1 June 2011

Wavefront propagation: diffraction from perfect crystals in the Bragg case.

References: "Multiple Diffraction of X-rays and the Phase Problem. Computational Procedures and Comparison with Experiment", R. Colella, Acta Cryst. A30, 413-423(1974).

Pseudocode: written in English, but (hopefully!) in a way that is simple enough for a programmer to convert into C code.

"User's Notes" provide extra information and need not be coded.

The procedure is as follows: All variables are real unless indicated otherwise. Complex variables are indicated with superscript C.

A.) Set the following constants for later use:

1.) $a_{Si} = 5.43102088$ = lattice constant of Si at 22.5°C in Å
2.) $\pi = 3.141592654...$
3.) Values $\Psi_H^C = -\frac{4\pi e^2 F_H^C}{m\omega_0^2 V}$ = Fourier components of the (periodic) electric susceptibility, where
   - e = electron charge
   - F_H^C = structure factor of Bragg reflection $\vec{H}$
   - m = electron mass
   - $\omega_0 = \frac{2\pi c}{\lambda}$: c = speed of light in vacuum, λ = photon wavelength
   - V = volume of unit cell of crystal.

   Two ways to deal with this:
   a.) Keep a lookup table of structure factors F_H^C.
   b.) Calculate F_H^C after the Miller indices of the Bragg reflection are input by the user.
4.) h = Planck's constant (eV·s)

B.) User inputs: Create a window that will ask the user for the following inputs:

1.) E_{cent} = photon energy at center of distribution (eV)
   → Program calculates
   - $k_0 = \frac{E_{cent}}{hc}$ - convert units to $Å^{-1}$
   - $\lambda = 1/k_0$ - units in Å
   - F_0^C (or finds it in lookup table)
   - $\Psi_0^C = -\frac{4\pi e^2 F_H^C}{m\omega_0^2 V} = -\frac{e^2\lambda^2 F_0^C}{\pi m c^2 V}$

2.) (hkl) [INTEGER] = Miller indices of Bragg reflection $\vec{H}$

→ Program calculates

- $d = a/\sqrt{h^2+k^2+l^2}$ in Å
- F^c_H (or finds it in lookup table)
- $\psi^c_H = -\dfrac{e^2\lambda^2 F^c_H}{\pi mc^2 V}$

- F^c_{-H} (or finds it in lookup table)
- $\psi^c_{-H} = -\dfrac{e^2\lambda^2 F^c_{-H}}{\pi mc^2 V}$

3.) In-plane asymmetry angle a^{deg} in degrees.

→ Program calculates

- $a = a^{deg}\pi/180$ (is in radians)

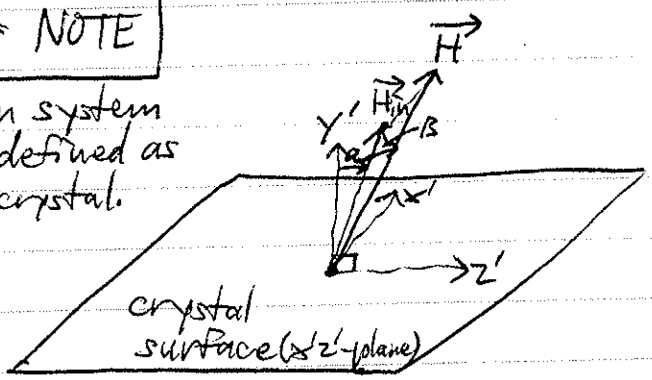
4.) Inclination angle β^{deg} of $\vec{H}$ in crystal $x'z'$-plane in degrees

→ Program calculates

- $\beta = \beta^{deg}\pi/180$ (is in radians)
- $\vec{H} = \frac{1}{d}(\sin a \sin\beta\,\hat{x}' + \cos a\,\hat{y}' + \sin a \cos\beta\,\hat{z}')$

USER's NOTE

Cartesian system $(x'y'z')$ defined as fixed to crystal.



