X-RAY DIFFRACTION IN A FINITE CRYSTAL WITH LINEAR LATTICE-CONSTANT VARIATION

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Vol. 39, No. 6, pp. 64-67, 1984

UDC 548.732

The dynamic theory of X-ray diffraction is considered for a crystal of finite thickness with linear variation in the lattice period for the Bragg case. There is shown to be an analogy between X-ray diffraction in such a crystal and light diffraction at a slit in the Fresnel case.

The epitaxial semiconductor films used in microelectronics may have composition inhomogeneity dependent on the production conditions. In some cases, there is a one-dimensional linear variation in the solid-solution concentration over the thickness [1,2], which in accordance with Vegard's law leads to linear lattice-constant variation (LLCV). LLCV arises also in an elastically bent crystal as used in X-ray monochromators. The LLCV model can be used in examining light scattering in cholesteric liquid crystals with variable spiral steps [3]. X-Ray diffraction is used in nondestructive examination of LLCV.

Solutions have previously been obtained numerically [4] and analytically [5,6] for dynamic X-ray diffraction in a semiinfinite crystal with one-dimensional LLCV in the Bragg case. The kinematic theory of diffraction in thin crystals showing LLCV is to be found in [1,2].

Here we consider X-ray diffraction in a crystal wafer of any thickness l showing LLCV. This displacement pattern u(z) in the crystal has a period that varies linearly, and this is a quadratic function of the coordinate z, which is directed into the crystal:

$$gu = -\pi (z/l_1)^2 (1 - a\cos\varphi/z), \qquad (1)$$

where g is the diffraction vector, $l_1 = a(n\Delta a/a)^{-1/2}$, Δa is the lattice-parameter discrepancy, ϕ is the angle between the input surface of the crystal and the reflecting planes, a is the lattice constant for the undistorted crystal, and n is the reflection order.

Simple replacement of the Takagi equation system [7] on the basis of [1] leads to the equation for a parabolic cylinder, whose solutions for the amplitudes of the transmitted wave Φ_0 and the diffracted wave Φ_g take the form

$$\Phi_0 = [M_1 D_{-\nu}(x) + M_2 D_{-\nu}(-x)] \exp \delta_0,$$
$$\Phi_g = -if\nu^{1/2} [M_1 D_{-\nu-1}(x) - M_2 D_{-\nu-1}(-x)] \exp \delta_g, \qquad (2)$$

where $D_\nu(x)$ are wave functions and the subscript $\nu=-i(\pi/2)(l_1/\Lambda_{ext})^2$ defines the dynamic interaction of the X-rays in the crystal with the LLCV, while Λ_{ext} is the extinction length, $\delta_0=x^2/4-(i/2\pi)^{1/2}(x-x_0)(l_1/l_0)$, $\delta_g=\delta_0+i(\mathbf{gu})$; $f=(\chi_g/\chi_{-g})^{1/2}(\gamma_0/|\gamma_g|)^{1/2}$; $l_0=\gamma_0\lambda(2\pi\chi_0)^{-1}$; and the parameter $x=x_0+(2\pi i)^{1/2}z/l_1$, where $x_0=-(2\pi i)\,l_1/\Lambda_{ext})y$, has the meaning of the angular discrepancy (the angular coordinate y is defined by expression (8.76) in [7]); $\chi_{0,g,-g}$ are the Fourier components of the polarizability in the forward direction (0) and in the diffraction directions (g, -g), $\gamma_{0,g}$ are the direction cosines of the rays, and λ is the X-ray wavelength.

The coefficients M_1 and M_2 are found from the boundary conditions, which take the form $\Phi_0(z=0)=1$, $\Phi_g(z=l)=0$ for the finite crystal in the Bragg case. Then the amplitude reflection coefficient (ARC) is defined by

$$R^g=-if\nu^{1/2}\frac{D_{-\nu-1}(-x_1)D_{-\nu-1}(x_0)-D_{-\nu-1}(x_1)D_{-\nu-1}(-x_0)}{D_{-\nu-1}(-x_1)D_{-\nu}(x_0)+D_{-\nu-1}(x_1)D_{-\nu}(-x_0)}, \qquad (3)$$

where $x_1=x_0+(2\pi i)^{1/2}l/l_1$.

