# Application of general quantum scattering theory to 1-D Bragg-Fresnel optics 

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#### Abstract

A scheme based on general quantum scattering theory is presented in this paper to describe the performance of 1-D Bragg-Fresnel optics recently developed for X-ray optics. The theory and method are valid as long as the working wavelength is smaller than the characteristic parameter (i.e. half-width of center zone) of the Bragg-Fresnel optics and this allows us to evaluate the performance of Bragg-Fresnel optics. Some simple numerical application results are also shown. © 1998 Elsevier Science B.V.


## 1. Introduction

X-ray optics is making an impressive breakthrough towards higher resolution and efficiency. The two competitive approaches in these efforts are reflection and diffraction optics. Grazing incidence optics was the first focusing device used in X-ray imaging systems. In the late 1970s, multilayer mirrors for X-ray were greatly developed. Compared to grazing incidence optics, a multilayer coating permits reduction in mirror size because of the possibility of a larger incidence angle. However, X-ray multilayer mirrors meet difficulties at manufacturing curve multilayer mirrors and getting essential reflectivity for shorter wavelength range (closely water window or hard X-ray). Due to its high spatial and spectrum resolution, diffraction optics was also developed. Nowadays transmission zone plates are widely used as objectives or condensers in X-ray imaging microscopes, but they are not strong enough to withdraw high mechanical and heat load. In 1986, Aristov et al. [1] advanced a new optics in X-ray range, i.e. Bragg-Fresnel optics (BFO) that patterned some kinds of diffraction graphs in Bragg reflectors (crystals or multilayer mirrors). In principle, BFOs maintain the advantages
of zone plates which offer high spatial resolution and of multilayer mirrors which offer high mechanical and heat stability. High mechanical and heat stability becomes especially important with the advance of ultrabright synchrotron sources. In addition, BFOs can be used either for hard (crystals as Bragg reflectors) or soft (multilayers as Bragg reflectors) X-ray regions.

During the past 10 years, BFOs have been proposed, realized and successfully tested in hard and soft X-ray regions [1,2], and some research groups have also tried different theories and methods to describe BFO performance [3-5]. Until now, however, all the theoretical methods have been based on considering X-ray as a wave front. In this paper, we consider X-ray as a particle-flow and evaluate BFO performance by using general quantum scattering theory, which is much simpler [4], for calculating BFO performance such as scattering power density. The only restrictive condition for our method to be valid is that the wavelength of radiation $\lambda$ is smaller than the half-width of the center zone of the diffraction pattern. This condition is generally fulfilled in the X-ray region.

In general quantum scattering theory, it is important first to decide the scattering potential function which inter-
acts with the incident particle flow; thus the result of interaction is expressed by a scattering amplitude. According to the BFO structure which couples multilayer (in-depth structure) and diffraction pattern (lateral structure), we describe it by using a three-dimensional (3-D) potential function. Then, due to separability of the electric susceptibility of the materials, calculation of the scattering amplitude is carried out laterally and in-depth, respectively.

As a special application of the method, the BFO scattering amplitude with a 1-D focusing diffraction pattern is derived in detail. Scattering power density and diffraction efficiency are calculated in connection with the scattering amplitude. The method can be easily generalized to other different diffraction patterns, the process will probably be complicated if the diffraction pattern is more complicated.

## 2. Fundamental theory

Considering incident X-ray radiation as a particle-flow which is scattered by the scattering potential, in general quantum scattering theory we solve such problems by obtaining the solution of the following Schrödinger equation,
$\left(\nabla^{2}+k^{2}\right) \varphi(\boldsymbol{R})=\frac{2 \mu}{\hbar^{2}} V(\boldsymbol{R}) \varphi(\boldsymbol{R})$,
where $2 \mu / \hbar^{2}$ is a constant related to particle energy, it will be zero when the incident particle-flow is a photonflow. However, $k^{2}$ related to the system energy is a complex term, the imaginary component of which is related to the interaction (expressed as $V(\boldsymbol{r})$ between photons and medium (i.e. BFOs), by moving this component to the right-hand side of Eq. (1), we obtain an inhomogeneous differential equation similar to Eq. (1):

$$
\begin{equation*}
\left(\nabla^{2}+k^{2}\right) \varphi(\boldsymbol{R})=V(\boldsymbol{R}) \varphi(\boldsymbol{R}) \tag{2}
\end{equation*}
$$

