Multifocus off-axis zone plates for x-ray free-electron laser experiments: supplement

FLORIAN DÖRING,* BENEDIKT RÖSNER, MANUEL LANGER, ADAM KUBEC, ARMIN KLEIBERT, JÖRG RAABE, CARLOS A. F. VAZ, MAXIME LEBUGLE, AND CHRISTIAN DAVID

Paul Scherrer Institut, Villigen-PSI 5232, Switzerland
*Corresponding author: florian.doering@psi.ch

This supplement published with The Optical Society on 14 August 2020 by The Authors under the terms of the Creative Commons Attribution 4.0 License in the format provided by the authors and unedited. Further distribution of this work must maintain attribution to the author(s) and the published article’s title, journal citation, and DOI.

Supplement DOI: https://doi.org/10.6084/m9.figshare.12657542

Parent Article DOI: https://doi.org/10.1364/OPTICA.398022
Supplementary Information on: Multi-focus off-axis zone plates for X-ray free-electron laser experiments

FLORIAN DÖRING*, BENEDIKT RÖSNER*, MANUEL LANGER, ADAM KUBEC, ARMIN KLEIBERT, JÖRG RAABE, CARLOS A. F. VAZ, MAXIME LEBUGLE, CHRISTIAN DAVID

Paul Scherrer Institut, Villigen-PSI 5232, Switzerland
*florian.doering@psi.ch, benedikt.rosner@psi.ch (theoretical part)

1. Theory

In accordance to J. Kirz, J. Opt. Soc. Am. 64, 3 (1974) [20], the diffraction efficiency of a one-dimensional binary grating can be calculated by integrating the wave functions that propagate through it in the Fourier space. The wave function is thereby expressed as $e^{i\Theta}$, and it is modified in accordance to the refractive index in the non-transparent, i.e., phase-shifting and absorbing part of the grating: $e^{i(\Theta-\delta kt+\beta kt)} = e^{i\Theta-\delta^{2}kt-\beta^{2}kt} = e^{i\Theta} \cdot e^{-\delta^{2}kt} \cdot e^{-\beta^{2}kt}$.

$$A_1 = \int_0^{d/m2\pi} e^{i\Theta} d\Theta = \int_0^{d/m2\pi} e^{i(m2\pi)\Theta} d\Theta = \frac{1}{im2\pi} \left[ e^{i(m2\pi)\Theta} \right]_0^d = \frac{1}{im2\pi} \left( e^{i(m2\pi)d} - 1 \right)$$

$$A_2 = \int_0^{d/m2\pi} e^{i\Theta} \cdot e^{-\delta^{2}kt} \cdot e^{-\beta^{2}kt} d\Theta = e^{-\delta^{2}kt} \cdot e^{-\beta^{2}kt} \int_0^{d/m2\pi} e^{i(m2\pi)\Theta} d\Theta$$

$$= \frac{e^{-\delta^{2}kt} \cdot e^{-\beta^{2}kt}}{im2\pi} \left[ e^{i(m2\pi)\Theta} \right]_0^d = e^{-\delta^{2}kt} \cdot e^{-\beta^{2}kt} \left( 1 - e^{i(m2\pi)d} \right) \frac{1}{im2\pi}$$

Fig. S 1. Unit cell of a binary grating in the Fourier space.

Figure S 1 shows the unit cell of a binary grating in Fourier space. Its length is $m \cdot 2\pi$, and it is divided into a transparent and a non-transparent part, whereas the border corresponds to the duty cycle of the grating.

1.1 Diffraction efficiencies for all non-zeroth diffraction orders

If we integrate the wave function over the size of the unit cell, we obtain the following coefficients:

$$A_1 = \int_0^{d/m2\pi} e^{i\Theta} d\Theta = \int_0^{d/m2\pi} e^{i(m2\pi)\Theta} d\Theta = \frac{1}{im2\pi} \left[ e^{i(m2\pi)\Theta} \right]_0^d = \frac{1}{im2\pi} \left( e^{i(m2\pi)d} - 1 \right)$$

$$A_2 = \int_0^{d/m2\pi} e^{i\Theta} \cdot e^{-\delta^{2}kt} \cdot e^{-\beta^{2}kt} d\Theta = e^{-\delta^{2}kt} \cdot e^{-\beta^{2}kt} \int_0^{d/m2\pi} e^{i(m2\pi)\Theta} d\Theta$$

$$= \frac{e^{-\delta^{2}kt} \cdot e^{-\beta^{2}kt}}{im2\pi} \left[ e^{i(m2\pi)\Theta} \right]_0^d = e^{-\delta^{2}kt} \cdot e^{-\beta^{2}kt} \left( 1 - e^{i(m2\pi)d} \right) \frac{1}{im2\pi}$$
For convenience, we will express $e^{-i\beta kt}$ as $e^{-i\phi}$, and $e^{-\beta kt}$ as $e^{-b}$ in the following.

