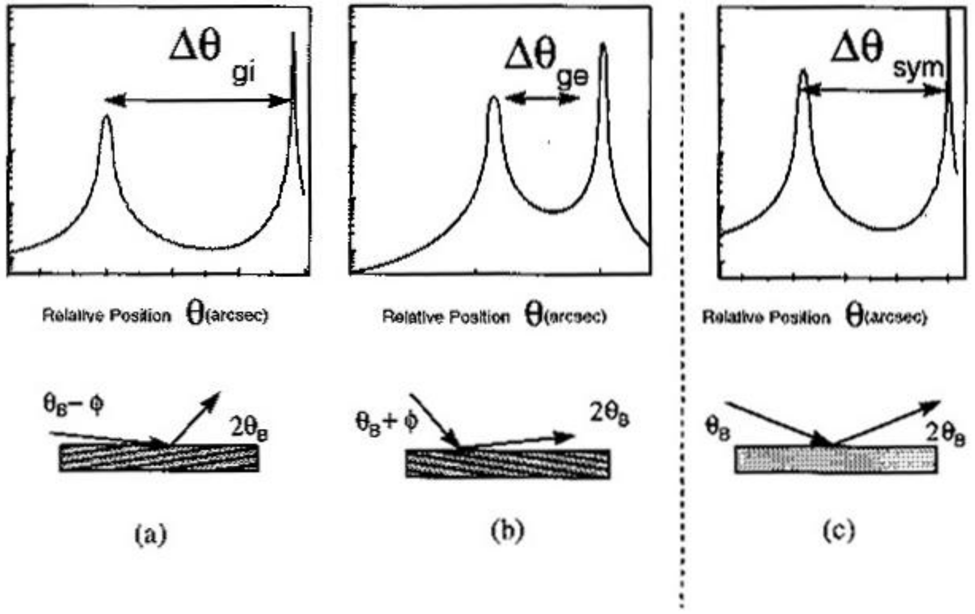
Relaxation

Need to measure misfit parallel to interface

Use grazing incidence e.g., (224) or (113)



(a) (b)



(a) (b) (c)

