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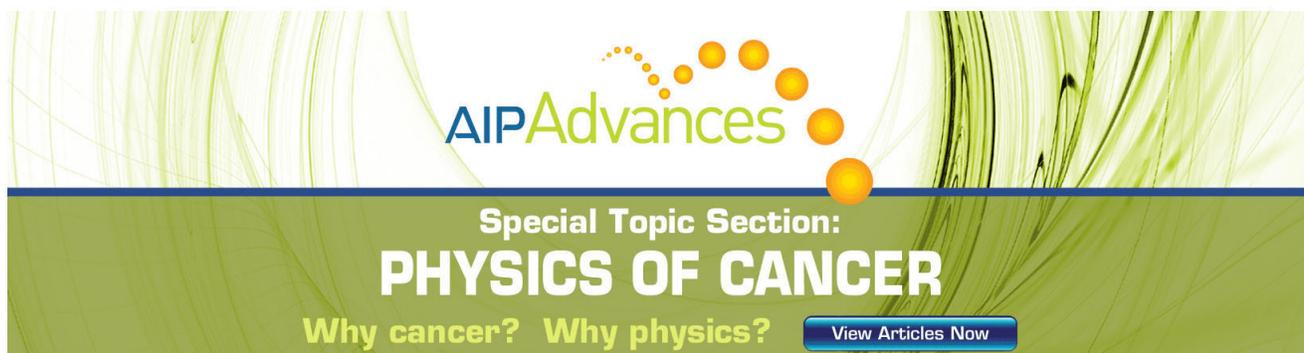
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X-ray interference in quantum-well laser structures

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X-ray interference effects are observed in the simulated rocking curves of quantum-well laser structures. It is shown that the interference effects appear in the cladding layer peak of rocking curves for a generic sample structure of a thin heterojunction layer of composition A cladded with two thicker layers of composition B. Depending on the detailed layer structure and the lattice mismatch, the sandwiched quantum-well layer can be as thin as 2–3 Å in order to affect the interference structure of the cladding layer peak. For a given mismatch, the interference effect occurs around a certain minimum thickness and similar interference structures appear periodically with increasing quantum-well layer thickness. This effect can be used to estimate the quantum-well layer thickness with a high accuracy. A simple model is used to calculate the thickness period as a function of lattice misfit and diffraction geometry. The calculation results explain the simulation results.

I. INTRODUCTION

It has been of a recent research interest to measure, non-destructively, the thicknesses of thin heterojunction epitaxial layers using the x-ray rocking curve (XRC) technique.^{1,2} Thickness measurement using the individual Bragg reflection peaks associated with each heterojunction layer is limited to fairly thick layers (> 500 Å) because of the difficulty of detecting low intensities. Other features in the rocking curve, such as the interference fringes, have also been used in the thickness measurements. For a $\text{Al}_{0.35}\text{Ga}_{0.65}\text{As}$ (1.3 μm)/ $\text{Al}_{0.09}\text{Ga}_{0.91}\text{As}$ (0.13 μm)/ $\text{Al}_{0.35}\text{Ga}_{0.65}\text{As}$ (1.3 μm) laser structure grown on a GaAs substrate, Chu and Tanner¹ reported that the 0.13-μm-thick AlGaAs active layer thickness can be measured within ± 200 Å using the interference structure on the cladding layer rocking curve peak. The interference is associated with the phase coherence of the x-ray waves across the thin active layer. More recently, for GaInAs/GaAs quantum-well structures, Jeong, Schlesinger, and Milnes² used the Pendellosung fringes of a thicker barrier layer (513-Å GaAs), which are modulated by a broad weak peak due mostly to a thin quantum-well layer (182-Å $\text{Ga}_{0.72}\text{In}_{0.28}\text{As}$), to estimate the quantum-well layer thickness. For the quantum-well devices whose structures are typified by a thin layer of composition A sandwiched between two thicker layers of composition B, we report here that the thicknesses can be estimated for the quantum wells as thin as a few Å by using the x-ray interference effects produced on the cladding layer peak. We also present a simple calculation which predicts the simulation results.