It follows from (3) for $l_1/\Lambda_{ext}\ll 1$ (dynamic interaction absent) that one has the ARC for a kinematic crystal showing LLCV [1,2], while for $l_1\gg\Lambda_{ext}$ (unperturbed dynamic interaction) one has the ARC for an ideal crystal of finite thickness [7]. For $l\to\infty$, (3) leads to the result of [5,6]. However, this transition to the limit of an ideal semiinfinite crystal ($\Delta a\to 0$) without absorption cannot be taken as correct, and also it does not lead to a single-valued expression for the ARC, because the boundary condition $\Phi_g(z=l)=0$, used in deriving (3) becomes meaningless for a semiinfinite crystal. This difficulty is overcome by specifying the boundary conditions only at the input surface: $\Phi_0(z=0)=1$, $|\Phi_g(z=0)|^2\leqslant 1$, and for $z\to\infty$ in the region of complete reflection, in (2) one should retain only the terms decreasing exponentially as z increases. Then we get the following expression for the ARC of a semiinfinite crystal showing LLCV:

$$R^g=\mp if\nu^{1/2}D_{-\nu-1}(\pm x_0)/D_{-\nu}(\pm x_0), \quad x_0\lesseqgtr 2i\nu^{1/2}. \qquad (4)$$

The signs in (4) are reversed for $x_0\lesseqgtr 2i\nu^{1/2}$, while in the solution obtained in [5, 6] and in that following from (3) ($l\to\infty$) they alter for $x_0\lesseqgtr 0$. Then (4) gives us an expression for the ARC single-valued with respect to y within the framework of the asymptotic expansion of the waver functions ($|\nu|\to\infty$) for an ideal semiinfinite crystal: $R^g=y\pm\sqrt{y^2-1}$, $y\lesseqgtr -1$.

One can interpret the one-sided oscillating profile for the diffraction curve DC for a crystal showing LLCV [4] in terms of the construction of [1,2], according to which the X-ray wave propagating in the crystal acquires an additional phase shift because of the presence of the lattice parameter discrepancy Δa. This enables one to split up the crystal into certain layers similar to Fresnel zones in optics, and l_1 has the meaning of the thickness of the first Fresnel layer. The deviation from the Bragg angle θ_0 corresponding to the first Fresnel layer transfer the diffraction reflection from one layer to another, while the interference of the X-rays from the other layers leads to oscillations on the DC. The peaks in the oscillations for a semiinfinite crystal correspond to the Bragg positions of the odd Fresnel layers, while the minima correspond to the even ones. From (4) we have that the angular position of maximum m is defined by the following in the kinematic approximation ($l_1\ll\Lambda_{ext}$):

$$\Delta\theta^m=(2m+1)^{1/2}a(2l_1 n\,\mathrm{ctg}\,\theta_0)^{-1}, \qquad (5)$$

which can also be derived by direct consideration of the Bragg condition for Fresnel layer 2m + 1.

According to (3), the oscillating DC profile from a finite crystal is substantially dependent on l. The period of the oscillations in that case is $\Delta\theta^k = [(2k+1)+(l/l_1)^2]a/(2ln \operatorname{ctg}\theta_0)$, $k=\pm 1, 2, 3 \ldots$. Therefore, for $\Delta a \to 0$, we get an expression for the secondary peaks for the thin ideal crystal, while (5) follows for $l=(2m+1)^{1/2}l_1$, $m \to \infty$.

The formula for the ARC for X-rays in a kinematically perfect crystal coincides with the expression for the amplitude of a light wave diffracted at a slit in the Fraunhofer case. The above interpretation of the DC by the construction of Fresnel zones enables one to extend the analogy to more complicated cases. In particular, it can be shown that kinematic diffraction in a crystal of finite thickness l showing LLCV is analogous to Fresnel diffraction at a slit. We established a correspondence between the angular distributions of the intensities for X-ray diffraction and the diffraction of light at a slit by the substitutions $b/L \to l/a$, $Y/r \to n \operatorname{ctg}\theta_0\Delta\theta$, $(r/L)^{1/2} \to l_1/a$, where b is slit width, L is light wavelength, r is the distance from slit to screen, and Y is the coordinate on the screen. Reducing the lattice-parameter discrepancy Δa ($\Delta a \to 0$) for X-ray diffraction is analogous to increasing r ($r \to \infty$), i.e., to transition from Fresnel diffraction to Fraunhofer diffraction. Kinematic X-ray diffraction in a semi-infinite crystal showing LLCV ($l_1 \ll \Lambda_{ext}$ in (4)) corresponds to the diffraction of light at a half-plane.

The above argument applies to nonabsorbing and absorbing crystals. In the latter case, the contributions from Fresnel layers lying far from the surface are small. Therefore, the oscillating DC profile falls rapidly in intensity as one deviates from θ_0.

The model for a crystal showing LLCV has been used to recover the structures of epitaxial films from X-ray diffraction data [8].

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