Thin films

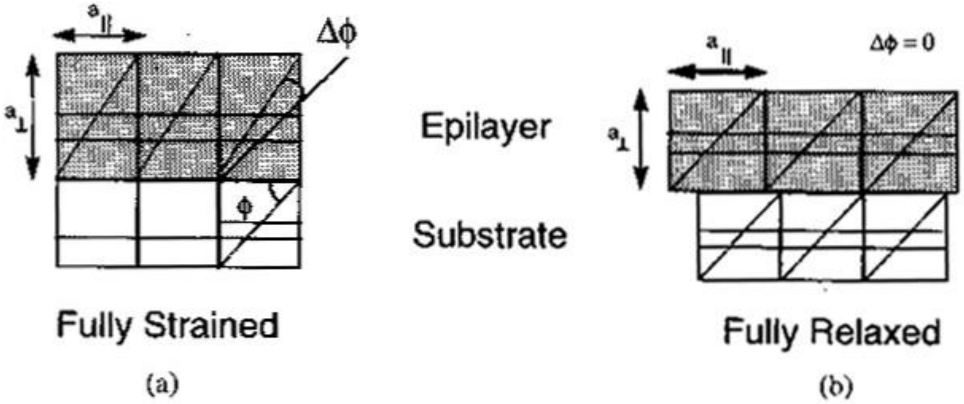
Relaxation

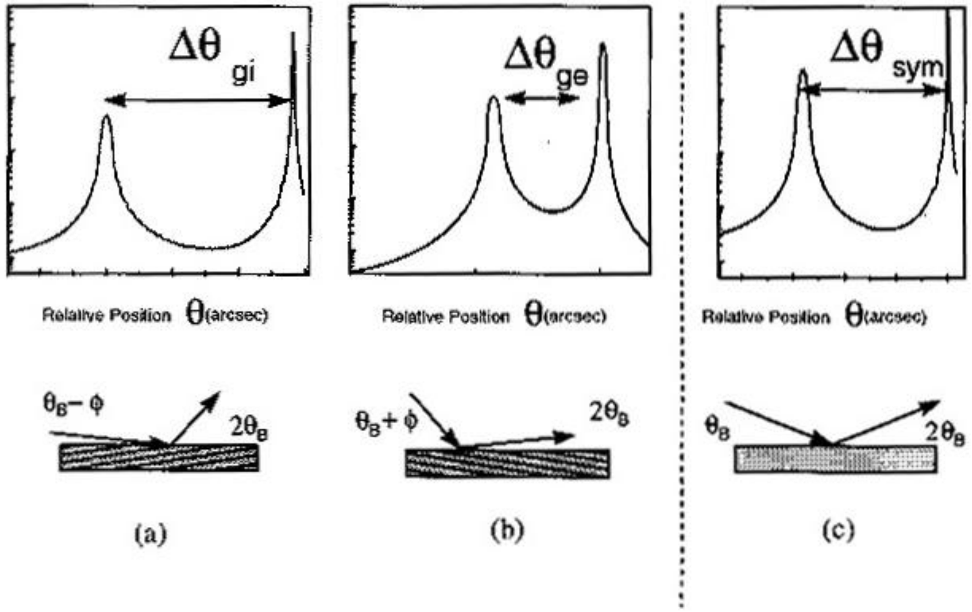
Use grazing incidence
e.g., (224) or (113)

Need to separate tilt
from true splitting

Tilt effect reversed
on rotation of φ = 180°

Mismatch splitting
unchanged on rotation





Thin films

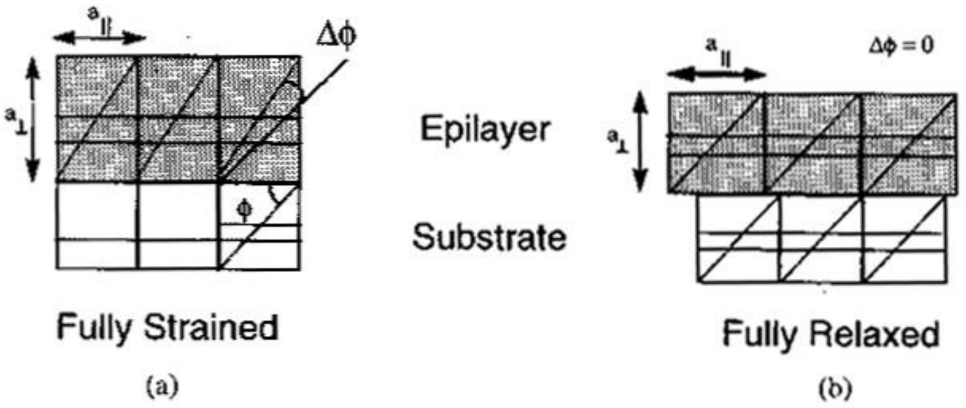
Relaxation

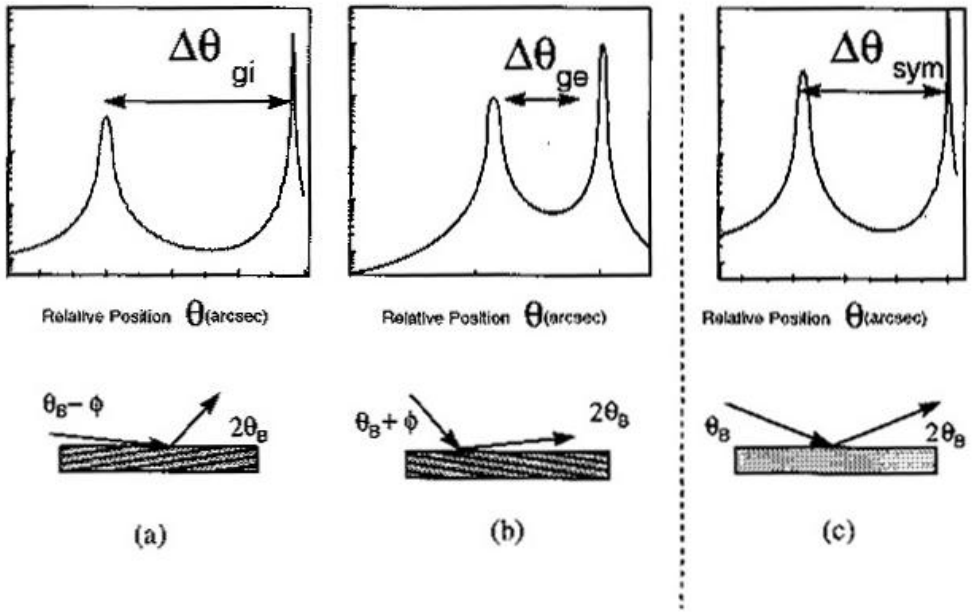
Use grazing incidence
e.g, (224) or (113)