Using the well-known derivation in general quantum scattering theory, we solve Eq. (2):

$$
\begin{align*}
\varphi(\boldsymbol{r})= & \exp (\mathrm{i} \boldsymbol{k} \cdot \boldsymbol{r}) \\
& -\frac{1}{4 \pi} \int \mathrm{~d} \boldsymbol{R} \frac{\exp (\mathrm{i} k|\boldsymbol{r}-\boldsymbol{R}|)}{|\boldsymbol{r}-\boldsymbol{R}|} V(\boldsymbol{R}) \varphi(\boldsymbol{R}) \tag{3}
\end{align*}
$$

Eq. (3) is a integral equation which is similar to the second kind Fredholm equation. Considering the interaction function (i.e. scattering potential) as a perturbation, we solve the equation term by term. First we define Green's function as
$G(E)[\varphi]=\int \mathrm{d} \boldsymbol{R} G(\boldsymbol{r}, \boldsymbol{R}, E) \varphi(\boldsymbol{R})$.

The solution of Eq. (3) can be expressed by a perturbation series:
$\varphi=\varphi_{0}(\boldsymbol{r})+\varphi_{1}(\boldsymbol{r}) V+\varphi_{2}(\boldsymbol{r}) V^{2}+\ldots$,
where
$\varphi_{0}(\boldsymbol{r})=\exp (\mathrm{i} \boldsymbol{k} \cdot \boldsymbol{r})$,
$\varphi_{n}(\boldsymbol{r})=\int G(\boldsymbol{r}, \boldsymbol{R}) \varphi_{n-1}(\boldsymbol{R}) \mathrm{d} \boldsymbol{R}$,
so the 1 st term of the solution should be:
$\varphi_{1}(\boldsymbol{r})=\int G(\boldsymbol{r}, \boldsymbol{R}) \varphi_{0}(\boldsymbol{R}) \mathrm{d} \boldsymbol{R}=G(E) \varphi_{0}(\boldsymbol{r})$,
$\varphi_{2}(\boldsymbol{r})=\int G(\boldsymbol{r}, \boldsymbol{R}) \varphi_{1}(\boldsymbol{R}) \mathrm{d} \boldsymbol{R}=G(E) G(E) \varphi_{0}(\boldsymbol{r})$.

Using the same reasoning, we finally get:

$$
\begin{align*}
\varphi(\boldsymbol{r})= & \varphi_{0}(\boldsymbol{r})+G(E) V \varphi_{0}(\boldsymbol{r})+G(E) V G(E) V \varphi_{0}(\boldsymbol{r}) \\
& +\ldots . \tag{10}
\end{align*}
$$

In this case, we define an operator $S(E)$ which is similar to the $S$ matrix in scattering theory, and a self-consistent equation follows:
$S(E)=V+V G(E) S(E)$.
Then Eq. (3) can be rewritten as

$$
\begin{align*}
\varphi(\boldsymbol{r})= & \exp (\mathrm{i} \boldsymbol{k} \cdot \boldsymbol{r})-\frac{1}{4 \pi} \int \mathrm{~d} \boldsymbol{R} \frac{\exp (\mathrm{i} k|\boldsymbol{r}-\boldsymbol{R}|)}{|\boldsymbol{r}-\boldsymbol{R}|} \\
& \times S(E) \exp (\mathrm{i} \boldsymbol{k} \cdot \boldsymbol{R}) \tag{12}
\end{align*}
$$

To continue, let us treat the term $\exp (\mathrm{i} k|\boldsymbol{r}-\boldsymbol{R}|) /|\boldsymbol{r}-\boldsymbol{R}|$ in Eq. (12). Due to $r>R$, we expand $|\boldsymbol{r}-\boldsymbol{R}|$ in terms of $R / r$ :
$|\boldsymbol{r}-\boldsymbol{R}|=r-\boldsymbol{R} \cdot \frac{\boldsymbol{r}}{r}+\frac{1}{2}\left[\frac{R^{2}}{r}-\frac{(\boldsymbol{R} \cdot \boldsymbol{r})^{2}}{r^{3}}\right]+\ldots$,
where $\boldsymbol{r}$ is regarded as the position vector corresponding to an observation point. Because we are interested in Fresnel diffraction, we thus restrict ourselves to the second order in $R$.