$\vec{H}_{in}$ = component of $\vec{H}$ in $y'z'$-plane

a = angle from y'-axis to $\vec{H}_{in}$

β = angle from $\vec{H}_{in}$ to $\vec{H}$.

$$\vec{H} = \frac{1}{d}\left(\sin a \sin\beta\,\hat{x}' + \cos a\,\hat{y}' + \sin a\cos\beta\,\hat{z}'\right)$$

5.) Pitch angle θ of $\vec{H}$ relative to central incident ray.

Two user modes: user should choose one.

a) AUTO: User inputs

- $\Delta\theta_B^{\mu r}$ = deviation from kinematic Bragg angle (in μrad)

→ Program calculates

- $\theta_B = \arcsin\left(\frac{\lambda}{2d}\right)$ = kinematic Bragg angle (in rad)
- $\theta = \theta_B + \Delta\theta_B^{\mu r}\cdot 10^{-6}$

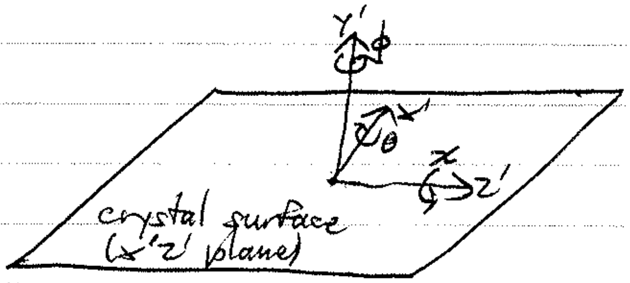
b.) ABSOLUTE: User inputs
- θ^{deg}

→ Program calculates
- $\theta = \theta^{deg}\pi/180$

6.) $\varkappa^{deg}$ = crystal's roll angle (in deg)
→ Program calculates
• $\varkappa = \varkappa^{deg}\pi/180$

7.) ϕ^{deg} = crystal's yaw angle (in deg)
→ Program calculates
• $\phi = \phi^{deg}\pi/180$

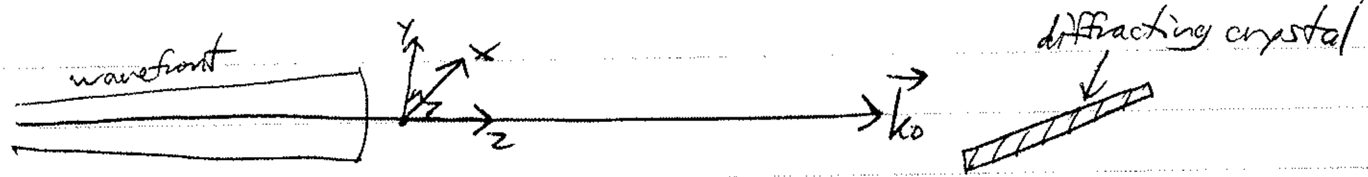
USER'S NOTE Definitions of pitch, roll and yaw rotation angles:



C.) Load properties of wavefront that is incident on the crystal.

The coding of this will depend on how SRW stores its wavefronts. However, at the end of this step, we should have a mesh of wave vector values (k_x, k_y), each associated with a pair of electric field coordinates (E_1^C, E_2^C).

USER'S NOTE Cartesian system $(x\,y\,z)$ is the lab frame in which the wavefront is initially defined.



The z-axis points along the central incident ray.
The wavefront is assumed monochromatic, so

$$k_x^2 + k_y^2 + k_z^2 = k_0^2 = 1/\lambda^2 .$$

E_1^c and E_2^c are electric field components along two orthogonal vectors $\hat{e}_1$ and $\hat{e}_2$, both of which are orthogonal to $\vec{k} = (k_x, k_y, k_z)$. See below for definitions.

