Improved models for synchrotron radiation sources in SHADOW

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Abstract. A technique to improve the description of synchrotron sources is proposed and applied to the ray tracing code SHADOW. Using a dedicated synchrotron radiation calculation code, it is possible to calculate the single electron emission, as well as the thick electron beam emission. Two methods will be introduced. The first simulates synchrotron radiation using the spatial electron distribution for the positions of the rays and the thick electron beam spectral-angular distribution in the far field for their directions and their energies. The second method derives the variation of the single electron spectral-angular distribution with respect to the electron direction and the electron energy, and simulates the rays emitted by each electron. A preprocessor for SHADOW has been developed to read the intensity distribution from an HDF5 file generated by SRW. The final rays have been used to simulate future beamlines and have been cross checked with the wavefront propagation method.

1. Introduction

The ongoing upgrades of synchrotrons around the world have increased the need for accurate and detailed description of synchrotron radiation (SR) sources for optical ray-tracing simulations. Formerly, tools embedded in SHADOW calculate the spectral-angular distribution using the analytical expression\cite{1}. We opted for a similar approach, but we obtain it from a dedicated synchrotron radiation calculation code: SRW\cite{2}\cite{3}. This code calculates the electromagnetic field of SR directly from the dynamics of the electrons, so it needs none of the approximations used in the analytical theory, and so the technique can simulate also more types of SR sources, since it is not limited by a particular form of the magnetic field.

2. Model

In the ray-tracing domain, the problem of generating a beam of X-rays is divided in two parts. First, one has to find the phase distribution for the rays and second, one implements a Monte-Carlo method to randomly select the rays.

We take a 5D phase distribution as we consider the transverse position, the horizontal and vertical angles, and the photon energy to be the relevant variables. The natural distribution to look for should be the brilliance, but this choice poses some problems. Sampling a 5D space is computationally expensive, as we need many rays to achieve a good statistics for the distribution. Moreover, in quantum mechanics it is not possible to measure simultaneously the position and the direction of a particle, and a distribution based on the brilliance can assume negative values\cite{4}.
To be consistent with a classical model, we introduce an approximation. We consider the spatial and the spectral-angular distribution of radiation to be separate and uncorrelated. The spectral-angular flux in the far field approximation for a single electron, or filament electron beam, is obtained from the electromagnetic field in the following way:

\[
\frac{d\Phi_{\text{single}}}{d\Omega}(\vec{r}',\omega) = C |\vec{E}(\vec{r}',\omega)|^2
\]

(1)

where \(\vec{r}'\) stands for the angles, \(\omega\) for the photon frequency and \(C\) is a convenient constant.

In storage rings the longitudinal distribution of the bunch is Gaussian and has a typical \(\sigma_s\) on the order of a few mm, while the emitted radiation has a much smaller wavelength. This fact ensures that no interference effects occur between the electromagnetic fields emitted by different electrons. Therefore the spectral-angular distribution of a thick electron beam is given by a convolution of the single electron spectral-angular distribution with the electron phase density:

\[
\frac{d\Phi_{\text{thick}}}{d\Omega}(\vec{r}',\omega) = \int_{\mathbb{R}^2} d^2\vec{R}' d\gamma \frac{d\Phi_{\text{single}}}{d\Omega}(\vec{r}' - \vec{R}',\omega,\gamma)\rho_e(\vec{R}',\gamma)
\]

(2)

where \(\vec{R}'\) stands for the direction of the electron, \(\gamma\) is the energy of the electron and \(\rho_e\) is the partial electron density, which is the electron phase density integrated over the positions.

We use the thick electron beam spectral-angular distribution to generate the horizontal and vertical angles, and the energy of the rays and the spatial part of the electron density to generate their transverse positions. Later on in the paper we will refer to this method as method 1. Part of the photons generated will fall out of the aperture slit, as we have imposed no correlations between the spatial and the angular distributions of the radiation. This correlation indeed exists, but it is hidden by the convolution in Eq. 2. In order to be consistent with the results obtained by the SR code, we remove these photons from the Monte Carlo sampling, as they are fictitious.

