Materials Analysis MATSCI 162/172
Laboratory Exercise No. 3
Analysis of epitaxial layers

Objectives:

To determine the mismatch, composition, thickness and strained lattice parameters of heteroepitaxial layers.

Background and Theory:

Determination of thickness from the fringes close to main scattering peaks

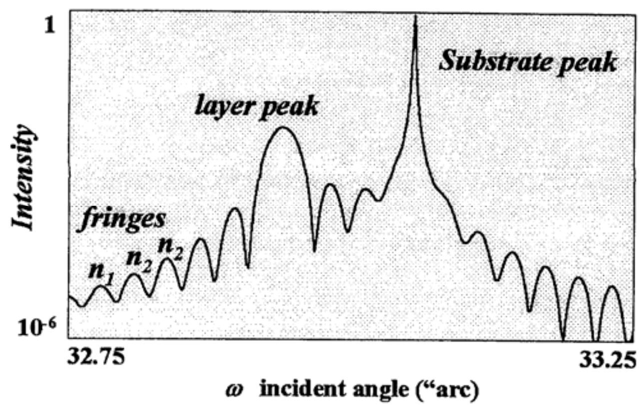
The most accurate way to determine thickness from x-ray diffraction is computer simulation of the whole XRD profile. Despite this it is often useful to get thickness by measuring the interference peak separation. Interference fringes observed in the scattering pattern, due to the different optical paths of the x-rays, are related to the thickness of the layers.

We can determine the thickness fringe peak positions n_1, n_2, n_3, ... etc., and determine a characteristic length scale, L, from Bragg equation. Now we can write for scattering from planes parallel to the surface:

$$2L\sin\omega_1 = n_1\lambda$$
$$2L\sin\omega_2 = n_2\lambda$$

Hence

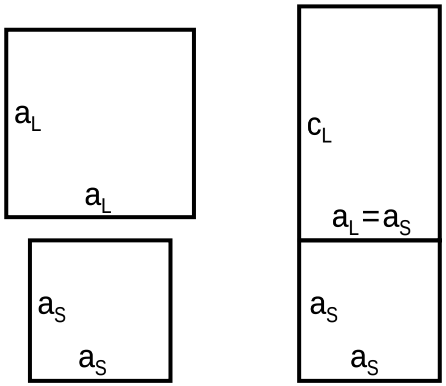
$$L = \frac{(n_1 - n_2)\lambda}{2(\sin\omega_1 - \sin\omega_2)} \approx \frac{(n_1 - n_2)\lambda}{2\Delta\omega\cos\omega}$$



where ω_1, ω_2, ...correspond to the angular positions of the peaks and $\Delta\omega = \omega_1 - \omega_2$, and ω is some average of the two values.
This equation is valid for scattering from planes parallel to the surface.

Determination of the mismatch

Any material phase will have overall characteristics associated with the periodic repeat unit, i.e. lattice parameters a, b, c, α, β, γ. For example AlAs, GaAs, InP, InAs, etc., all have the same atomic arrangements in their unit cells yet atomic radii differ and consequently lengths $a = b = c$ are different for each phase. The angles α, β, γ are all 90°.



These differences in lattice parameter through Bragg's equation give rise to different scattering angles. For nearly perfect layers this difference in lattice parameter is accommodated by elastic distortion. The strain in the layer can be expressed as a function of Δθ from Bragg equation. For cubic (001) oriented material the experimentally measured normal component of the mismatch:

$$m_{\perp} = \frac{a_{\perp} - a_S}{a_S} = \left(\frac{\Delta a}{a}\right)_{\perp} = \frac{\sin\theta_S - \sin(\theta_S + \Delta\theta)}{\sin(\theta_S + \Delta\theta)} \approx -\frac{\Delta\theta}{\tan\theta_S}$$

The experimental mismatch, $m_{\perp}$, can be related to the mismatch through the equation:

$$m = \frac{a_L - a_S}{a_S} = \frac{1-\nu}{1+\nu} m_{\perp}$$

where ν is Poisson ratio.
For Si, ν = 0.28.

Determination of the layer composition

The composition of the $A_{1-x}B_x$ alloy can be calculated from Vegard's law, which states that the lattice parameter of a solid solution alloy will be given by a linear dependence of lattice parameter on composition:

$$a_L(x) = (1-x)a_A + xa_B$$

The fractional composition in the strained alloy layer can be obtained from the mismatch.

Let say our substrate has the lattice parameter a_A. Layer grown coherently on that substrate has composition $A_{1-x}B_x$ and relaxed lattice parameter a_L.Then:

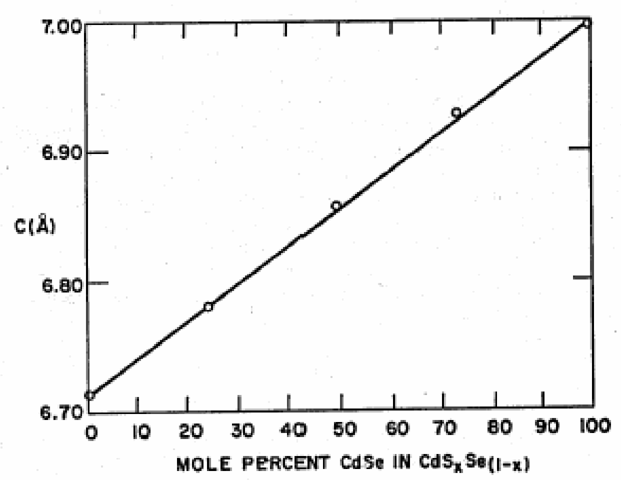
$$a_L = a_A + x(a_B - a_A) \rightarrow x = \frac{a_L - a_A}{a_B - a_A}$$

From the mismatch we may write:

$$m = \frac{a_L - a_A}{a_A} \rightarrow (a_L - a_A) = a_A m$$

then

$$x = m\frac{a_A}{a_B - a_A}$$



For SiGe system:

$$a_{Ge_xSi_{1-x}} = xa_{Ge} + (1-x)a_{Si} + 0.007\left[(2x-1)^2 - 1\right]$$

where lattice parameters are in Å.

Lab report:

You are to prepare a formal lab report in which you demonstrate the technique that you use to get parameters of the heteropeitaxial layers. Your report should contain a title, author name and affiliation, introduction, experimental, results and discussion section. Following a brief description of the experimental method, discuss how you made your calculations.

The results section should contain a table showing your experimentally determined values. The discussion section should briefly explain any deviations of your calculated values. Comment also on the effects of random and systematic errors.