As implied by Fig. 6.3.2, the diffraction peak of the thin film appears on the lower angle side of the sharp diffraction peak of the substrate and the diffraction intensity oscillates on both sides of the diffraction peak. This oscillation corresponds to the Pendellosung fringes related to the reflected wave moving from the interface between the film and the substrate.

6.3.3 Rocking Curve Analysis

In general, the thickness and composition of the multilayer film cannot be determined directly from the measured rocking curve. In actual analysis, we must simulate the rocking curve of a multilayer film model (of hypothetical film thickness and composition) as described in the previous section and change the thickness and the composition to reproduce the measured rocking curve in the analysis. This section presents several examples to help clarify the relationship between the rocking curve and the layer structure.

1. Single layer film
   Fig. 6.3.3 (a) shows the assumed layer structure, while Fig. 6.3.3 (b) shows the rocking curve for the (004) plane calculated with this model.

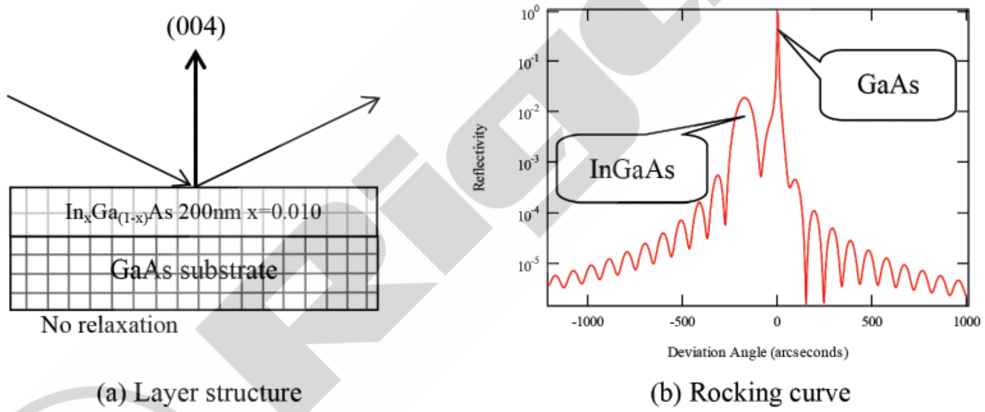
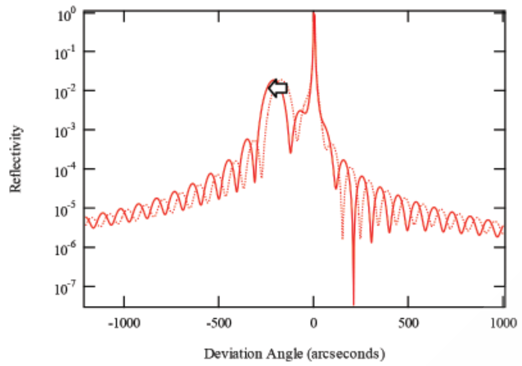


*Fig. 6.3.3 **Layer structure and rocking curve***

As shown in Fig. 6.3.3, the diffraction peak of the film appears at a lower diffraction angle with wider width and lower intensity than the diffraction peak of the substrate. This is because the film has a wider interplanar spacing in the (004) direction and because the crystal has a lesser volume contributing to the diffraction than the substrate. From the shift of the diffraction peaks of the substrate and the film, we can calculate the lattice constants of the film if the lattice constants of the substrate are known. If the presence or absence of lattice relaxation and the elastic constant are known, we can use the lattice constants to determine the composition ratio of the mixed crystal (in this example, the ratio of InAs and GaAs) based on Vegard's law. Additionally, the diffraction intensity oscillates on both sides of the diffraction peak of the film. We can obtain the thickness of the film based on the period of this oscillation.

Fig. 6.3.4 shows the changes in the rocking curve when x (the ratio of InAs and GaAs) of $In_xGa_{(1-x)}As$ (x = 0.010) is changed from 1.0% to 1.2% (when we increase the interplanar spacing).