The expression $\exp (\mathrm{i} k|\boldsymbol{r}-\boldsymbol{R}|)$ is a function which changes fast along with $\boldsymbol{R}$. By substituting Eq. (13) in this expression, we obtain:

$$
\begin{align*}
\exp (\mathrm{i} k|\boldsymbol{r}-\boldsymbol{R}|)= & \exp (\mathrm{i} k r) \exp \left(\frac{\mathrm{i} k}{r}(\boldsymbol{R} \cdot \boldsymbol{r})\right) \\
& \times \exp \left[\mathrm{i} k\left(\frac{R^{2}}{2 r}-\frac{(\boldsymbol{R} \cdot \boldsymbol{r})^{2}}{2 r^{3}}\right)\right] \tag{14}
\end{align*}
$$

Then we introduce a new physical parameter $\boldsymbol{k}^{s}$,
$\boldsymbol{k}^{s}=(k / r) \boldsymbol{r}$
for the elasticity scattering, $\left|\boldsymbol{k}^{s}\right|=k$, and by using the calculation rules for vectors,
$\boldsymbol{a} \cdot \boldsymbol{b}=a b \cos (\vartheta), \quad|\boldsymbol{a} \times \boldsymbol{b}|=a b \sin (\vartheta)$,
$|\boldsymbol{a}|=a, \quad|\boldsymbol{b}|=b$,
where $\vartheta$ is the angle between vectors $\boldsymbol{a}$ and $\boldsymbol{b}$. Finally Eq. (14) is rewritten as
$\exp (\mathrm{i} k|\boldsymbol{r}-\boldsymbol{R}|)=\exp (\mathrm{i} k r) \exp \left(-\mathrm{i} \boldsymbol{k}^{s} \cdot \boldsymbol{R}\right) \exp \left(\frac{\mathrm{i} k^{\prime} R^{2}}{2 r}\right)$,
where
$k^{\prime}=\frac{1}{k R^{2}}\left(\left|\boldsymbol{k}^{s} \times \boldsymbol{R}\right|\right)^{2}$.
Because the denominator $|\boldsymbol{r}-\boldsymbol{R}|$ is a function which changes smoothly and slowly, we may use just $r$ instead of $|\boldsymbol{r}-\boldsymbol{R}|$; therefore we finally get:

$$
\begin{align*}
\varphi(\boldsymbol{r})= & \exp (\mathrm{i} \boldsymbol{k} \cdot \boldsymbol{r})-\frac{\exp (\mathrm{i} k r)}{4 \pi r} \int \mathrm{~d} \boldsymbol{R} \exp \left(-\mathrm{i} \boldsymbol{k}^{s} \cdot \boldsymbol{R}\right) \\
& \times \exp \left(\frac{\mathrm{i} k^{\prime} R^{2}}{2 r}\right) S(E) \exp (\mathrm{i} \boldsymbol{k} \cdot \boldsymbol{R}) . \tag{19}
\end{align*}
$$

By using the closure relation $\int \mathrm{d} \boldsymbol{R}|\boldsymbol{R}\rangle\langle\boldsymbol{R}|=1$ and Dirac bracket notation, we obtain
$\varphi(\boldsymbol{r})=\exp (\mathrm{i} \boldsymbol{k} \cdot \boldsymbol{r})-\frac{1}{4 \pi} \frac{\exp (\mathrm{i} k r)}{r}\left\langle\boldsymbol{k}^{s}\right| S^{\prime}(E)|\boldsymbol{k}\rangle$,
where
$S^{\prime}(E)=V^{\prime}+V G(E) V^{\prime}+V G(E) V G(E) V^{\prime}+\ldots$,
$V^{\prime}(\boldsymbol{R}, r)=\exp \left(\mathrm{i} k^{\prime}\left(R^{2} / 2 r\right)\right] V(\boldsymbol{R})$.
Physically the pertinent quantity in Eq. (20) is the scattering amplitude $f\left(\boldsymbol{k}^{s}, \boldsymbol{k}, r\right)$, which we can define by setting
$\varphi(\boldsymbol{r})=\exp (\mathrm{i} \boldsymbol{k} \cdot \boldsymbol{r})+\frac{\exp (\mathrm{i} k r)}{r} f\left(\boldsymbol{k}^{s}, \boldsymbol{k}, r\right)$,
so that we get the expression of the scattering amplitude
$f\left(\boldsymbol{k}^{s}, \boldsymbol{k}, r\right)=-\frac{1}{4 \pi}\left\langle\boldsymbol{k}^{s}\right| S^{\prime}(E)|\boldsymbol{k}\rangle$.
In order to obtain the solution of scattering amplitude conveniently, we express $f\left(\boldsymbol{k}^{s}, \boldsymbol{k}, r\right)$ as