For grazing incidence:

$\Delta\theta_i = \delta\theta + \delta\phi$

$\delta\theta$ – θ splittting
betwn substrate
& layer





Thin films

Relaxation

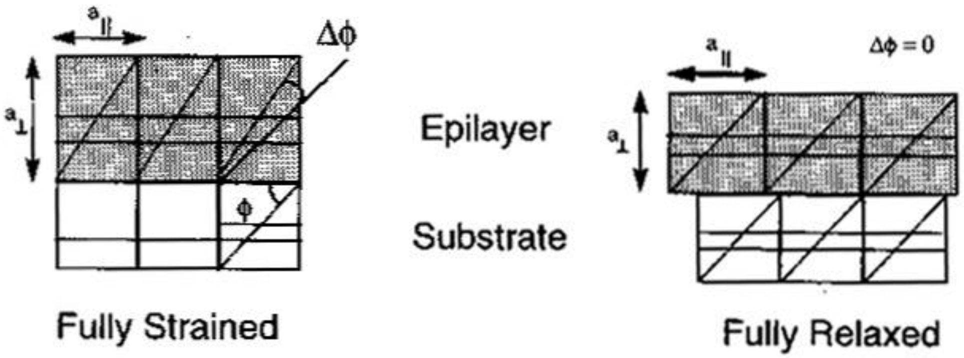
Use grazing incidence
e.g, (224) or (113)

For grazing incidence:

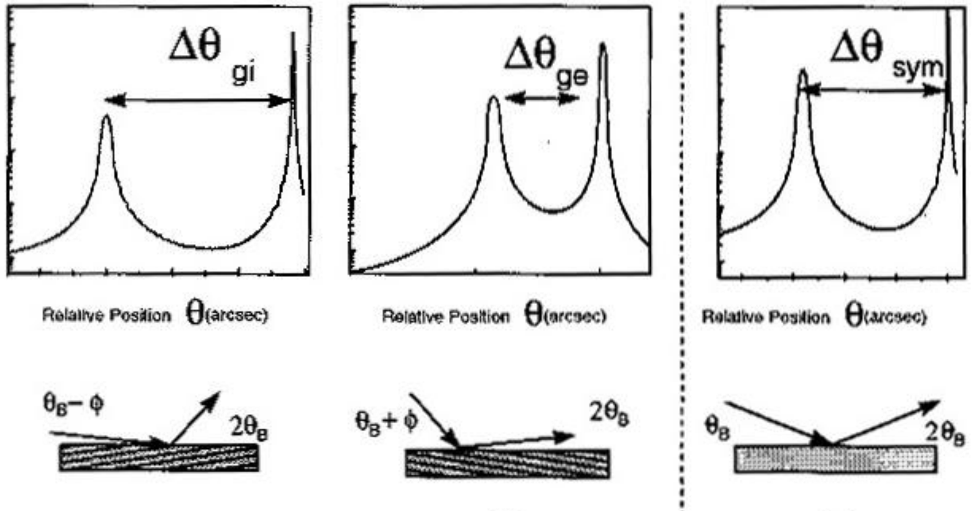
$$\Delta\theta_i = \delta\theta + \delta\phi$$