6.3 Dynamical Theory of Diffraction in Multilayer Film Crystals

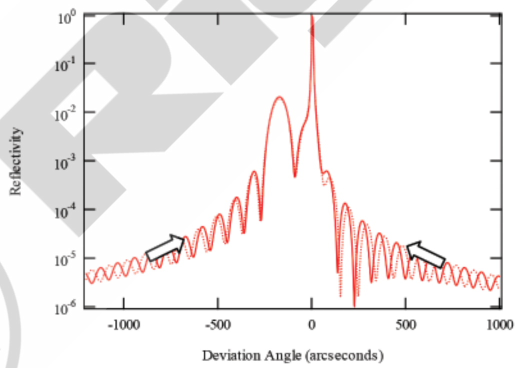


(Dashed curve: 1.0%, solid curve: 1.2%)

Fig. 6.3.4 Rocking curve

As shown by Fig. 6.3.4, when the interplanar spacing increases, the diffraction peak of the InGaAs film shifts to the lower angle side, and the position of the oscillation in the diffraction intensity shifts accordingly. If the position of the diffraction peak of the thin film does not agree for the measurement and simulation, adjust the model using the composition ratio and lattice relaxation rate so that the interplanar spacing of the film changes.

Fig. 6.3.5 shows the changes in the rocking curve when the thickness of the $In_xGa_{(1-x)}As$ (x = 0.010) film increases from 200 nm to 210 nm.



(Dashed curve: 200 nm, solid curve: 210 nm)

Fig. 6.3.5 Rocking curve

Fig. 6.3.5 shows that when the film thickness increases, the period of the oscillation in the diffraction intensity decreases. If the period of the oscillation in the diffraction intensity of the thin film does not agree for the measurement and simulation, adjust the model by changing the film thickness.

2. Multilayer film
   Fig. 6.3.6 (a) shows the layer structure assumed, and Fig. 6.3.6 (b) shows the rocking curve for the (004) plane calculated with this model.

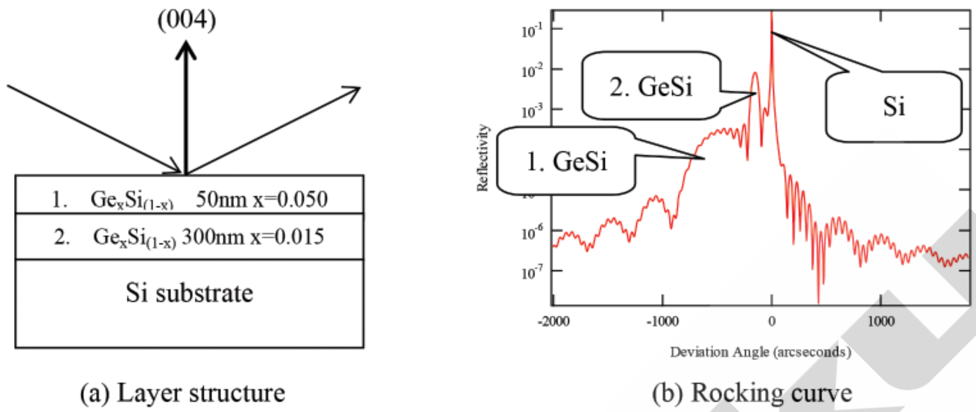


Fig. 6.3.6 Layer structure and rocking curve

As shown in Fig. 6.3.6, the diffraction peaks of Film 1 and Film 2 and the oscillation in the diffraction intensity appear superposed in the rocking curve. The wide diffraction peak appearing farther on the lower angle side of the diffraction peak of the substrate is considered attributable to Film 1 based on its characteristics of a larger Ge composition ratio (high difference in interplanar spacing compared to Si substrate) and lower film thickness. The oscillation in the diffraction intensity accompanying this diffraction peak appears at a larger period because the film is thinner. The diffraction peak relatively narrower and closer to the substrate peak is considered attributable to Film 2 based on its characteristics with a smaller Ge composition ratio (low difference in interplanar spacing compared to Si substrate) and greater film thickness. The oscillation in the diffraction intensity accompanying this diffraction peak appears at a smaller period because the film is thicker.