II. DYNAMICAL X-RAY DIFFRACTION THEORY SIMULATION

In Fig. 1 we show the quantum-well laser structure, together with the nominal compositions and thicknesses, which is grown on a (001) face GaAs substrate. This structure was actually used for fabrication of a quantum-well laser.³ The rocking curves of the quantum-well laser structure in Fig. 1 are simulated using the computer programs developed by us based on a dynamical diffraction theory.⁴ Figure

2 shows the simulated rocking curves taken with 004 reflection, $\text{CuK}\alpha_1$ radiation, and the GaAs substrate crystal as the reference. In each rocking curve, the peak "s" on the right corresponds to the GaAs substrate (and layers) and the peak "c" on the left corresponds to the cladding AlGaAs layers. In Fig. 2, the rocking curves are for varying thicknesses of the active layer with all other layer parameters kept the same as in Fig. 1. The feature "a" in the cladding layer peak is due to the interference of the x-ray waves across the active layer, and its angular position within the cladding layer peak changes with a 2–3-Å change in the active layer thickness. The cladding layer peak in Fig. 2 is similar in shape to the cladding layer peak obtained by Chu and Tanner¹ for their laser structure which had a 0.13-μm-thick active layer. Figure 2 shows the active layer thicknesses at which the same interference structures appear in the cladding layer peak. The period is 25.5 Å with respect to the active layer thickness of the sample in Fig. 1 and 004 rocking curves. The interference structure in the cladding layer peak is sensitive to a 2–3-Å change in the active layer thickness, which can be utilized for accurate measurements of the active layer thickness. The fringes "pf" between the substrate

0.1 μm	GaAs	cap layer
0.2 μm	$\text{Al}_x\text{Ga}_{1-x}\text{As}$	$x = 0.4 \rightarrow 0$
1.5 μm	$\text{Al}_{0.4}\text{Ga}_{0.6}\text{As}$	cladding layer
0.2 μm	$\text{Al}_x\text{Ga}_{1-x}\text{As}$	$x = 0 \rightarrow 0.4$
100 Å	GaAs	
t_a	$\text{Ga}_{0.63}\text{In}_{0.37}\text{As}$	active layer
100 Å	GaAs	
0.2 μm	$\text{Al}_x\text{Ga}_{1-x}\text{As}$	$x = 0.4 \rightarrow 0$
1.5 μm	$\text{Al}_{0.4}\text{Ga}_{0.6}\text{As}$	cladding layer
0.2 μm	$\text{Al}_x\text{Ga}_{1-x}\text{As}$	$x = 0 \rightarrow 0.4$
0.5 μm	GaAs	buffer
GaAs (001) substrate		

FIG. 1. The quantum-well laser structure. Simulated rocking curves for this device with varying active layer thickness are shown in Figs. 2 and 3, and with varying active layer composition in Fig. 5.

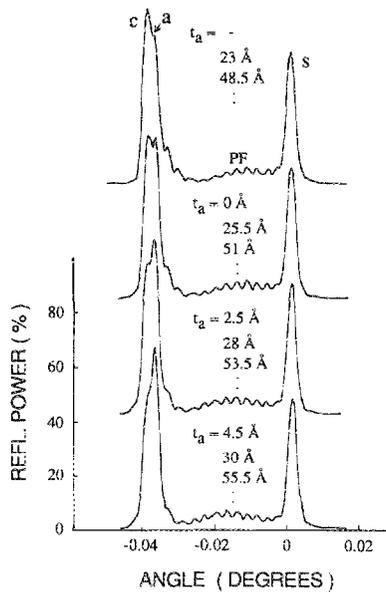


FIG. 2. Simulated 004 rocking curves of the quantum-well laser in Fig. 1. Half width of the convolution function was 3 arcsec. Peak "s" is from the GaAs substrate and peak "c" is mostly from the 1.5- μm cladding layers. The "a" is the interference kink due to the active layer. Note that the location of "a" changes with the active layer thickness, within the cladding layer peak. For each rocking curve, the active layer thicknesses are given for similar interference structures in the cladding layer peak. The period is 25.5 \AA .

and cladding layer peaks are the Pendellosung fringes of the top AlGaAs cladding layer in Fig. 1. The layer thickness calculated from the fringe period is consistent with the top cladding layer thickness.⁵ Figure 3 shows the simulated 115 asymmetric rocking curves (with a large incidence angle) for the sample in Fig. 1. The minimum thickness, for the interference kink to appear at the peak maximum, is around 5 \AA for the 115 reflection as opposed to 0 \AA for the 004 reflection. The thickness period for similar interference effect is about 22 \AA for the 115 reflection.