$$\Delta\theta_e = \delta\theta - \delta\phi$$

Can thus get both
$\delta\theta$ and $\delta\phi$



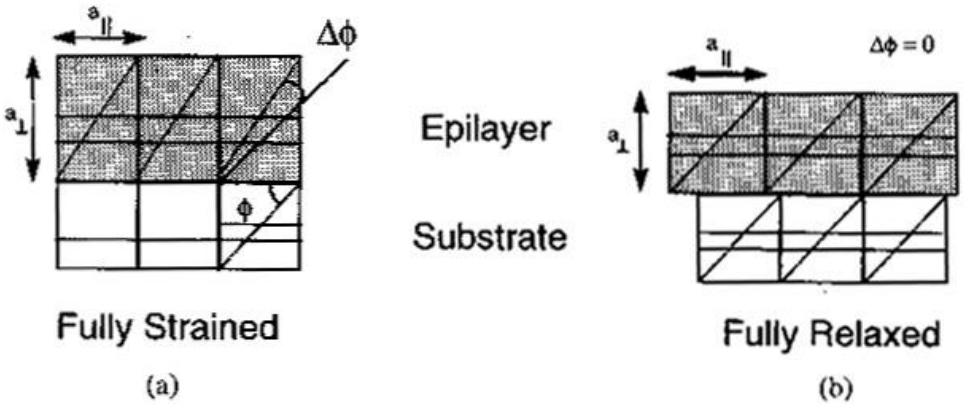
(a) (b)



(a) (b) (c)

Thin films

Relaxation



Fully Strained

(a)

Fully Relaxed

(b)

Also,

$$\theta_l = \theta_s + \delta\theta$$

$$\phi_l = \phi_s + \delta\phi$$

And

$$\frac{4\sin^2\theta_l}{\lambda^2} = \frac{h^2+k^2}{a_l^2} + \frac{l^2}{c_l^2}$$

$$\sec^2\phi_l = \frac{c_l^2}{l^2}\left\{\frac{h^2+k^2}{a_l^2} + \frac{l^2}{c_l^2}\right\}$$

Thin films

Relaxation

Also,

$$\theta_l = \theta_s + \delta\theta$$

$$\phi_l = \phi_s + \delta\phi$$

And

$$\frac{4\sin^2\theta_l}{\lambda^2} = \frac{h^2+k^2}{a_l^2} + \frac{l^2}{c_l^2} \qquad \sec^2\phi_l = \frac{c_l^2}{l^2}\left\{\frac{h^2+k^2}{a_l^2} + \frac{l^2}{c_l^2}\right\}$$

Finally

$$c_l = \frac{l\lambda}{2\sin\theta_l\cos\phi_l} \qquad a_l = \frac{l\lambda}{2\sin\theta_l}\sqrt{\frac{h^2+k^2}{l^2}}$$

$$R = \frac{a_l - a_s}{a_l^R - a_s} \times 100$$

Thin films

Homogeneity

Measure any significant parameter over a grid on specimen

Ex: compositional variation

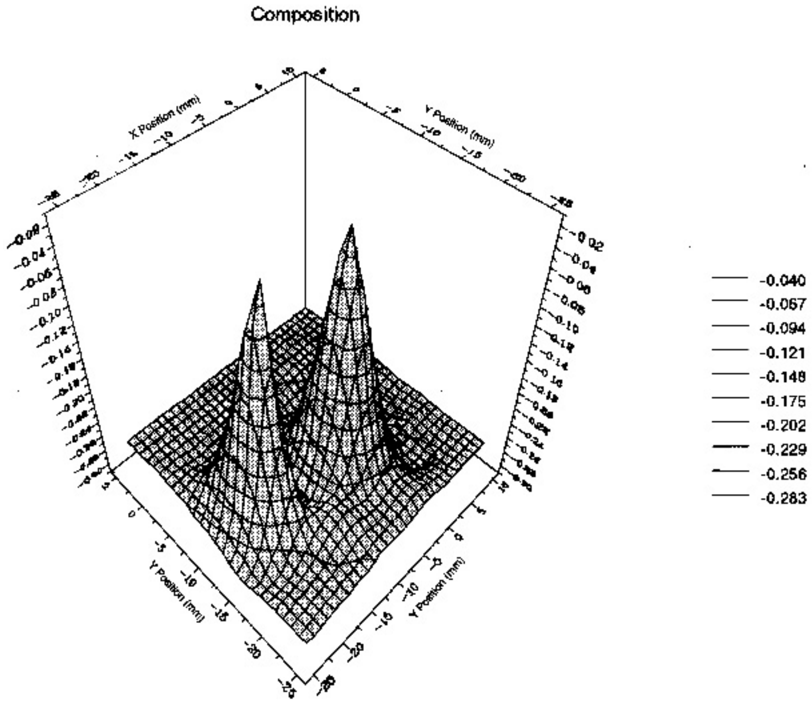
get composition using Vegards law
measure lattice parameter(s) – calculate relaxed mismatch

