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Brief Communication

Rate of X-ray Beam Confinement in Absorbing Crystal

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In order to explain the X-ray beam confinement in a thin absorbing crystal and its emission from the edge observed in experiments, we study the rate of beam confinement on the base of a resonant dynamical theory of X-ray diffraction. The rate is related to the absorption factor, which shows that the confinement occurs for an absorbing crystal but not for a nonabsorbing crystal. The confinement can be maximized when the linear absorption coefficient is effectively diminished by the dynamical diffraction effect in the Bragg case. The optimum condition for the confinement is estimated as a function of crystal thickness as well as scattering factor. [DOI: 10.1143/JJAP.45.2830]

KEYWORDS: X-ray waveguide, X-ray amplifier, X-ray condenser, X-ray beam confinement, X-ray beam condensation, Borrmann effect

In recent years, X-ray diffraction with resonant scattering has been studied, and several characteristic phenomena have been reported. For example, Kato,[1)] and Fukamachi and Kawamura,[2)] have studied the dynamical diffraction caused by only the imaginary part of the anomalous scattering factor in the Bragg case and pointed out that the rocking curve becomes very sharp. Using a complex dispersion surface, Fukamachi *et al.*[3)] have investigated that the sharp rocking curve is caused by an ensemble scattering of all the resonant atoms in the crystal when the linear absorption coefficient μ is effectively diminished by the anomalous transmission due to the Borrmann effect. Fukamachi *et al.*[4,5)] have pointed out that some of the incident X-rays can be confined in a thin finite crystal just like a crystal waveguide when absorption is effectively diminished by the dynamical diffraction effect in the Bragg case. They have observed the emission of the confined beams from the side edge of a thin Ge crystal by using X-rays from synchrotron radiation. The schematic diagram of the incident, diffracted, transmitted and emitted beams for a crystal waveguide is shown in Fig. 1. The enhancement of the X-rays emitted from the side edge has also been observed by increasing the width of the incident X-rays along the direction from the incident point to the edge of the crystal. In this paper, we report on the rate of the confinement based on a resonant dynamical theory of diffraction (RDT) to clarify the condition of the confinement.

We denote the atomic scattering factor as $f = f^0 + f' + if''$ with f^0 being the normal scattering factor and $f' + if''$ the anomalous scattering factor. The $\boldsymbol{h}$-th Fourier component of X-ray polarizability χ_h is expressed as

$$\chi_h = \chi_{hr} + i\chi_{hi} = |\chi_{hr}|\exp(i\alpha_{hr}) + i|\chi_{hi}|\exp(i\alpha_{hi}), \quad (1a)$$

with

$$\chi_{hr} = -\frac{4\pi}{\omega^2 V}\sum_{j=1}^{n}(f_j^0 + f_j')\exp(i\boldsymbol{h}\cdot\boldsymbol{r}_j)\Theta_j \quad (1b)$$

and

$$\chi_{hi} = -\frac{4\pi}{\omega^2 V}\sum_{j=1}^{n} f_j''\exp(i\boldsymbol{h}\cdot\boldsymbol{r}_j)\Theta_j. \quad (1c)$$

Here, the atomic units ($\hbar = e = m = 1$) are used. α_{hr} and α_{hi} are the phases of χ_{hr} and χ_{hi}, respectively. ω is the X-ray energy, V the unit cell volume, $\boldsymbol{r}_j$ the position of the j-th atom in a unit cell, Θ_j the temperature correction factor for the j-th atom, and n the number of atoms in a unit cell. We define an absorption factor k as

$$k = |\chi_{hi}|/|\chi_{hr}|. \quad (2)$$

k is zero when $f^0 \neq 0$ and $f' = f'' = 0$ (in the case of only Thomson scattering), and $k = \infty$ when $f^0 + f' = 0$ ($\chi_{hr} = 0$) and $f'' \neq 0$. In the following, we will study the symmetric Bragg case for X-rays of σ-polarization, while ignoring the temperature correction ($\Theta_j = 1$). In addition, for a crystal having a center of symmetry, χ_{hr} and χ_{hi} are both real, and the relation $\chi_h = \chi_{-h}$ holds. Then χ_h is given by

$$\begin{aligned}\chi_h &= |\chi_{hr}|\exp(i\alpha_{hr})[1 + ik\exp(i\delta)] \\ &= |\chi_{hr}|(1 + k^2)^{1/2}\exp(i\alpha_{hr})\exp(\pm i\theta),\end{aligned} \quad (3)$$

where

$$\theta = \tan^{-1} k, \quad (4)$$

and

$$\delta = \alpha_{hi} - \alpha_{hr} = 0 \quad \text{or} \quad \pm\pi, \quad (5)$$

In eq. (3), the positive sign is taken if $\delta = 0$ and the negative sign is taken if $\delta = \pm\pi$.