III. KINEMATICAL MODEL FOR X-RAY INTERFERENCE

In order to derive a formula which will predict the minimum active layer thickness and the thickness periodicity for the appearance of the interference structures, we consider a simpler sample structure in Fig. 4. Simulated 004 rocking curve peaks for the cladding layer showed essentially the same features as those in Fig. 2, but with an interference period of 18.6 \AA with respect to the active layer thickness. Subsidiary peaks also appeared around the cladding layer peak which are the Pendellosung fringes due to the top AlGaAs cladding layer. The interference structure on the

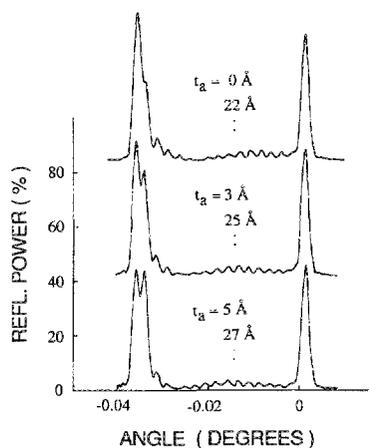


FIG. 3. Simulated 115 rocking curves of Fig. 1 taken at the large incidence angle. The Gaussian function for convolution is 2 arcsec half width. Compare the active layer thickness minimum and period for the appearance of interference in the cladding layer peak with the 004 rocking curves.

1.5 μm Al _{0.5} Ga _{0.5} As	cladding layer
t _a Ga _{0.5} In _{0.5} As	active layer
1.5 μm Al _{0.5} Ga _{0.5} As	cladding layer
GeAs (001) substrate	

FIG. 4. A simple strained layer quantum-well structure. The active layer thickness t_a can be 0 \AA and up. This structure is for Eqs. (1), (2), and (3) in the text.

cladding layer peak can be most easily understood using the kinematical diffraction theory.⁶ Assuming that the layers are thin enough so that the kinematical diffraction theory is applicable and neglecting the normal absorption, it can be shown for the sample in Fig. 4 that the reflecting power near the cladding layer Bragg angle is approximately

$$\begin{aligned} \text{Reflecting power} \\ \text{(cladding layer)} &\approx 4[\sin^2(A_c Y_c)/Y_c^2] \\ &\quad \times \cos^2(A_c Y_c + A_a Y_a), \end{aligned} \quad (1)$$

where

$$\begin{aligned} A &= (\lambda r_c f_H' t) / (V \sqrt{\gamma_0 \gamma_H}), \\ Y &\approx [\pi V \sin(2\Theta_B) / (\lambda^2 r_c f_H')] \sqrt{|\gamma_0 / \gamma_H|} \\ &\quad \times (\Delta\Theta_B + k_1 \epsilon_1^{\text{nr}} + k_2 \epsilon_2^{\text{nr}}) \end{aligned}$$

(Ref. 7), and other parameters are defined as follows: λ = x-ray wavelength, Θ_B = substrate Bragg angle, r_c = classical electron radius, f_H' = real part of the structure factor, V = unit cell volume, γ_0, γ_H = direction cosines of the incident and diffracted wave vectors, t = layer thickness, $\Delta\Theta_B = \Theta - \Theta_B$, $k_{1,2}$ = geometrical factors, $\epsilon_1^{\text{nr}} = (a_1 - a_s)/a_s$, $\epsilon_2^{\text{nr}} = (a_{\parallel} - a_s)/a_s$, a_1, a_{\parallel} = layer lattice constants normal and parallel to the plane, a_s = substrate lattice constant, and the subscripts "a" and "c" in Eq. (1) correspond to the active and cladding layers, respectively. For most strained quantum-well structures the epitaxial layers are pseudomorphic and $\epsilon_2^{\text{nr}} = 0$.

The cosine term in Eq. (1) contains the phase shift $A_a Y_a$ due to the active quantum-well layer. For real samples, the plane wave rocking curve, Eq. (1), is convolved with a Gaussian broadening function. Therefore, when the condition that $\cos^2(A_c Y_c + A_a Y_a) = 0$ occurs within the cladding layer peak, the rocking curve will show a "kink" at a corresponding location in the peak. In order for this kink to be observable in the experimental rocking curve, the epitaxial layer must be of a high quality and the incident x-ray beam spot needs to be as small as possible in order to avoid the additional broadening due to the wafer curvature. The interference kink is not clearly visible in the simulated rocking curves when the half width of the convolution function is greater than 4 arcsec.