$$
\begin{align*}
f\left(\boldsymbol{k}^{s}, \boldsymbol{k}, r\right) & =-\frac{1}{4 \pi} \sum_{j}^{\infty} f_{j}\left(\boldsymbol{k}^{s}, \boldsymbol{k}, r\right) \\
& =-\frac{1}{4 \pi} \sum_{j=1}^{\infty}\left\langle\boldsymbol{k}^{s}\right|[V G(E)]^{j-1} V^{\prime}|\boldsymbol{k}\rangle . \tag{25}
\end{align*}
$$

By inserting the closure relation $\int \mathrm{d} \boldsymbol{q}|\boldsymbol{q}\rangle\langle\boldsymbol{q}|=1$, and using the Fourier transform expression of Green's function,
$\tilde{G}(\boldsymbol{q})=-\frac{1}{(2 \pi)^{3}} \frac{1}{q^{2}-k^{2}}$,
we express $f_{j}\left(\boldsymbol{k}^{s}, \boldsymbol{k}, r\right)$ as

$$
\begin{align*}
f_{j}\left(\boldsymbol{k}^{s}, \boldsymbol{k}, r\right) & =\left\langle\boldsymbol{k}^{s}\right|[V G(E)]^{j-1} V^{\prime}|\boldsymbol{k}\rangle \\
& =-\frac{1}{(2 \pi)^{3}} \int \mathrm{~d} \boldsymbol{q} \frac{\tilde{V}\left(\boldsymbol{k}^{s}-\boldsymbol{q}\right)}{q^{2}-k^{2}} \tilde{f}_{j-1}(\boldsymbol{q}, \boldsymbol{k}, r) . \tag{27}
\end{align*}
$$

The tilde above the functions is used to express their Fourier transforms.

## 3. Special application to 1-D BFOs

The 3-D geometric scheme of 1-D focusing BraggFresnel optics is shown in Fig. 1. Due to separability of the electric susceptibility and the linear diffraction pattern, the complex dielectric constant does not change along the $y$ axis. We can assume that the spatial dependence of the electric susceptibility $\chi(x, z)$ of the medium satisfies the following condition,
$\chi(x, z)=\chi_{x}(x) \chi_{z}(z)$.
Then the scattering potential $V(\boldsymbol{R})$ can be written as
$V(\boldsymbol{R})=V_{x}(x) V_{z}(z)$.
For the 1-D focusing diffraction pattern we chose, its Fourier transform (i.e. the lateral component of the Fourier transform of the scattering potential) behaves as a distribution which is similar to a Dirac distribution. Thus we obtain the following Fourier transform of $V(\boldsymbol{R})$ :
$\tilde{V}(\boldsymbol{q})=2 \pi \alpha \delta\left(q_{x}\right) \tilde{V}_{z}\left(q_{z}\right)$,
where $\boldsymbol{q}=\left(q_{x}, q_{z}\right)$ and $\alpha$ is a constant.


Fig. 1. The 3-D geometric scheme of 1-D Bragg-Fresnel optics.