When X-rays satisfying the condition $k = \infty$ are incident on an infinitely extended thin parallel crystal of thickness H at a Bragg condition, the reflection rate R and transmission rate T are given by

$$R = [sH/(1 + sH)]^2 \quad (6)$$

$$T = 1/(1 + sH)^2, \quad (7)$$

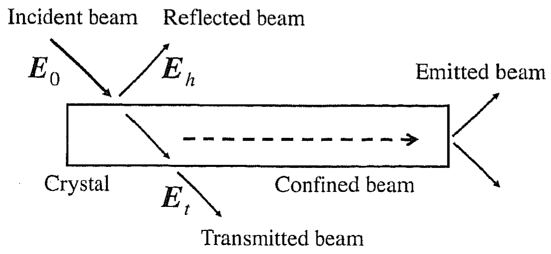

Fig. 1. Schematic diagram of diffraction geometry. The confined beam is indicated by the dashed arrow.

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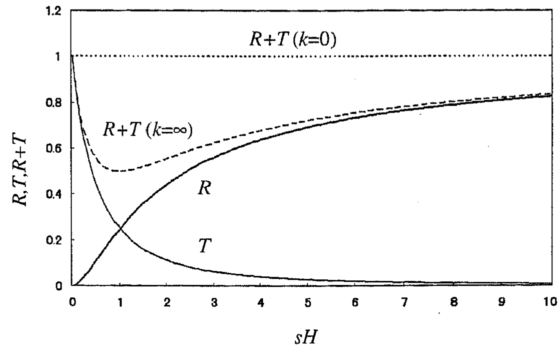

Fig. 2. Variations of R, T, and $R+T$ for $k=\infty$ (f'' only). The dotted line shows $R+T$ for $k=0$.

according to eqs. (3) and (4) of Negishi *et al.*[6] Here, s is given by

$$s = \kappa_{0r}(|\chi_{hr}|^2 + |\chi_{hi}|^2)^{1/2}/(2\sin\theta'_B), \qquad (8)$$

and κ_{0r} is the real part of the average wavenumber in the crystal and θ'_B the Bragg angle. In Fig. 2, variations of R, T, and $R+T$ are shown as functions of sH. When sH increases from 0, T decreases rapidly from 1, whereas R increases slowly from 0. $R+T$ decreases from 1 at $sH=0$ to 0.5 at $sH=1$, then it increases gradually up to 1 for $sH=\infty$. We define the rate η by

$$\eta = 1-(R+T) = 2sH/(1+sH)^2, \qquad (9)$$

which gives the amount of X-rays that do not come out of the crystal (referred as the rate of confinement). When $k=\infty$, η is not zero for $0<sH<\infty$. When $k=0$, on the other hand,

$$R = (sH)^2/[1+(sH)^2] \qquad (10)$$

and

$$T = 1/[1+(sH)^2] \qquad (11)$$

at the normalized Bragg angle (defined later) $W=\pm 1$. The relation $R+T=1$ always holds and the flux is conserved. Then $\eta=0$ and no beams are confined in a crystal.

In order to study the difference between these two cases, i.e., diffraction only by f'' ($k=\infty$) and that only by f^0 ($k=0$), the complex dispersion surfaces are shown in Fig. 3(a) for $k=0$, (b) for $k=\infty$ and (c) for $k=0.1$. The real part Y_{0r} is shown by the thick line and the imaginary part Y_{0i} by the dotted line. The abscissa is the distance W defined by

$$W = -2X\cos\theta'_B/[\kappa_{0r}(|\chi_{hr}|^2 + |\chi_{hi}|^2)^{1/2}]. \qquad (12)$$

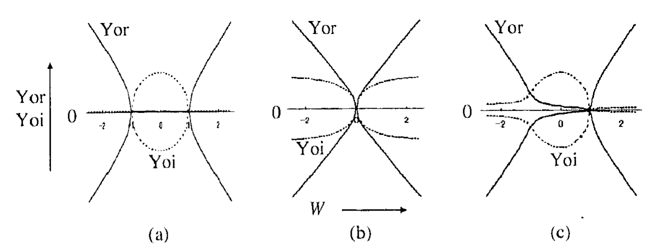

Fig. 3. Complex dispersion surfaces for (a) $k=0$, (b) $k=\infty$, and (c) $k=0.1$. Thick solid lines show the real part, and the dashed lines the imaginary part. The ordinate is Y_{0r} and Y_{0i}, and the abscissa is W.