The intensity of a non-zero diffraction order $m \neq 0$ is then:

$$A_m(d, k, \delta, \beta) = (A_1 + A_2)(A_1 + A_2)$$

$$= \left( \frac{1}{4\pi} \right)^2 \left\{ \left( \frac{e^{-i(m2\pi)d}}{i} - e^{i\phi}e^{-b} \left( \frac{(1 - e^{-i(m2\pi)d})}{i} \right) \right) \left( \frac{e^{i(m2\pi)d}}{i} - \right. \right.$$  

$$+ e^{-i\phi}e^{-b} \left( \frac{1 - e^{i(m2\pi)d}}{i} \right) \right\}$$

$$= \left( \frac{1}{4\pi} \right)^2 \left[ (e^{-i(m2\pi)d} - 1) - e^{i\phi}e^{-b}(e^{-i(m2\pi)d} - 1)] \right] \left[ (e^{i(m2\pi)d} - 1) - e^{-i\phi}e^{-b}(e^{i(m2\pi)d} - 1) \right]$$

$$= \left( \frac{1}{4\pi} \right)^2 \left( 1 - e^{-i(m2\pi)d} - e^{i(m2\pi)d} + 1) \right] \left[ 1 - e^{-b}(e^{-i\phi} + e^{i\phi}) + e^{-2b} \right]$$

$$= \left( \frac{1}{4\pi} \right)^2 \left( 2 - 2 \cos(m2\pi d)) \right] \left[ 1 - e^{-b} \cos(\phi) + e^{-2b} \right]$$

$$= \frac{\sin(m\pi d)}{m\pi} \left[ 1 + e^{-\beta kt} - 2e^{-\beta kt} \cos(\delta kt) \right]$$

The following relations were used:

$$e^{i\phi} \cdot e^{-i\phi} = 1.$$  

$$e^{ix} + e^{-ix} = 2 \cos(x) \text{ with } e^\pm ix = \cos(x) \pm i \sin(x), \text{ and } \cos(2x) = 1 - 2\sin^2(x).$$

The first term of this expression is material independent, and thus only corresponds to the pattern of the grating, i.e., it is the form factor. The second term depends on the material, its height, and the photon energy. It is the structure factor, and will be part of all other equations as well.

1.2 Diffraction efficiency for the zeroth diffraction order

For $m = 0$, the integrals of the kind $\int_{x_1}^{x_2} e^{im2\pi \theta} d\theta$ simplify to $\int_{x_1}^{x_2} \theta = (x_2 - x_1)$. Consequently, the terms $A_1$ and $A_2$ simplify to:

$$A_1 = d,$$

$$A_2 = e^{-i\phi}e^{-b}(1 - d).$$

$$A_0(d, k, \delta, \beta) = (A_1 + A_2)(A_1 + A_2)$$

$$= \left[ d + e^{i\phi}e^{-b}(1 - d) \right] \left[ d + e^{-i\phi}e^{-b}(1 - d) \right]$$

$$= d^2 + d(1 - d)e^{-i\phi}e^{-b} + d(1 - d)e^{-i\phi}e^{-b} + e^{-2b}d(1 - d)^2$$

$$= d^2 + 2d(1 - d)e^{-b}\cos(\phi) + (1 - d)^2e^{-2b}$$

2. Theory of a two-dimensional grating

2.1 The general case non-zeroth diffraction orders in a two-dimensional grating with variable duty cycles $d_1, d_2$

The efficiency of the diffraction orders of a two-dimensional grating can be calculated in a similar way by integration of its unit cell in the Fourier space. Figure S2a shows the unit cell...
of a two-dimensional, rectangular grating with an orthogonal basis. We see that the unit cell divides into four regions. The coefficients for a particular diffraction order \(A_{m,n}\) contain then the product of the complex conjugated sum and the sum \(A_1 + A_2 + A_3 + A_4\). If we assume that the unit cell of the grating is fully orthogonal, the integrals in both directions can be separated in the following way:

\[
A_1 = \int_0^{d_1} e^{i(m2\pi)\theta} d\theta \int_0^{d_2} e^{i(n2\pi)\theta} d\theta = -\frac{1}{m\pi} \int_0^{d_1} e^{i(m2\pi)\theta} d\theta \int_0^{d_2} e^{i(n2\pi)\theta} d\theta
\]

\[
= -\frac{1}{m\pi} \left(e^{i(m2\pi)d_1} - 1\right) \left(e^{i(n2\pi)d_2} - 1\right)
\]

If this is performed for all four regions, we see immediately that the terms of the kind \(e^{i(m2\pi)d_1} - 1\) and their complex conjugated can be factorized as in the one-dimensional case, leaving the same structure factor, and a form factor that is simply supplemented by \(\left(e^{-i(n2\pi)d_2} - 1\right) \cdot \left(e^{i(n2\pi)d_2} - 1\right) = 4\sin^2(n\pi d_2)\):

\[
A_{m,n} = \left[\frac{\sin(m\pi d_1)\sin(n\pi d_2)}{m\pi n\pi}\right]^2 \left[1 + e^{-2\phi k t} - 2e^{-\phi k t \cos(\delta k t)}\right]
\]

![Fig. S 2. a) Unit cell of a two-dimensional, rectangular grating with an orthogonal basis. b) Specific case for \(m = 1\), \(d_1 = 0.3\), and a shift \(s\) of the second row by a fraction of \(\frac{d}{\lambda}\).](image)

### 2.2 The specific case for a focusing off-axis zone plate with variable duty cycles \(d_2\) and shifted zones

For the application of an off-axis zone plate, we can concentrate on the first, focusing diffraction order of the zone plate functionality, and fix the parameters \(m = 1\) and \(d_1 = 0.5\) (see Figure 2b). In addition, we introduce the shift of one row of the zones for the terms \(A_2\) and \(A_4\), leading to a change in the limits of the Fourier integrals.