D.) Calculate the transformation matrix $R = R(\theta, \chi, \phi)$, which converts crystal coordinates $(x'\,y'\,z')$ into lab coordinates $(x\,y\,z)$:

$$R(\theta,\chi,\phi) = \begin{bmatrix} \cos\chi\cos\phi & -\sin\chi & \cos\chi\sin\phi \\ \cos\theta\sin\chi\cos\phi - \sin\theta\sin\phi & \cos\theta\cos\chi & \cos\theta\sin\chi\sin\phi + \sin\theta\cos\phi \\ -\sin\theta\sin\chi\cos\phi - \cos\theta\sin\phi & -\sin\theta\cos\chi & -\sin\theta\sin\chi\sin\phi + \cos\theta\cos\phi \end{bmatrix}$$

USER'S NOTE: for an arbitrary 3-D vector $\vec{A}$,

$$\begin{bmatrix} A_x \\ A_y \\ A_z \end{bmatrix} = R(\theta,\chi,\phi) \begin{bmatrix} A_{x'} \\ A_{y'} \\ A_{z'} \end{bmatrix} , \quad \begin{bmatrix} A_{x'} \\ A_{y'} \\ A_{z'} \end{bmatrix} = R^T(\theta,\chi,\phi) \begin{bmatrix} A_x \\ A_y \\ A_z \end{bmatrix}$$

R is orthogonal, so $R^{-1} = R^T$.

BEGIN LOOP OVER ALL VALUES (k_x, k_y): For each,

E.) 1) Calculate the lab frame polarization vectors $\hat{e}_1, \hat{e}_2$:

$$\hat{e}_1(k_x,k_y) = \frac{\sqrt{k_0^2-k_x^2-k_y^2}}{\sqrt{k_0^2-k_y^2}}\hat{x} - \frac{k_x}{\sqrt{k_0^2-k_y^2}}\hat{z}$$

$$\hat{e}_2(k_x,k_y) = \frac{-k_x k_y}{k_0\sqrt{k_0^2-k_y^2}}\hat{x} + \frac{\sqrt{k_0^2-k_y^2}}{k_0}\hat{y} - \frac{k_y\sqrt{k_0^2-k_x^2-k_y^2}}{k_0\sqrt{k_0^2-k_y^2}}\hat{z}$$

2.) Convert $\hat{e}_1, \hat{e}_2$ to the crystal coordinate system.
<u>NOTE</u>: All vectors with a prime (′) have their components given in the crystal coordinate system.

$$\hat{e}_1'(k_x,k_y) = R^T\hat{e}_1(k_x,k_y)$$
$$\hat{e}_2'(k_x,k_y) = R^T\hat{e}_2(k_x,k_y)$$

3.) Calculate the following vectors for the incident beam:

a.) $\hat{u}_0 = \frac{1}{k_0}\left(k_x\hat{x} + k_y\hat{y} + \sqrt{k_0^2-k_x^2-k_y^2}\,\hat{z}\right)$

b.) $\hat{u}_0' = R^T\hat{u}_0$ <u>and</u> $\vec{k}_0' = k_0\hat{u}_0'$

c.) $\hat{\sigma}_0' = \frac{\vec{H}'\times\hat{u}_0'}{|\vec{H}'\times\hat{u}_0'|}$

d.) $\hat{\pi}_0' = \hat{u}_0'\times\hat{\sigma}_0'$

4.) Calculate the following vectors for the diffracted beam:

a.) $\hat{u}_H' = \frac{\vec{k}_0'+\vec{H}'}{|\vec{k}_0'+\vec{H}'|}$

b.) $\hat{\sigma}_H' = \frac{\hat{u}_H'\times\hat{u}_0'}{|\hat{u}_H'\times\hat{u}_0'|}$

c.) $\hat{\pi}_H' = \hat{u}_H'\times\hat{\sigma}_H'$

5.) Define the following vectors:

a) $\hat{x}_0' = \dfrac{\hat{u}_0' - (\hat{u}_0' \cdot \hat{y}')\hat{y}'}{|\hat{u}_0' - (\hat{u}_0' \cdot \hat{y}')\hat{y}'|}$; $\hat{x}_H' = \dfrac{\hat{u}_H' - (\hat{u}_H' \cdot \hat{y}')\hat{y}'}{|\hat{u}_H' - (\hat{u}_H' \cdot \hat{y}')\hat{y}'|}$

b) $\hat{z}_0' = \dfrac{\hat{x}_0' \times (-\hat{y}')}{|\hat{x}_0' \times (-\hat{y}')|}$; $\hat{z}_H' = \dfrac{\hat{x}_H' \times (-\hat{y}')}{|\hat{x}_H' \times (-\hat{y}')|}$

USER'S NOTE: These choices will not work well if either the incident or the diffracted beam is very nearly normal to the crystal surface.