The details of the dispersion surface and the related notations are given in ref. 3. For $k=\infty$, $Y_{0r}=Y_{0i}=0$ is satisfied at $W=0$, i.e., at an exact Bragg condition. As the absorption coefficient μ is proportional to Y_{0i}, $Y_{0i}=0$ means $\mu=0$. For $k=0$, on the other hand, $Y_{0r}=Y_{0i}=0$ is satisfied at $W=\pm 1$, and for $k=0.1$ at $W=0.995$. Among these three cases, the beam confinement is not expected for $k=0$, as shown above. For $k=0.1$, the beam confinement has been observed at $W=0.995$ in experiments.[4,5] $Y_{0r}=Y_{0i}=0$ is a necessary but not sufficient condition for the beam confinement. At the condition $Y_{0r}=Y_{0i}=0$, $W_{\mu=0}$ is given by

$$W_{\mu=0} = \pm 1/(1+k^2)^{1/2}. \qquad (13)$$

Here, $W_{\mu=0}\le 0$ if $\delta=0$ and $W_{\mu=0}\ge 0$ if $\delta=\pm\pi$.

According to RDT, the electric fields for the incident ($\boldsymbol{E}_0^\sigma$: σ polarization), transmitted ($\boldsymbol{E}_t$) and diffracted ($\boldsymbol{E}_h$) beams near the condition $Y_{0r}=Y_{0i}=0$ are given by

$$\boldsymbol{E}_t(\boldsymbol{r},t) = \boldsymbol{E}_0^\sigma \frac{1}{1+sH\exp(\pm i\varphi)} \exp[i(\omega t - \boldsymbol{k}\cdot\boldsymbol{r})] \qquad (14a)$$

and

$$\boldsymbol{E}_h(\boldsymbol{r},t) = \boldsymbol{E}_0^\sigma \frac{(\pm)sH\exp(\pm i\varphi)}{1+sH\exp(\pm i\varphi)} \exp[i(\omega t - \boldsymbol{k}\cdot\boldsymbol{r})]. \qquad (14b)$$

The phase factor φ is related to θ as

$$\varphi = \pi/2 - \theta. \qquad (15)$$

As for the double sign before $i\varphi$ in eqs. (14a) and (14b), the negative sign is taken if $\delta=0$ and the positive sign if $\delta=\pm\pi$. As for the double sign in the parentheses in eq. (14b), the positive sign is taken if $\alpha_{hi}=0$ and the negative sign is taken if $\alpha_{hi}=\pi$.

For any value of k, the reflection and transmission rates are given by

$$R = (sH)^2/[1+(sH)^2+2sH\sin\theta] \qquad (16)$$

and

$$T = 1/[1+(sH)^2+2sH\sin\theta]. \qquad (17)$$

The rate of confinement η becomes

$$\eta = 2sH\sin\theta/[1+(sH)^2+2sH\sin\theta]. \qquad (18)$$

For $k=0$, $\theta=0$, $\varphi=\pi/2$, and $\sin\theta=0$, no confinement occurs ($\eta=0$). If $k=\infty$, $\theta=\pi/2$, $\varphi=0$, and $\sin\theta=1$, then η is maximized. In Fig. 4, variations of η are shown as a

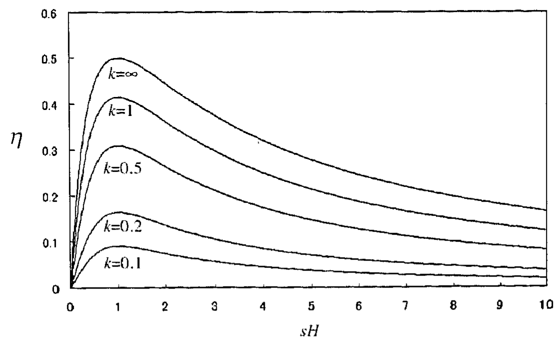

Fig. 4. Calculated curves of confinement rate as a function of sH for $k=0.1$, 0.2, 0.5, 1.0, and ∞.

function of sH for $k = 0.1$, 0.2, 0.5, 1.0, and ∞. We can see that η becomes large as k increases. For any k (except for $k = 0$), η becomes maximum at $sH = 1$, then decreases gradually as sH increases. We can expect the beam confinement for a thicker crystal ($sH > 1$) to a certain extent.

In summary, we have obtained the following results.

1) We have derived the diffraction condition for the beam confinement.
2) The rate of confinement is given in terms of $\sin\theta$ as given in eq. (18).
3) The rate of confinement is given in terms of absorption factor k [eqs. (2), (4), (15), and (18)].
4) The beam confinement can be observed for any absorbing crystal.
5) When sH is constant, the confinement becomes maximum for $k = \infty$. When k is constant, it becomes maximum for $sH = 1$.

In the previous work,[4,5] the confinement was observed for $k \approx 0.1$–0.2 and $sH \approx 20$. The rate of confinement is estimated to be approximately 1–2%. If k is increased and sH is decreased by thinning a crystal, a much higher rate is expected. It is noted that the present study can be applied to explain the interference fringes observed in the emitted beams from the side edge.[5] Because the beam confinement is observed when μ becomes minimum at room temperature, the analysis including the temperature factor should be needed. The beam confinement at a finite temperature and the electric flux in a crystal under the confinement are to be investigated in our future work.

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