For this purpose, we can utilize the periodicity of the Fourier space: we will have a look at the integral \(\int_{s+0.5}^{s+1} e^{i2\pi\theta} d\theta\):

\[
\int_{s+0.5}^{s+1} e^{i2\pi\theta} d\theta = \frac{1}{i2\pi} \left(e^{i2\pi(s+1)} - e^{i2\pi(s+0.5)}\right) = \frac{1}{i2\pi} \left(e^{i2\pi s}e^{-i2\pi} - e^{i2\pi s}e^{-i\pi}\right) = e^{i2\pi s} \frac{e^{-i\pi}}{i\pi},
\]

in comparison to the sum of the parts within an interval between 0 and 1 (see the shaded parts in Figure S2b):

\[
\int_{s+0.5}^{s+1} e^{i2\pi\theta} d\theta + \int_0^{s} e^{i2\pi\theta} d\theta = \frac{1}{i2\pi} \left[\left(e^{i2\pi} - e^{i2\pi(s+0.5)}\right) + \left(e^{i2\pi s} - e^{i2\pi s} e^{0}\right)\right]
\]

This means that we can compose the Fourier space of the following four terms:

\[
A_1 = \int_0^{0.5} e^{i(2\pi)\theta} d\theta \int_0^{d_2} e^{i(n2\pi)\theta} d\theta = \frac{1}{n4\pi^2} \left[ e^{i(2\pi)\theta} \right]_{0}^{s+0.5} \left[ e^{i(n2\pi)\theta} \right]_{d_2}^{1} = \frac{e^{i\pi}}{2\pi^2} \left( 1 - e^{i(n2\pi)d_2} \right)
\]

\[
A_2 = \int_s^{0.5} e^{i(2\pi)\theta} d\theta \int_0^{1} e^{i(n2\pi)\theta} d\theta = -\frac{1}{n4\pi^2} \left[ e^{i(2\pi)\theta} \right]_{s}^{s+0.5} \left[ e^{i(n2\pi)\theta} \right]_{d_2}^{1} = \frac{e^{i\pi}}{2\pi^2} \left( 1 - e^{i(n2\pi)d_2} \right)
\]

\[
A_3 = e^{-i\phi} e^{-b} \int_0^{1} e^{i(2\pi)\theta} d\theta \int_0^{d_2} e^{i(n2\pi)\theta} d\theta = \frac{e^{-i\phi} e^{-b}}{n4\pi^2} \left[ e^{i(2\pi)\theta} \right]_{0}^{s+0.5} \left[ e^{i(n2\pi)\theta} \right]_{d_2}^{1} = \frac{e^{-i\phi} e^{-b}}{2\pi^2} \left( 1 - e^{i(n2\pi)d_2} \right)
\]

\[
A_4 = e^{-i\phi} e^{-b} \int_s^{0.5} e^{i(2\pi)\theta} d\theta \int_0^{1} e^{i(n2\pi)\theta} d\theta = \frac{e^{-i\phi} e^{-b}}{n4\pi^2} \left[ e^{i(2\pi)\theta} \right]_{s}^{s+0.5} \left[ e^{i(n2\pi)\theta} \right]_{d_2}^{1} = \frac{e^{-i\phi} e^{-b}}{2\pi^2} \left( 1 - e^{i(n2\pi)d_2} \right)
\]

In essence, the form factor just contains an additional term for the shift: \(\sin(\pi s)\), whereas \(\sin(n\pi d_2)\) and \(m^2\) become unity.

For the case of \(n = 0\), the integral \(\int_0^{d_2} e^{i(n2\pi)\theta} d\theta\) simplifies to \(d_2\), and \(\int_0^{1} e^{i(n2\pi)\theta} d\theta\) to \(1 - d_2\).

Calculating the product of the different regions, we can derive the same structure factor, whereas the form factors differs for the pattern inversion and the pattern shift approaches. For the pattern inversion case, we obtain:

\[
A_{1,0} = \left[ \frac{2d_2 - 1}{\pi} \right]^2 \cdot \left[ 1 + e^{-2\beta k t} - 2e^{-\beta k t} \cos(\delta k t) \right]
\]
For the case of *pattern shift*, we obtain:

\[ A_{1,0} = \left( \frac{\cos(s\pi)}{\pi} \right)^2 \cdot [1 + e^{-2\beta kt} - 2e^{-\beta kt} \cos(\delta kt)] \]