Thin films

Homogeneity

Measure any significant parameter over a grid on specimen

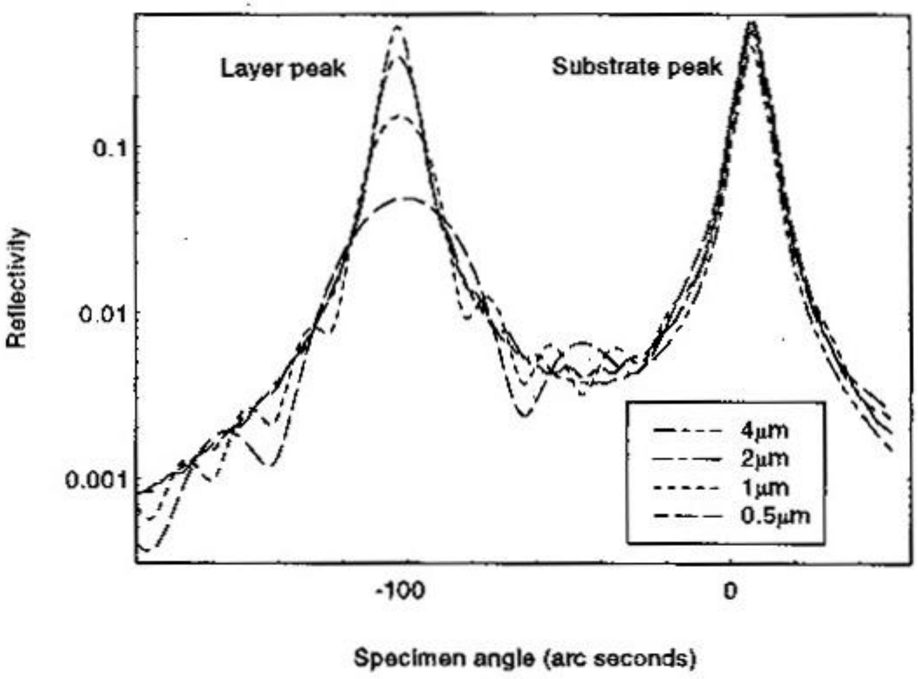
Ex: variation of In content in InAlAs layer on GaAs



Thin films

Thickness

For simple structure layer, layer peak integrated intensity increases monotonically w/ thickness