Since the X-rays in each layer are related by boundary conditions and are not independent, the rocking curve of a multilayer film is not a superposition of the rocking curves of the independent layers in the strictest sense. However, if we have a rough idea of the layer structure, the diffraction peaks and oscillating components of the diffraction intensity can be assigned to each layer as above.

3. Superlattice
   Fig. 6.3.7 (a) shows the superlattice structure assumed, while Fig. 6.3.7 (b) shows the rocking curve for the (004) plane calculated with this model.

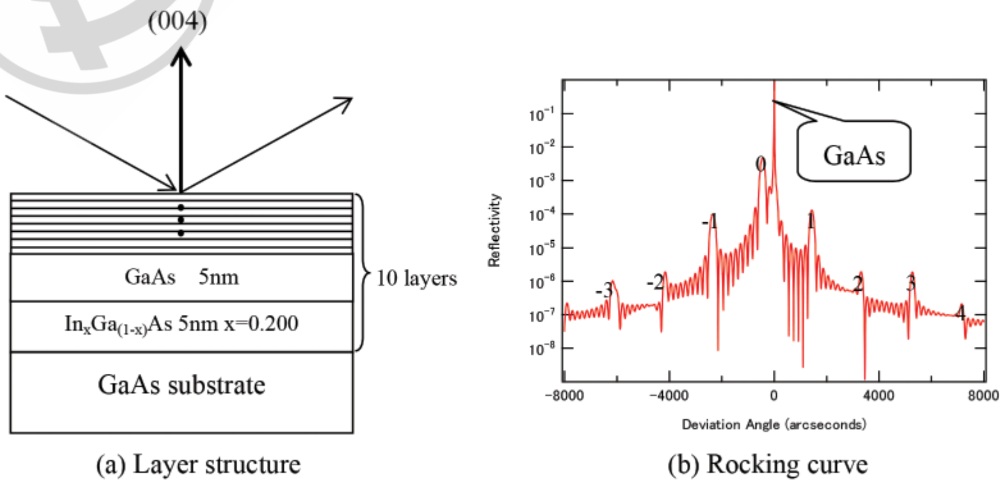


Fig. 6.3.7 Layer structure and rocking curve

6.3 Dynamical Theory of Diffraction in Multilayer Film Crystals

As shown in Fig. 6.3.7, the rocking curve of a superlattice has many diffraction peaks called **satellite peaks**. Of these satellite peaks, the peak appearing at the position corresponding to the average lattice constant of the two layers constituting the superlattice, GaAs and $In_{0.2}Ga_{0.8}As$, is called the zeroth order satellite peak. From the position of the zeroth order satellite peak, we can obtain the average lattice constant of the superlattice. For this example, we can use the lattice constant to obtain the composition ratio x. On both sides of the zeroth order satellite peak, the n-th order satellite peaks appear at the interval corresponding to the thickness of the entire superlattice film. This interval can be used to determine the thickness of the entire superlattice film. Generally speaking, the number of repetitions in a superlattice film is known from film growth conditions. In this case, we can obtain the thickness of a unit of the superlattice structure—the period of the superlattice.

If the positions of the diffraction peaks do not agree for the measurement and simulation, adjust the model by changing the average lattice constant for the position of the zeroth order satellite peak and by changing the superlattice period for the interval of the satellite peaks. Since the ratio of the thickness of the two layers constituting a unit of the superlattice structure influences the relative intensity ratio of the satellite peaks, adjusting the model to reproduce the entire rocking curve measured can provide detailed information on the superlattice.

6.4 Summary

This chapter discussed the dynamical theory of diffraction, which is applied to perfect crystals (e.g., Si, Ge, and GaAs). Summarized below are the important formulas described in this chapter.

