6.2 Basic Equation of Dynamical Theory of Diffraction

6.2.8 Extinction Distance

When X-rays enter a crystal and are diffracted, the intensity of the X-ray beam propagating in the incident direction decays as the X-ray beam propagates farther into the crystal. Here, the **extinction distance** is the quantity used as a guide to the degree of X-ray penetration depth into the crystal. The extinction distance l_B for the Bragg case is defined as the depth at which X-ray intensity declines to 1/e for W = 0, as expressed below:

$$l_{B} = \frac{\Lambda \tan \theta_{B}}{2\pi} = \frac{\lambda \sin \theta_{B}}{2\pi |P| |\chi_{g}|} = \frac{v_{c} \sin \theta_{B}}{2|P| r_{e} \lambda |F_{g}|} = \frac{v_{c}}{4|P| dr_{e} |F_{g}|}$$

Formula 6.2.68

The value is generally several micrometers to several dozen micrometers.

6.3 Dynamical Theory of Diffraction in Multilayer Film Crystals

In general, for a multilayer film sample of a heteroepitaxial crystal, the lattice constants differ in the substrate and in the film. In such cases, X-rays behave as if the lattice is strained at the interface between the substrate and the film and between the layers in the film. To understand dynamical diffraction phenomena in multilayer films and interpret measurement results, we must apply the dynamical theory of diffraction in a strained crystal. Numerous theories have been proposed depending on the type of strain in question. This chapter uses one of the theories, called Darwin's approach, to calculate the rocking curve, and discusses the relationship between this theory and evaluations of epitaxial crystals.

6.3.1 Dynamical Theory of Diffraction for Strained Crystal

Given below are examples of dynamical theories of diffraction for strained crystals.

1. Darwin's method

Darwin's method regards a multilayer film crystal as a combination of perfect crystals with different interplanar spacings, and the diffraction theory for a perfect crystal is repeated. It is applied to local defects and planar defects, including stacking faults, multilayer films, twin crystals, and grazing boundaries.

2. Eikonal theory

The eikonal theory is also called the beam theory. It describes the process whereby the X-rays propagate in the crystal while being bent. It is applied to gradual elastic strain over a wide region.

3. Takagi-Taupin theory

The Takagi-Taupin theory describes the propagation of the wave field in the strained crystal as a differential equation. It can be applied to both elastic strain and local strain.

Here, we describe 1 **Darwin's method**, which can be used to handle multilayer films and allows for relatively quick calculations. Note that all theories use approximation, although Theory 3 is considered more widely applicable, since it requires less rigorous conditions for valid approximations than Theory 1 or 2. Theory 2 cannot be applied to a crystal containing large local strains.

6.3.2 Rocking Curve of Multilayer Film

A multilayer film can be regarded as two or more thin crystals overlaid. For example, consider the sample shown in Fig. 6.3.1, in which the substrate is numbered n = 0 and each layer of the multilayer film over the substrate is numbered from n = 1 to n = N. When we take an arbitrary layer n = m, it can be regarded as a thin perfect crystal, to

which the dynamical theory of diffraction for a thin crystal as discussed in 2. of Section 6.2.6 applies. If we obtain the ratio E_{gJ}^{n}/E_{oJ}^{m} of the amplitude of the electric field of the wave (O wave) propagating in the transmission direction and the amplitude of the wave (G wave) propagating in the diffraction direction, we can use it as a recurrence formula and calculate the amplitude ratio from the substrate, n = 0, to the topmost layer, n = N. In this manner, we can obtain the amplitude ratio of the electric fields of the incident X-rays entering the surface and the diffracted X-rays exiting from the surface. By squaring the amplitude ratio, we obtain the intensity ratio of the incident and diffracted X-rays, or the rocking curve.



Fig. 6.3.1 X-rays in multilayer film

As indicated to the right of Fig. 6.3.1, E_{oj}^{m+1} is incident on the *m*-th layer in the incident direction from the (m + 1)-th layer nearer to the surface, while E_{gj}^{m} exits into the (m + 1)-th layer in a similar manner. Further, E_{gj}^{m-1} is incident on the *m*-th layer in the diffraction direction from the (m - 1)-th layer nearer to the substrate, and E_{oj}^{m} exits into the (m - 1)-th layer in a similar manner. Here, the waves E_{oj}^{m} and E_{gj}^{m} exist in the *m*-th layer and satisfy the boundary conditions at the interfaces on the surface and substrate sides. In the case of a multilayer film, boundary conditions must be satisfied at all interfaces between the layers as well as at the crystal surface.