calculated curves

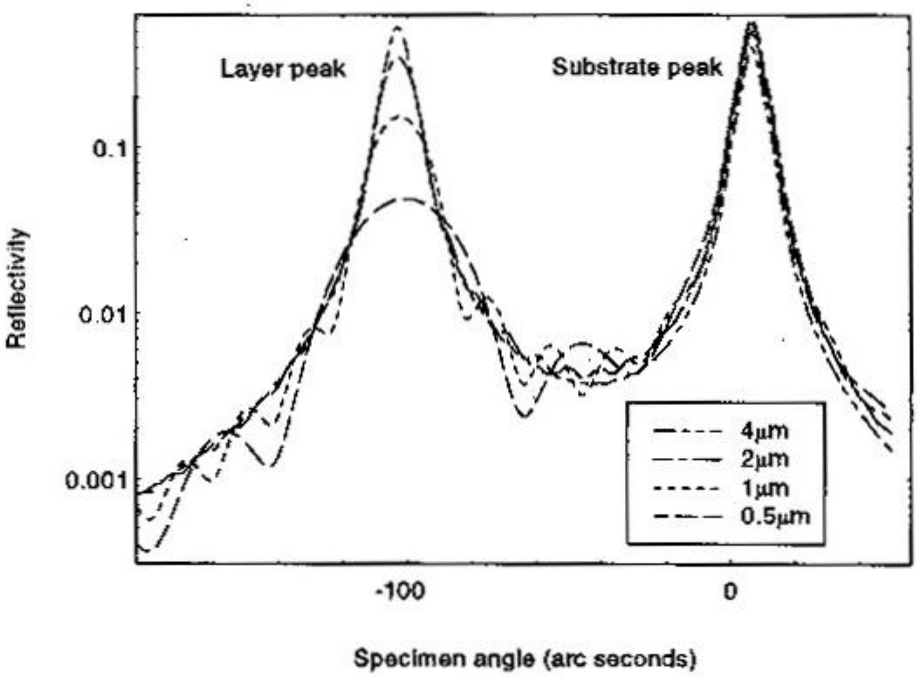
Thin films

Thickness

For simple structure layer, layer peak integrated intensity increases monotonically w/ thickness

Note thickness fringes

Can use to estimate thickness



calculated curves

Thin films

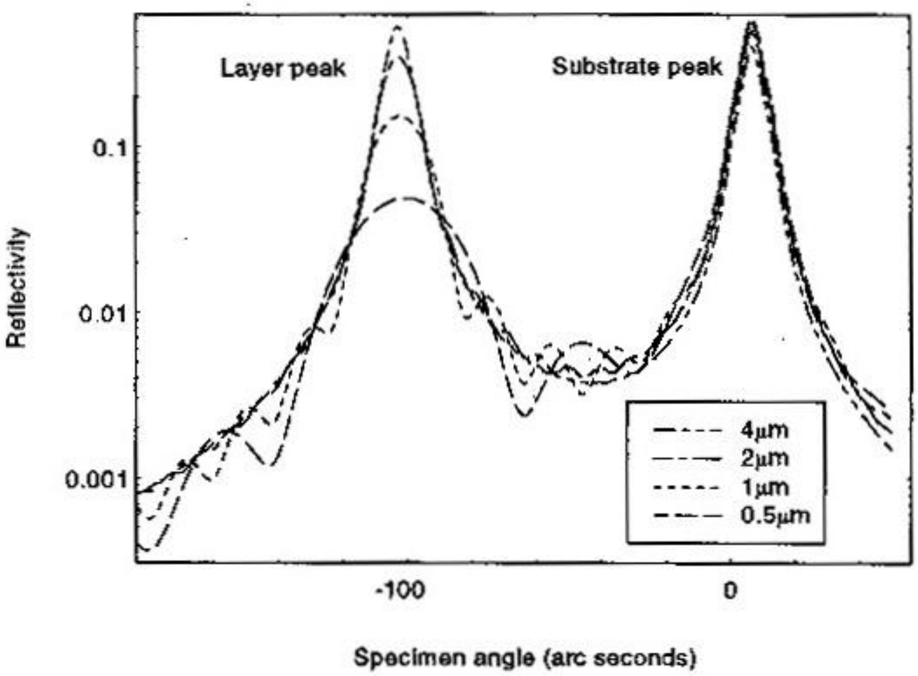
Thickness

For simple structure layer, layer peak integrated intensity increases monotonically w/ thickness

$$\Delta\theta_p = \frac{\lambda \gamma_g}{t \sin 2\theta}$$

$$\Delta\theta_p = \frac{\lambda \sin(\theta \pm \phi)}{t \sin 2\theta}$$

$$t = \frac{\lambda}{2\Delta\theta_p \cos\theta}$$



calculated curves