6.) Calculate 2 parameters:

a) $b = \left(1 + \dfrac{\hat{y}' \cdot \vec{H}'}{\hat{y}' \cdot \vec{k}_0'}\right)^{-1}$

b) $A = \dfrac{1}{k_0^2}\left(\dfrac{1}{d^2} + 2\vec{k}_0' \cdot \vec{H}'\right)$

7.) Calculate the following dot products:

a) $a_{OH}^{\sigma\sigma} = \hat{\sigma}_0' \cdot \hat{\sigma}_H'$

b) $a_{OH}^{\pi\pi} = \hat{\pi}_0' \cdot \hat{\pi}_H'$

8.) Calculate
- the 2 eigen~~vectors~~ values $2\delta_{01}^{\sigma c}$, $2\delta_{02}^{\sigma c}$ and
- the 2 eigenvectors $\begin{bmatrix} D_{O01}^{c} \\ D_{HO1}^{c} \end{bmatrix}$, $\begin{bmatrix} D_{O02}^{c} \\ D_{HO2}^{c} \end{bmatrix}$ of the matrix

$$\begin{bmatrix} \psi_0^c & \psi_{-H}^c a_{OH}^{\sigma\sigma} \\ b\,\psi_H^c a_{OH}^{\sigma\sigma} & b(\psi_0^c - A) \end{bmatrix}$$

9.) Calculate

- the 2 eigenvalues $2\delta_{01}^{\pi C}$, $2\delta_{02}^{\pi C}$ and
- the 2 eigenvectors $\begin{bmatrix} D_{0\pi 1}^{C} \\ D_{H\pi 1}^{C} \end{bmatrix}$, $\begin{bmatrix} D_{0\pi 2}^{C} \\ D_{H\pi 2}^{C} \end{bmatrix}$ of the matrix

$$\begin{bmatrix} \psi_0^C & \psi_{-H}^C a_{OH}^{\pi\pi} \\ \\ b\psi_H^C a_{OH}^{\pi\pi} & b(\psi_0^C - A) \end{bmatrix}$$

10.) Calculate the index of refraction increments of the H beam inside the crystal:

a.) $\delta_{H1}^{\sigma C} = \frac{1}{b}\delta_{01}^{\sigma C} + \frac{1}{2}A$

b.) $\delta_{H2}^{\sigma C} = \frac{1}{b}\delta_{02}^{\sigma C} + \frac{1}{2}A$

c.) $\delta_{H1}^{\pi C} = \frac{1}{b}\delta_{01}^{\pi C} + \frac{1}{2}A$

d.) $\delta_{H2}^{\pi C} = \frac{1}{b}\delta_{02}^{\pi C} + \frac{1}{2}A$

11.) Calculate the incident beam propagation vectors inside the crystal:

a.) $\gamma_0 = -\hat{y}' \cdot \vec{k}_0'$

b.) $\vec{\beta}_{01}^{\sigma C\prime} = \vec{k}_0' - \frac{k_0 \delta_{01}^{\sigma C}}{\gamma_0}\hat{y}'$ d.) $\vec{\beta}_{01}^{\pi C\prime} = \vec{k}_0' - \frac{k_0 \delta_{01}^{\pi C}}{\gamma_0}\hat{y}'$

c.) $\vec{\beta}_{02}^{\sigma C\prime} = \vec{k}_0' - \frac{k_0 \delta_{02}^{\sigma C}}{\gamma_0}\hat{y}'$ e.) $\vec{\beta}_{02}^{\pi C\prime} = \vec{k}_0' - \frac{k_0 \delta_{02}^{\pi C}}{\gamma_0}\hat{y}'$

12.) Calculate the diffracted beam propagation vectors inside the crystal a.) $\vec{B}^{\sigma C'}_{H1} = \vec{B}^{\sigma C'}_{01} + \vec{H}'$ c.) $\vec{B}^{\pi C'}_{H1} = \vec{B}^{\pi C'}_{01} + \vec{H}'$

b.) $\vec{B}^{\sigma C'}_{H2} = \vec{B}^{\sigma C'}_{02} + \vec{H}'$ d.) $\vec{B}^{\pi C'}_{H2} = \vec{B}^{\pi C'}_{02} + \vec{H}'$