The boundary conditions for a multilayer film are more complex than those for the substrate alone. However, we can simplify the boundary conditions by assuming that the wave vectors of the incident and diffracted X-rays are the same in all layers.

When we take z = 0 for the interface on the surface side of the *m*-th layer and $z = T_m$ for the interface on the substrate side of the *m*-th layer, the boundary conditions at each interface are given by the following formula:

$$z = 0:$$

$$E_{o}^{m+1} = E_{o1}^{m} + E_{o2}^{m}$$

$$Formula 6.3.1$$

$$z = T_{m}:$$

$$E_{o1}^{m} \exp(ik_{o1z}T_{m}) + E_{o2}^{m} \exp(ik_{o1z}T_{m}) = E_{o}^{m-1} \exp(ik_{oz}T_{m})$$

$$E_{o1}^{m} \exp(ik_{o1z}T_{m}) + E_{o2}^{m} \exp(ik_{o1z}T_{m}) = E_{o}^{m-1} \exp(ik_{oz}T_{m})$$
Formula 6.3.2

6.3 Dynamical Theory of Diffraction in Multilayer Film Crystals

Here, using the expressions below,

$$r_{j}^{n} = \frac{E_{gj}^{n}}{E_{oj}^{n}}$$
Formula 6.3.3
$$e = \exp(i(k_{o2z} - k_{o1z})T_{m})$$

$$e_{o2} = \exp(ik_{o2z}T_{m}), \quad e_{g2} = \exp(ik_{g2z}T_{m})$$
Formula 6.3.4

Formula 6.3.2 can be expressed in matrix form. We use a matrix to easily calculate the recurrence formula.

$$\begin{pmatrix} E_{g}^{n} \\ E_{o}^{n} \end{pmatrix} = \frac{1}{r_{1}^{n} - r_{2}^{n}} \begin{pmatrix} r_{1}^{n}e - r_{2}^{n} & r_{1}^{n}r_{2}^{n}(1-e) \\ e - 1 & r_{1}^{n} - r_{2}^{n}e \end{pmatrix} \begin{pmatrix} e_{g2} & 0 \\ 0 & e_{o2} \end{pmatrix} \begin{pmatrix} E_{g}^{n-1} \\ E_{o}^{n-1} \end{pmatrix} = \mathbf{M}_{n} \begin{pmatrix} E_{g}^{n-1} \\ E_{o}^{n-1} \end{pmatrix}$$

$$\mathbf{M}_{n} \equiv \frac{1}{r_{1}^{n} - r_{2}^{n}} \begin{pmatrix} r_{1}^{n}e - r_{2}^{n} & r_{1}^{n}r_{2}^{n}(1-e) \\ e - 1 & r_{1}^{n} - r_{2}^{n}e \end{pmatrix} \begin{pmatrix} e_{g2} & 0 \\ 0 & e_{o2} \end{pmatrix} \begin{pmatrix} e_{g2} & 0 \\ 0 & e_{o2} \end{pmatrix}$$
Formula 6.3.5

If we assume no X-rays enter the substrate from the rear surface ($E_{g^{-1}} = 0$ and $E_{o^{-1}} = 1$), we can apply Formula 6.3.5 from the substrate toward the surface layer one by one to obtain the amplitude ratio of the electric fields of the incident and diffracted X-rays and the corresponding intensity ratio: in short, the rocking curve.

$$\begin{pmatrix} E_{g}^{N+1} \\ E_{o}^{N+1} \end{pmatrix} = \prod_{n=N}^{0} (\mathbf{M}_{n}) \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$
Formula 6.3.6
$$\frac{I_{g}}{I_{o}} = \left| \frac{E_{g}^{N+1}}{E_{o}^{N+1}} \right|^{2}$$
Formula 6.3.7

The rocking curve expressed by Formula 6.3.7 changes in various ways depending on the layer structure. Fig. 6.3.2 shows the example of the rocking curve calculated for the (004) plane of the sample consisting of a GaAs (001) substrate and 200 nm of $In_{0.01}Ga_{0.99}As$ film. Here, we assume that the crystal axes of the substrate crystal and the thin film crystal are not tilted with respect to each other and that the lattice of the film is not relaxed.



Fig. 6.3.2 Rocking curve of GaAs/GaAs (004)

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.