In order to calculate the scattering amplitude, we deduce each component of Eq. (25), in a first stage, according to Eqs. (22), (25) and (30). We get:

$$
\begin{align*}
\tilde{f}_{1}(\boldsymbol{q}, \boldsymbol{k}, r)= & -\frac{1}{4 \pi} \tilde{V}^{\prime}(\boldsymbol{q}-\boldsymbol{k}, r) \\
= & -\frac{1}{4 \pi}\left[\frac{\tilde{V}_{x}^{\prime}\left(q_{x}-k_{x}, r\right)}{2 \pi \alpha}\right] \\
& \times\left[2 \pi \alpha \tilde{V}_{z}^{\prime}\left(q_{z}-k_{z}, r\right)\right] \tag{31}
\end{align*}
$$

where we may replace $\tilde{V}_{z}^{\prime}\left(q_{z}-k_{z}, r\right)$ by $\tilde{V}\left(q_{z}-k_{z}\right)$, which is valid because the penetration depth of radiation is of the same order as the wavelength in our case. By using Eq. (27) and (30), we obtain
$\tilde{f}_{2}(\boldsymbol{q}, \boldsymbol{k}, r)=-\frac{1}{4 \pi} \frac{\tilde{V}_{x}^{\prime}\left(q_{x}^{s}-k_{x}, r\right)}{\alpha}$

$$
\begin{equation*}
\times \int \frac{\mathrm{d} q_{z}}{2 \pi} \frac{\alpha \tilde{V}_{z}\left(q_{z}^{s}-q_{z}\right)}{\left(q_{z}\right)^{2}-\left(q_{z}^{s}\right)^{2}} \alpha \tilde{V}_{z}\left(q_{z}-k_{z}\right) \tag{32}
\end{equation*}
$$

that is
$\tilde{f}_{2}(\boldsymbol{q}, \boldsymbol{k}, r)=-\frac{1}{4 \pi} \frac{\tilde{V}_{x}^{\prime}\left(q_{x}^{s}-k_{x}, r\right)}{\alpha} \tilde{f}_{2}^{z}\left(q_{z}, k_{z}\right)$,
where
$\tilde{f}_{z}^{z}\left(q_{z}, k_{z}\right)=\alpha^{2} \int \frac{\mathrm{~d} q_{z}}{2 \pi} \frac{\tilde{V}_{z}\left(q_{z}^{s}-q_{z}\right)}{\left(q_{z}\right)^{2}-\left(q_{z}^{s}\right)^{2}} \tilde{V}_{z}\left(q_{z}-k_{z}\right)$,
where $q_{x}^{s}$ and $q_{z}^{s}$ correspond, respectively, to the frequency representation of $k_{x}^{s}$ and $k_{z}^{s}$.

It is obviously that the integrator on the right-hand side of Eq. (34) is only related to the variable $z$, so it stands for an unpatterned multilayer structure and is expressed as $\tilde{f}_{2, \mathrm{UE}}^{z}\left(q_{z}, k_{z}\right)$.

Using the same reasoning and assumptions, we can get
$\tilde{f}_{j}^{z}\left(q_{z}, k_{z}\right)=\alpha^{j} \tilde{f}_{j, \mathrm{UE}}^{z}\left(q_{z}, k_{z}\right)$,
$\tilde{f_{j}}(\boldsymbol{q}, \boldsymbol{k}, r)=-\frac{1}{4 \pi} \frac{\tilde{V}_{x}^{\prime}\left(q_{x}^{s}-k_{x}, r\right)}{\alpha} \tilde{f}_{j}^{z}\left(q_{z}, k_{z}\right)$.
By performing the summation over $j$ and by factorizing the term corresponding to the lateral component, we can finally get:
$f\left(\boldsymbol{k}^{s}, \boldsymbol{k}, r\right)=-\frac{1}{4 \pi} \frac{\tilde{V}_{x}^{\prime}\left(q_{x}^{s}-k_{x}, r\right)}{\alpha} \tilde{f}_{\mathrm{eff}, \mathrm{UE}}^{z}\left(q_{z}^{s}, k_{z}\right)$,
where $\tilde{V}_{x}^{\prime}\left(q_{x}^{s}-k_{x}, r\right)$ is related to the Fourier transform of the lateral component of the scattering potential and
$\tilde{f}_{\mathrm{eff}, \mathrm{UE}}^{z}\left(q_{z}^{s}, k_{z}\right)=\sum_{j=1}^{+\infty} \alpha^{j} f_{j, \mathrm{UE}}^{z}\left(q_{z}, k_{z}\right)$
can be described by calculating the reflectivity of the multilayer.
3.1. Lateral component of scattering potential of $1-D$ BFOs and its Fourier transform