13.) Calculate the unit vectors of propagation:

a.) $\hat{u}^{\sigma C'}_{01} = \vec{B}^{\sigma C'}_{01} / |\vec{B}^{\sigma C'}_{01}|$; $\hat{u}^{\sigma C'}_{H1} = \vec{B}^{\sigma C'}_{H1} / |\vec{B}^{\sigma C'}_{H1}|$

b.) $\hat{u}^{\sigma C'}_{02} = \vec{B}^{\sigma C'}_{02} / |\vec{B}^{\sigma C'}_{02}|$; $\hat{u}^{\sigma C'}_{H2} = \vec{B}^{\sigma C'}_{H2} / |\vec{B}^{\sigma C'}_{H2}|$

c.) $\hat{u}^{\pi C'}_{01} = \vec{B}^{\pi C'}_{01} / |\vec{B}^{\pi C'}_{01}|$; $\hat{u}^{\pi C'}_{H1} = \vec{B}^{\pi C'}_{H1} / |\vec{B}^{\pi C'}_{H1}|$

d.) $\hat{u}^{\pi C'}_{02} = \vec{B}^{\pi C'}_{02} / |\vec{B}^{\pi C'}_{02}|$; $\hat{u}^{\pi C'}_{H2} = \vec{B}^{\pi C'}_{H2} / |\vec{B}^{\pi C'}_{H2}|$

14.) Calculate the polarization vectors of the O and H beams:

a.) $\hat{\sigma}^{\sigma C'}_{01} = \dfrac{\vec{H}' \times \hat{u}^{\sigma C'}_{01}}{|\vec{H}' \times \hat{u}^{\sigma C'}_{01}|}$; $\hat{\pi}^{\sigma C'}_{01} = \hat{u}^{\sigma C'}_{01} \times \hat{\sigma}^{\sigma C'}_{01}$

b.) $\hat{\sigma}^{\sigma C'}_{02} = \dfrac{\vec{H}' \times \hat{u}^{\sigma C'}_{02}}{|\vec{H}' \times \hat{u}^{\sigma C'}_{02}|}$; $\hat{\pi}^{\sigma C'}_{02} = \hat{u}^{\sigma C'}_{02} \times \hat{\sigma}^{\sigma C'}_{02}$

c.) $\hat{\sigma}^{\pi C'}_{01} = \dfrac{\vec{H}' \times \hat{u}^{\pi C'}_{01}}{|\vec{H}' \times \hat{u}^{\pi C'}_{01}|}$; $\hat{\pi}^{\pi C'}_{01} = \hat{u}^{\pi C'}_{01} \times \hat{\sigma}^{\pi C'}_{01}$

d.) $\hat{\sigma}^{\pi C'}_{02} = \dfrac{\vec{H}' \times \hat{u}^{\pi C'}_{02}}{|\vec{H}' \times \hat{u}^{\pi C'}_{02}|}$; $\hat{\pi}^{\pi C'}_{02} = \hat{u}^{\pi C'}_{02} \times \hat{\sigma}^{\pi C'}_{02}$

and analogous formulas with the subscript O replaced by H.

15.) Calculate the following dot products:

a.) $\sigma^{\sigma C}_{01x} = \hat{\sigma}^{\sigma C'}_{01} \cdot \hat{\underline{x}}'_0$; $\sigma^{\pi C}_{01x} = \hat{\sigma}^{\pi C'}_{01} \cdot \hat{\underline{x}}'_0$

b.) $\sigma^{\sigma C}_{01z} = \hat{\sigma}^{\sigma C'}_{01} \cdot \hat{\underline{z}}'_0$; $\sigma^{\pi C}_{01z} = \hat{\sigma}^{\pi C'}_{01} \cdot \hat{\underline{z}}'_0$

c.) $\sigma^{\sigma C}_{02x} = \hat{\sigma}^{\sigma C'}_{02} \cdot \hat{\underline{x}}'_0$; $\sigma^{\pi C}_{02x} = \hat{\sigma}^{\pi C'}_{02} \cdot \hat{\underline{x}}'_0$

d.) $\sigma^{\sigma C}_{02z} = \hat{\sigma}^{\sigma C'}_{02} \cdot \hat{\underline{z}}'_0$; $\sigma^{\pi C}_{02z} = \hat{\sigma}^{\pi C'}_{02} \cdot \hat{\underline{z}}'_0$

and analogous formulas with the subscript O replaced by H.