One way to treat the correlation between space and angles, which was avoided in the previous method, is implemented in method 2. We use the single electron spectral-angular distribution calculated by SRW, and we derive the effects induced to the radiation emitted, when the electron has a different energy and direction. We deduce, from scaling considerations of the electric field expression, that given an electron with energy \(\gamma = \gamma_0(1 + \delta)\), the spectrum is “stretched” by a factor \(1 + 2\delta\) for all the observed directions. From geometrical considerations we find that the radiation of an electron with direction \(\vec{u}\), not parallel to the longitudinal axis \(\vec{v}\), is shifted by \(\vec{u} - \vec{v}\). This method correctly takes into account the correlation between source size and spectral-angular distribution of the emitted radiation.

3. Applications

The tool has been developed and has already been used in the simulation of future NSLS-II beamlines. In this context we present two studies, where we compare distribution of radiation generated by SRW, and by the two methods when propagated to the beamline aperture slit.

3.1. NSLS-II FMX beamline

The frontier macromolecular crystallography undulator beamline (FMX) will produce a tunable beam down to one micron in dimension, with variable divergence, to address the most difficult problems in MX: small, weakly diffracting crystals, and very large unit cells.

The source has been simulated with method 2 using three millions rays sampling a narrow bandwidth between 12.65 ± 0.05 keV. For the purpose of this paper we also simulate the source using method 1, but on a broader energy window. The properties of the electron beam are listed in Table 1. The FMX undulator is long 2.5 m, its period length is 2.1 cm, the magnetic field is vertical, with a peak of 0.80371 T. Figure 1 shows the accuracy of the two methods for
Table 1. electron beam properties at FMX and 3PW beamlines.

|     | \(\sigma_x\), \(\mu\)m | \(\sigma'_x\), \(\mu\)rad | \(\langle xx'\rangle\), nm rad | \(\sigma_y\), \(\mu\)m | \(\sigma'_y\), \(\mu\)rad | \(\langle yy'\rangle\), nm rad | \(\sigma_E\), p.n. |
|-----|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| FMX | 39.2            | 16.5            | 0.34            | 4.50            | 2.75            | 9 \(10^{-3}\)    | 0.089%          |
| 3PW | 128.4           | 98.0            | -12.46          | 12.53           | 0.82            | 6.454 \(10^{-3}\)| 0.089%          |

The spectral flux on a slit of 5.0x2.5 mm\(^2\), 42.0 m away from the source. Figure 2 illustrates the intensities on the slit for two different photon energies. Near the peak of the spectral flux, the undulator radiation shows a complex pattern consisting of two lobes, while at the resonant energy of the harmonic the shape is one lobe, close to Gaussian. These features are represented by both methods.

Figure 1. Spectral flux at 42.0 m from the source for a 5.0x2.5 mm\(^2\) slit. (right) Closeup on the peak of intensity.

Figure 2. Intensity distribution at 42.0 m. (right) Vertical cut for x=0. For the legend, see Figure 1.

3.2. NSLS-II Three-Pole Wiggler beamlines

We apply method 1 to a three pole wiggler (3PW), which is a replacement for high field bending magnet source at NSLS-II. As NSLS-II will have about ten 3PW beamlines, it is of paramount importance to correctly represent these sources.

We sample the spectral flux generated by SRW with three millions rays for different photon energies: 5, 10, and 20 keV. The electron beam parameters are listed in Table 1. The 3PW spatial distribution is composed by a central pole and two side poles. In this simulation we approximate the spatial distribution with the central pole. In fact, most of the beamlines will use the radiation coming from the central pole. It is possible to refine this model by representing the source as a sum of incoherent contributions from each pole. The 3PW magnetic field modeled had a 1.2 T central pole and two 0.4 T side poles, each one at 7 cm from the central pole. Figure
3 shows the intensities at a slit 30.0 m away from the 3PW. Figure 4 shows the horizontal and vertical cuts of the previous intensities. The results are in good agreement.

![Intensity profile at 30.0 m from the central pole.](image)

**Figure 3.** Intensity profile at 30.0 m from the central pole.

![Horizontal (left) and vertical (right) cuts of the distribution presented in Figure 3 by planes passing by the origin (x=y=0).](image)

**Figure 4.** Horizontal (left) and vertical (right) cuts of the distribution presented in Figure 3 by planes passing by the origin (x=y=0).

4. Conclusion
Two methods have been introduced to treat SR sources for ray tracing codes. The two methods give similar results in the performed simulations. We have shown that the technique can be applied to generate a source, such as a 3PW, which has different magnetic field from undulators. We are currently working to include the polarization in the model. The tool soon will be included in the SHADOW package. The same results can be obtained by generating the spectral-angular flux with other SR dedicated codes, such as SPECTRA and WAVE.

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