We have chosen a square-wave profile with straight edges unbounded in the $y$ direction, as shown in Fig. 1. In such a diffraction pattern, the multilayer structure forms strips along the $y$ axis. We can describe its lateral profile by the 'rect' function,
$I=\operatorname{rect}\left(\frac{x}{a \sqrt{2 j+1}}\right)-\operatorname{rect}\left(\frac{x}{a \sqrt{2 j}}\right)$,
where $a$ is the half-width of the center zone in the diffraction pattern, $j$ is a positive integer within the range $[0, N]$ ( $N$ is used to describe zone numbers). The 'rect' function is generally defined as follows:
$\operatorname{rect}\left(\frac{x}{b}\right)= \begin{cases}0 & |x| \geq b, \\ 1 & |x|<b .\end{cases}$
Then the lateral component of the scattering potential can be written as
$V_{x}(x)=\sum_{j=0}^{N}\left[\operatorname{rect}\left(\frac{x}{a \sqrt{2 j+1}}\right)-\operatorname{rect}\left(\frac{x}{a \sqrt{2 j}}\right)\right]$.
Now we calculate the Fourier transform of the scattering potential, Generally the Fourier transforms of scattering potential are described as follows:

$$
\begin{equation*}
\tilde{V}(\boldsymbol{q})=\int_{-\infty}^{+\infty} \mathrm{d} x \int_{-\infty}^{+\infty} \mathrm{d} z V(x, z) \exp \left(\mathrm{i}\left(q_{x} x+q_{z} z\right)\right), \tag{42}
\end{equation*}
$$

$$
\begin{align*}
\tilde{V}^{\prime}(\boldsymbol{q}, r)= & \int_{-\infty}^{+\infty} \mathrm{d} x \int_{-\infty}^{+\infty} \mathrm{d} z \exp \left(\mathrm{i} \frac{k^{\prime}\left(x^{2}+z^{2}\right)}{2 r}\right) V(x, z) \\
& \times \exp \left[\mathrm{i}\left(q_{x} x+q_{z} z\right)\right] \tag{43}
\end{align*}
$$

and the Fourier transforms of the scattering potential can be separated because scattering potential function can be separated.
$\tilde{V}(\boldsymbol{q})=\tilde{V}_{x}\left(q_{x}\right) \tilde{V}_{z}\left(q_{z}\right)$,
$\tilde{V}^{\prime}(\boldsymbol{q}, r)=\tilde{V}_{x}^{\prime}\left(q_{x}, r\right) \tilde{V}_{z}^{\prime}\left(q_{z}, r\right)$,
where

$$
\begin{align*}
\tilde{V}_{x}^{\prime}\left(q_{x}, r\right)= & \exp \left(-\mathrm{i} \frac{r}{2 k^{\prime}} q_{x}^{2}\right) \\
& \times \int_{-\infty}^{+\infty} \exp \left[\frac{\mathrm{i} k^{\prime}}{2 r}\left(x+\frac{r}{k^{\prime}} q_{x}\right)^{2}\right] V_{x}(x) \mathrm{d} x \tag{46}
\end{align*}
$$

By substituting Eq. (41) into Eq. (46) and using a Fresnel integrated formula (written as Fr):
$C_{f}=\int \cos \left(\frac{\pi}{2} t^{2}\right) \mathrm{d} t, \quad S_{f}=\int \sin \left(\frac{\pi}{2} t^{2}\right) \mathrm{d} t$,
we finally get:

$$
\begin{align*}
\tilde{V}_{x}^{\prime}\left(q_{x}, r\right)= & \sqrt{\frac{\pi r}{k^{\prime}}} \exp \left(-\mathrm{i} \frac{r}{2 k^{\prime}} q_{x}^{2}\right) \\
& \times \sum_{j}(-1)^{j+1}\left\{\operatorname{Fr}\left[\left(a \sqrt{j}+\frac{r q_{x}}{k^{\prime}}\right) \sqrt{\frac{k^{\prime}}{\pi r}}\right]\right. \\
& \left.+\operatorname{Fr}\left[\left(a \sqrt{j}-\frac{r q_{x}}{k^{\prime}}\right) \sqrt{\frac{k^{\prime}}{\pi r}}\right]\right\} \tag{48}
\end{align*}
$$

where the range of the summations is $[0,2 N+1]$. Because every zone in diffraction pattern has to be calculated, the calculation is very much time consuming with large zone numbers.