16.) Calculate the following dot products:

a.) $\Pi_{01x}^{\sigma e} = \hat{\pi}_{01}^{\sigma e\prime} \cdot \hat{\hat{x}}_0^{\prime}$; $\Pi_{01x}^{\pi e} = \hat{\pi}_{01}^{\pi e\prime} \cdot \hat{\hat{x}}_0^{\prime}$

b.) $\Pi_{01z}^{\sigma e} = \hat{\pi}_{01}^{\sigma e\prime} \cdot \hat{\hat{z}}_0^{\prime}$; $\Pi_{01z}^{\pi e} = \hat{\pi}_{01}^{\pi e\prime} \cdot \hat{\hat{z}}_0^{\prime}$

c.) $\Pi_{02x}^{\sigma e} = \hat{\pi}_{02}^{\sigma e\prime} \cdot \hat{\hat{x}}_0^{\prime}$; $\Pi_{02x}^{\sigma e} = \hat{\pi}_{02}^{\pi e\prime} \cdot \hat{\hat{x}}_0^{\prime}$

d.) $\Pi_{02z}^{\sigma e} = \hat{\pi}_{02}^{\sigma e\prime} \cdot \hat{\hat{z}}_0^{\prime}$; $\Pi_{02z}^{\pi e} = \hat{\pi}_{02}^{\pi e\prime} \cdot \hat{\hat{z}}_0^{\prime}$

and analogous formulas with subscripts 0 replaced by H.

17.) Calculate

a.) $\vec{k}_{0t}^{\prime} = \vec{k}_0^{\prime} - (\vec{k}_0^{\prime} \cdot \hat{y}^{\prime})\hat{y}^{\prime}$ (tangential component of $\vec{k}_0^{\prime}$)

b.) $\vec{k}_{Ht}^{\prime} = \vec{\beta}_{H1}^{\sigma e\prime} - (\vec{\beta}_{H1}^{\sigma e\prime} \cdot \hat{y}^{\prime})\hat{y}^{\prime}$

c.) $\vec{k}_{\bar{0}}^{\prime} = \vec{k}_{0t}^{\prime} + \hat{y}^{\prime}(k_0^2 - \vec{k}_{0t}^{\prime} \cdot \vec{k}_{0t}^{\prime})$

d.) $\vec{k}_{\bar{H}}^{\prime} = \vec{k}_{Ht}^{\prime} + \hat{y}^{\prime}(k_0^2 - \vec{k}_{Ht}^{\prime} \cdot \vec{k}_{Ht}^{\prime})$

e.) $\hat{\pi}_{\bar{0}}^{\prime} = \dfrac{\vec{k}_{\bar{0}}^{\prime} \times \hat{\hat{z}}_0^{\prime}}{|\vec{k}_{\bar{0}}^{\prime} \times \hat{\hat{z}}_0^{\prime}|}$; $\hat{\pi}_{\bar{H}}^{\prime} = \dfrac{\vec{k}_{\bar{H}}^{\prime} \times \hat{\hat{z}}_H^{\prime}}{|\vec{k}_{\bar{H}}^{\prime} \times \hat{\hat{z}}_H^{\prime}|}$

f.) $\Pi_{\bar{0}x} = \hat{\pi}_{\bar{0}}^{\prime} \cdot \hat{\hat{x}}_0^{\prime}$; $\Pi_{\bar{H}x} = \hat{\pi}_{\bar{H}}^{\prime} \cdot \hat{\hat{x}}_H^{\prime}$