1. Fundamental equation of dynamical theory of diffraction

$$\frac{k_g{}^2 - K^2}{K^2}\mathbf{E}_g = \sum_h \chi_{g-h}\mathbf{E}_h$$

2. Boundary conditions

$$E_{\mathrm{t}} = E_{\mathrm{t}}^{\mathrm{a}}, \quad D_{\mathrm{z}} = D_{\mathrm{z}}^{\mathrm{a}}$$

$$\sum_{k_{g\mathrm{t}}=K_{m\mathrm{t}}} E_g \exp(ik_{g\mathrm{z}}Z_{\mathrm{s}}) = \sum_{k_{g\mathrm{t}}=K_{m\mathrm{t}}} E_m^{\mathrm{a}} \exp(iK_{m\mathrm{z}}Z_{\mathrm{s}})$$

3. Wave field in crystal under two-wave approximation

$$\mathbf{E} = \mathbf{E}_o \exp(i\mathbf{k}_o \cdot \mathbf{r}) + \mathbf{E}_g \exp(i\mathbf{k}_g \cdot \mathbf{r})$$

4. Rocking curve
Bragg case, infinitely thick crystal, absorption disregarded

$$\frac{I_g^W}{I_o} = \left|\frac{E_g^{\mathrm{a}}}{E_o^{\mathrm{a}}}\right|^2 = \begin{cases} \left(|W| - \sqrt{W^2 - 1}\right)^2 & : |W| \ge 1 \\ 1 & : |W| < 1 \end{cases}$$

Bragg case, thin crystal, absorption disregarded

$$\frac{I_g^W}{I_o} = \left|\frac{E_g^{\mathrm{a}}}{E_o^{\mathrm{a}}}\right|^2 = \begin{cases} \dfrac{\sin^2\left(\pi T\sqrt{W^2-1}/\Lambda\right)}{W^2-1+\sin^2\left(\pi T\sqrt{W^2-1}/\Lambda\right)} & :|W|\geq 1 \\ \dfrac{\sinh^2\left(\pi T\sqrt{1-W^2}/\Lambda\right)}{1-W^2+\sinh^2\left(\pi T\sqrt{1-W^2}/\Lambda\right)} & :|W|<1 \end{cases}$$

Bragg case, infinitely thick crystal, absorption considered

$$\frac{I_g}{I_o} = L - \sqrt{L^2-1}$$

$$L = \frac{W^2+g^2+\sqrt{(W^2-g^2-1+\kappa^2)^2+4(gW-\kappa)^2}}{1+\kappa^2}, \quad g = \frac{\chi_o''}{|P||\chi_g'|}, \quad \kappa = \frac{\chi_g''}{\chi_g'}$$

5. Extinction distance

$$l_B = \frac{\Lambda\tan\theta_B}{2\pi} = \frac{\lambda\sin\theta_B}{2\pi|P||\chi_g|} = \frac{v_c\sin\theta_B}{2|P|r_e\lambda|F_g|} = \frac{v_c}{4|P|dr_e|F_g|}$$

6. Rocking curve of multilayer film (Darwin’s approach)

$$\begin{pmatrix} E_g^{N+1} \\ E_o^{N+1} \end{pmatrix} = \prod_{n=N}^{0}(\mathbf{M}_n)\begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$\frac{I_g}{I_o} = \left|\frac{E_g^{N+1}}{E_o^{N+1}}\right|^2$$

$$\begin{pmatrix} E_g^{n} \\ E_o^{n} \end{pmatrix} = \frac{1}{r_1^n - r_2^n}\begin{pmatrix} r_1^n e - r_2^n & r_1^n r_2^n(1-e) \\ e-1 & r_1^n - r_2^n e \end{pmatrix}\begin{pmatrix} e_{g2} & 0 \\ 0 & e_{o2} \end{pmatrix}\begin{pmatrix} E_g^{n-1} \\ E_o^{n-1} \end{pmatrix} = \mathbf{M}_n\begin{pmatrix} E_g^{n-1} \\ E_o^{n-1} \end{pmatrix}$$

$$\mathbf{M}_n \equiv \frac{1}{r_1^n - r_2^n}\begin{pmatrix} r_1^n e - r_2^n & r_1^n r_2^n(1-e) \\ e-1 & r_1^n - r_2^n e \end{pmatrix}\begin{pmatrix} e_{g2} & 0 \\ 0 & e_{o2} \end{pmatrix}$$