### 3.2. Reflectivity of unpatterned multilayer structure

There have been many methods to calculate the reflectivity of a multilayer structure; a review of the various methods was given by Pardo et al. [6]. Our research group has developed a method to calculate the performances of a multilayer, and we describe it here briefly.

When a plane wave with wavelength $\lambda$ acts on the multilayer mirror, the reflectivity of the multilayer mirror can be described by the Bernning formula:

$$
\begin{align*}
R_{j} & =\frac{r_{j}\left(1-r_{j} R_{j-1}\right)+\left(R_{j-1}-r_{j}\right) \exp \left(-\mathrm{i} \delta_{j}\right)}{1-r_{j} R_{j-1}+r_{j}\left(R_{j-1}-r_{j}\right) \exp \left(-\mathrm{i} \delta_{j}\right)} \\
j & =1,2, \ldots, m \tag{49}
\end{align*}
$$

with

$$
\begin{equation*}
\delta_{j}=\frac{4 \pi N_{j} d_{j} \cos \left(\varphi_{j}\right)}{\lambda}, \quad \sin \left(\varphi_{j}\right)=\frac{\sin (\vartheta)}{N_{j}} \tag{50}
\end{equation*}
$$

$N_{j}=n_{j}-i k_{j}$,
where $R_{j}, R_{j-1}$ are, respectively, the reflectivity of a multilayer structure with $j$ layers and with $j-1$ layers, $r_{j}$ is the Fresnel reflective factor of the material of the $j$ th layer. The successive iterations go from 1 to $j . \vartheta$ is the incoming angle, $N_{j}$ is the complex index of refraction, $d_{j}$ is the thickness of each layer.

Because $\left|r_{j}\right| \ll 1$ is valid for all materials in the X-ray region, we can simplify Eq. (49) to

$$
\begin{align*}
R_{j} & =r_{j}+\left(R_{j-1}-r_{j}\right) \exp \left(-\mathrm{i} \delta_{j}\right) \\
& =r_{j}+D_{j}\left(R_{j-1}-r_{j}\right) \exp \left(-\mathrm{i} \beta_{j}\right) \tag{51}
\end{align*}
$$

where
$D_{j}=\exp \left(-4 \pi b_{j} d_{j} / \lambda\right), \quad \beta_{j}=4 \pi a_{j} d_{j} / \lambda$,
$N_{j} \cos \left(\varphi_{j}\right)=a_{j}-\mathrm{i} b_{j}$.
According to the theory above, we developed a set of numerical programs to calculate the reflectivity of a multilayer mirror and optimum thickness of each layer, etc. This method has been described in more detail in Ref. [7].

### 3.3. Diffraction efficiency and scattered power density of 1-D BFOs

After obtaining the scattering amplitude results, we will calculate the diffraction efficiency and scattered power density of BFOs in connection with the scattering amplitude $f\left(\boldsymbol{k}^{s}, \boldsymbol{k}, r\right)$. The calculation is more complicated than for mirrors, diffraction gratings and other optical systems involving Fraunhofer diffraction. When we deal with a quantum scattering problem, we consider the angular dispersion and different qualities of the scattering particles but not the energy eigenvalue. Because the position of the observation point $r \gg \lambda$ (the wavelength of the radiation particles), the angular dispersion function depends on the performance of the wave function at $r \rightarrow \infty$ and is related to the energy of the radiation particles and the interaction between radiation particles and scattering potential. From Eq. (23), we know that the scattering wave function is described by
$\varphi(\boldsymbol{r})=\exp (\mathrm{i} \boldsymbol{k} \cdot \boldsymbol{r})+\frac{1}{r} f\left(\boldsymbol{k}^{s}, \boldsymbol{k}, r\right) \exp (\mathrm{i} k r)$,
where the first term refers to the incident wave and the second term to the outgoing scattering spherical wave. If the incident particle flow density is defined as $J_{i}$, then the outgoing particle flow density $J_{s}$ is:
$J_{s}=J_{i}\left|f\left(\boldsymbol{k}^{s}, \boldsymbol{k}, r\right)\right|^{2} / r^{2}$.
Thus, the scattered power density can be described as follows:
$\frac{\mathrm{d} W\left(\boldsymbol{k}^{s}, \boldsymbol{k}, r\right)}{\mathrm{d} s}=C\left|f\left(\boldsymbol{k}^{s}, \boldsymbol{k}, r\right)\right|^{2} / r^{2}$,
where $C$ is a constant. For a perfect diffraction pattern, we consider $\alpha=1 / 2$. Then we get
$f\left(\boldsymbol{k}^{s}, \boldsymbol{k}, r\right)=-\frac{1}{2 \pi} \tilde{V}_{x}^{\prime}\left(q_{x}^{s}-k_{x}, r\right) \tilde{f}_{\text {eff, UE }}^{z}\left(q_{z}^{s}, k_{z}\right)$.