g.) $\hat{\Sigma}_{\bar{0}}^{\prime} = \hat{\hat{z}}_0^{\prime}$; $\hat{\Pi}_{\bar{0}}^{\prime} = \dfrac{\vec{k}_{\bar{0}}^{\prime} \times \hat{\hat{z}}_0^{\prime}}{|\vec{k}_{\bar{0}}^{\prime} \times \hat{\hat{z}}_0^{\prime}|}$

h.) $\hat{\Sigma}_{\bar{H}}^{\prime} = \hat{\hat{z}}_H^{\prime}$; $\hat{\Pi}_{\bar{H}}^{\prime} = \dfrac{\vec{k}_{\bar{H}}^{\prime} \times \hat{\hat{z}}_H^{\prime}}{|\vec{k}_{\bar{H}}^{\prime} \times \hat{\hat{z}}_H^{\prime}|}$

USER'S NOTE: Polarization vectors of vacuum incident (0) and vacuum diffracted (H) beams, for use with boundary conditions

18.) Calculate indices of refraction (n) and dielectric constants (ϵ):

a.) $n_{01}^{\sigma e} = 1 + \delta_{01}^{\sigma e}$; $n_{01}^{\pi e} = 1 + \delta_{01}^{\pi e}$

$\epsilon_{01}^{\sigma e} = 1 + 2\delta_{01}^{\sigma e}$; $\epsilon_{01}^{\pi e} = 1 + 2\delta_{01}^{\pi e}$

la) $\eta_{02}^{\sigma c} = 1 + \delta_{02}^{\sigma c}$; $\eta_{02}^{\pi c} = 1 + \delta_{02}^{\pi c}$
$\epsilon_{02}^{\sigma c} = 1 + 2\delta_{02}^{\sigma c}$; $\epsilon_{02}^{\pi c} = 1 + 2\delta_{02}^{\pi c}$

and analogous formulas with subscripts 0 replaced by H.

19.) Create the matrix $\underline{F^c}$ = (4x4 complex matrix)

$$
\begin{bmatrix}
D^c_{0\sigma 1}\left(\frac{\sigma_{01z}^{\sigma c}}{\epsilon_{01}^{\sigma c}} - \frac{\pi_{01x}^{\sigma c}}{\pi_{0x}}\frac{1}{\eta_{01}^{\sigma c}}\right) & D^c_{0\sigma 2}\left(\frac{\sigma_{02z}^{\sigma c}}{\epsilon_{02}^{\sigma c}} - \frac{\pi_{02x}^{\sigma c}}{\pi_{0x}}\frac{1}{\eta_{02}^{\sigma c}}\right) & D^c_{0\pi 1}\left(\frac{\pi_{01z}^{\pi c}}{\epsilon_{01}^{\pi c}} + \frac{\sigma_{01x}^{\pi c}}{\pi_{0x}}\frac{1}{\eta_{01}^{\pi c}}\right) & D^c_{0\pi 2}\left(\frac{\pi_{02z}^{\pi c}}{\epsilon_{02}^{\pi c}} + \frac{\sigma_{02x}^{\pi c}}{\pi_{0x}}\frac{1}{\eta_{02}^{\pi c}}\right) \\
D^c_{0\sigma 1}\left(-\frac{\pi_{01z}^{\sigma c}}{\eta_{01}^{\sigma c}} - \frac{\sigma_{01x}^{\sigma c}}{\pi_{0x}}\frac{1}{\epsilon_{01}^{\sigma c}}\right) & D^c_{0\sigma 2}\left(-\frac{\pi_{02z}^{\sigma c}}{\eta_{02}^{\sigma c}} - \frac{\sigma_{02x}^{\sigma c}}{\pi_{0x}}\frac{1}{\epsilon_{02}^{\sigma c}}\right) & D^c_{0\pi 1}\left(\frac{\sigma_{01z}^{\pi c}}{\eta_{01}^{\pi c}} - \frac{\pi_{01x}^{\pi c}}{\pi_{0x}}\frac{1}{\epsilon_{01}^{\pi c}}\right) & D^c_{0\pi 2}\left(\frac{\sigma_{02z}^{\pi c}}{\eta_{02}^{\pi c}} - \frac{\pi_{02x}^{\pi c}}{\pi_{0x}}\frac{1}{\epsilon_{02}^{\pi c}}\right) \\
\multicolumn{4}{l}{\text{same as 1st row except subscript 0 changed to H}} \\
\multicolumn{4}{l}{\text{same as 2nd row except subscript 0 changed to H}}
\end{bmatrix}
$$