The condition that the kink occurs at the intensity maximum of the cladding layer peak (i.e., $Y_c = 0$) is

$$A_a Y_a = 2\pi t \Delta\epsilon_1^{\text{nr}} \sin \Theta_B \cos \phi / \lambda = (n + \frac{1}{2})\pi, \quad (2)$$

where $\Delta\epsilon_1^{\text{nr}}$ = the difference in the ϵ_1^{nr} between the active layer and the cladding layer, n = integer, and ϕ = the angle

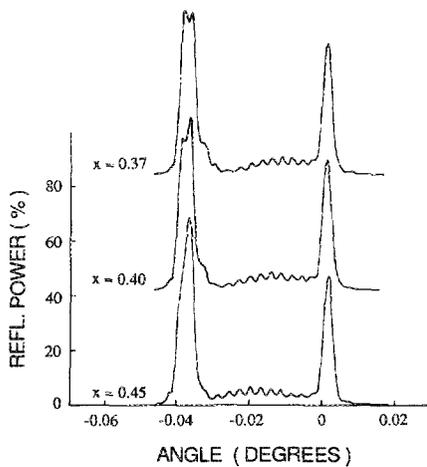


FIG. 5. Simulated 004 rocking curves of Fig. 1 at 25.5-Å active layer thickness for varying x in $\text{Ga}_{1-x}\text{In}_x\text{As}$ active layer.

between the lattice plane and sample surface. In Eq. (2), we assumed $\epsilon_{\parallel}^{\text{nr}} = 0$ for the quantum-well samples. For a given lattice mismatch between the active layer and the cladding layer (i.e., given $\Delta\epsilon_{\parallel}^{\text{nr}}$), Eq. (2) predicts that, for the sample in Fig. 4, similar interference structures will appear in the cladding layer peak with the active layer thickness of

$$\text{Period} = \lambda / (2\Delta\epsilon_{\parallel}^{\text{nr}} \sin \Theta_B \cos \phi) = d_{hkl} / (\Delta\epsilon_{\parallel}^{\text{nr}} \cos \phi), \quad (3)$$

where d_{hkl} is the spacing of the reflecting lattice planes (hkl). Different reflection geometry (different ϕ) can show the interference effects at different thicknesses as seen in the simulated rocking curves (Figs. 2 and 3), but the period does not depend on the wavelength explicitly. For the sample in Fig. 4, Eq. (3) gives a period of 20.3 Å as compared to the simulation result 18.6 Å. For the sample in Fig. 1, Eq. (1) gives a period of 27.8 Å as compared to the simulation result 25.5 Å. In Fig. 1, the additional layers between the quantum-well active layer and the thick uniform cladding layers induce additional phase shifts and affect the minimum active layer thickness at which the kink appears at the top of the cladding layer peak. According to the dynamical diffraction theory simulation, the thickness minimum was 9.5 Å for the sample in Fig. 4 [which agrees with Eq. (2) within 1 Å] and 0 Å for the sample in Fig. 1 (due to the many additional layers).

Finally, we present in Fig. 5 the simulated 004 rocking curves at three different compositions of the active layer (thickness = 25.5 Å) for the sample in Fig. 1. Figure 5 shows that the interference structure in the cladding layer peak can be used to estimate the composition of the active layer. In order to induce a phase shift equivalent to a decrease of 3 Å from the active layer thickness of 25.5 Å, the x in $\text{Ga}_{1-x}\text{In}_x\text{As}$ must increase by 0.043 from Eq. (2). However, the change in x needed for the equivalent phase shift is inversely proportional to the active layer thickness.

IV. CONCLUSION

In summary, using the x-ray interference effect in rocking curves, it is possible to estimate the quantum-well layer thicknesses with a high accuracy. Actual measurements shall depend on the lattice mismatch, diffraction geometry, layer quality, and x-ray beam size, but not on the wavelength. We presented the theoretical formula for the interference period, with respect to the quantum-well layer thickness, as a function of the lattice mismatch and the diffraction geometry.

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