According to Eq. (30), for the real foci at the specular direction case, the power density can be described by
$\frac{\mathrm{d} W\left(\boldsymbol{k}^{s}, \boldsymbol{k}, r\right)}{\mathrm{d} s}=C^{\prime}\left|B_{j}\right|^{2}\left|\tilde{f}_{\text {eff, UE }}^{z}\left(q_{z}^{s}, k_{z}\right)\right|^{2} \delta\left(k_{x}^{s}, k_{x}\right)$,
where $B_{j}$ is a factor which can be obtained by Eq. (48). By analogy with the diffraction theory of gratings, we can describe the notion of efficiency $\eta_{j}$ of a focus $j$ for a perfect diffraction pattern as follows:
$\eta_{j}=C^{\prime}\left|B_{j}\right|^{2} \frac{\left|f_{\mathrm{eff}, \mathrm{UE}}^{z}\left(-k_{z}, k_{z}\right)\right|^{2}}{(2 \pi)^{2}}$.
According to

$$
\begin{equation*}
\sum_{m=-\infty}^{+\infty} \frac{1}{(2 m+1)^{2}}=\frac{\pi^{2}}{4} \tag{59}
\end{equation*}
$$

we finally obtain the total efficiency for all the foci:
$\eta=\left|f_{\text {eff,UE }}^{z}\left(-k_{z}, k_{z}\right)\right|^{2}$.

## 4. Numerical application results

The parameters of the 1-D BFO that we designed are as follows. The multilayer structure consists of 40 molybdenum/silicon layers at 18 nm wavelength. The molybdenum ( Mo ) layers are 3.04 nm thick and the silicon $(\mathrm{Si})$ layers are 6.36 nm thick. The diffraction pattern consists of 99 zones; the half-width of the center zone is $60.45 \mu \mathrm{~m}$ and the outermost zone is $3.045 \mu \mathrm{~m}$.

In Fig. 2, we show the curves of efficiency at the first focus, second focus and all the foci of 1-D BFO versus the incoming angle. For sake of comparison, we also present


Fig. 2. (a) Multilayer structure reflectivity versus the incoming angle. BFO efficiency versus the incoming angle for: (b) All foci: (c) 1st focus; (d) 2 nd focus at wavelength of 18 nm . The multilayer structure consists of $40 \mathrm{Mo}(3.04 \mathrm{~nm}) / \mathrm{Si}(6.36 \mathrm{~nm})$ layers.


Fig. 3. Curve 1: efficiency of BFO versus the number of layers of the multilayer structure. Curve 2 : reflectivity versus the number of layers of the multilayer structure; the multilayer structure consists of $40 \mathrm{Mo}(3.04 \mathrm{~nm}) / \mathrm{Si}(6.36 \mathrm{~nm})$ layers.


Fig. 4. Power density of the light diffracted in the specular direction versus the distance of observation.
the theoretical reflectivity of the corresponding multilayer structure. Fig. 3 gives the reflectivity of the multilayer structure together with the efficiency of the 1-D BFO versus the number of layers. Fig. 4 gives the power density of the light diffracted in the specular direction versus the distance of observation.

## 5. Conclusion

The quantum model that we have presented in this paper is valid under the condition $(\lambda / a)^{2} \ll 1$, and a completely mathematical process and some essentially numerical applications would confirm this assertion. An example of the simplest diffraction pattern, i.e. 1-D diffraction pattern, is described in detail. The method can be easily generalized to other different diffraction patterns (circular or elliptical, etc.), but the mathematical process will probably be complicated.

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