20.) Invert F^c to find $(F^c)^{-1}$. Then, define a 4x2 matrix $\mathcal{W}^c$ as follows:

$$
\mathcal{W}^c = \begin{bmatrix}
[(F^c)^{-1}]_{11} & [(F^c)^{-1}]_{12} \\
[(F^c)^{-1}]_{21} & [(F^c)^{-1}]_{22} \\
[(F^c)^{-1}]_{31} & [(F^c)^{-1}]_{32} \\
[(F^c)^{-1}]_{41} & [(F^c)^{-1}]_{42}
\end{bmatrix}
$$

21.) Calculate a 2×4 matrix $\wp^c =$

$$\begin{bmatrix} \dfrac{D^c_{H\sigma 1}\,\sigma^{\sigma c}_{H12}}{G^{\sigma c}_{H1}} & \dfrac{D^c_{H\sigma 2}\,\sigma^{\sigma c}_{H22}}{G^{\sigma c}_{H2}} & \dfrac{D^c_{H\pi 1}\,\pi^{\pi c}_{H12}}{G^{\pi c}_{H1}} & \dfrac{D^c_{H\pi 2}\,\pi^{\pi c}_{H22}}{G^{\pi c}_{H2}} \\ -\dfrac{D^c_{H\sigma 1}\,\pi^{\sigma c}_{H12}}{\sqrt{G^{\sigma c}_{H1}}} & -\dfrac{D^c_{H\sigma 2}\,\pi^{\sigma c}_{H22}}{\sqrt{G^{\sigma c}_{H2}}} & \dfrac{D^c_{H\pi 1}\,\sigma^{\pi c}_{H12}}{\sqrt{G^{\pi c}_{H1}}} & \dfrac{D^c_{H\pi 2}\,\sigma^{\pi c}_{H22}}{\sqrt{G^{\pi c}_{H2}}} \end{bmatrix};$$

22.) Calculate the 2×2 matrix

$$T^c = 2\wp^c W^c.$$

<u>USER'S NOTE</u>: T^c is the "transmission function" of the diffracting crystal.

23.) Convert the incident beam polarization amplitudes (E_1, E_2) to the $\hat{\Sigma}_0'$, $\hat{\Pi}_0'$ directions: The results will be E^c_Σ, E^c_π:

$$\begin{bmatrix} E^c_\Sigma \\ E^c_\pi \end{bmatrix} = \begin{bmatrix} \hat{e}_1'\cdot\hat{\Sigma}_0' & \hat{e}_2'\cdot\hat{\Sigma}_0' \\ \hat{e}_1'\cdot\hat{\Pi}_0' & \hat{e}_2'\cdot\hat{\Pi}_0' \end{bmatrix} \begin{bmatrix} E^c_1 \\ E^c_2 \end{bmatrix}$$

24.) Calculate the diffracted beam amplitudes $E^c_{\bar{H}\Sigma}, E^c_{\bar{H}\pi}$ in vacuum along the directions $\hat{\Sigma}_0'$, $\hat{\Pi}_0'$:

$$\begin{bmatrix} E^c_{\bar{H}\Sigma} \\ E^c_{\bar{H}\pi} \end{bmatrix} = T^c \begin{bmatrix} E^c_\Sigma \\ E^c_\pi \end{bmatrix}$$

25.) Convert all vectors to the lab frame:

a.) $\vec{k}_{\bar{H}} = R\vec{k}_{\bar{H}}'$

b.) $\hat{\Sigma}_{\bar{H}} = R\hat{\Sigma}_{\bar{H}}'$

c.) $\hat{\Pi}_{\bar{H}} = R\hat{\Pi}_{\bar{H}}'$

26.) Store the results in a table.
END LOOP OVER ALL VALUES (k_x, k_y).

F.) Conversion of generated table into "propagat-able" SRW wavefront. To be discussed with Oleg Chubar.

END OF PSEUDOCODE (1 June 2011)