Novel x-ray optics for imaging XPDC

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Abstract

In the present work an introduction to the x-ray parametric down-conversion (XPDC) processes is given. The aim of the project was to develop a bent-analyzer setup, which can resolve x-ray-to-visible XPDC on top of elastic background scattering. For this it was necessary to create a beam object first, which resembles the emission cone of the XPDC effect. The object was simulated using XRT-software. Since simulation of nonlinear effects is not integrated in XRT, a code in python environment was created that would allow to simulate such tasks.

Contents

1 Introduction

Parametric down conversion (PDC) is the effect of a spontaneous decay of an incident photon (referred to as "pump" photon) into a pair of correlated photons ("signal" and "idler"). X-ray parametric down conversion denotes a process of PDC of x-rays into longer wavelengths. The initial pump beam interacts with nonlinear crystal to generate two photons: one is in the x-ray range ("signal") and the second one is in the UV or visible range ("idler"), which satisfies energy conservation [1].

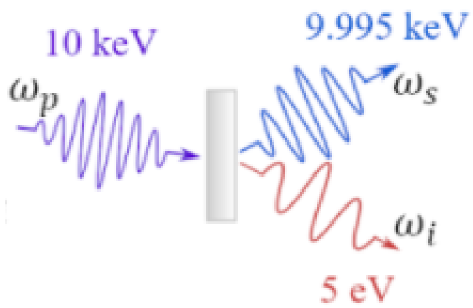

Figure 1: Image shows a schematic representation of XPDC. Here ω_p, ω_s and ω_i represent pump, signal and idler energies respectively. As x-ray photon interacts with crystal (a gray block) it is converted into two other with lower energies.

In 1969 Freud and Levine [2] first proposed an approach to consider PDC in the x-ray regime and to use nonlinear wave mixing of x-ray and UV or visible light to resolve microscopic properties of valence electrons. Later in 1970 Eisenberger and McCall [3] demonstrated the parametric down-conversion of x-rays in their experiment with an x-ray tube.

The detection of such nonlinear scattering is still very challenging as signals are very weak and are accompanied by strong background effects like elastic diffraction.
At the same time, in comparison to conventional (i.e. elastic) scattering processes, the nonlinear scattering provides specific access to the valence charges. This suggests a promising application of XPDC for studying valence electrons, which is of importance since the behaviour of valence electrons determines the properties of a material.

2 Theory

2.1 Phase matching for XPDC

The frequency selection of the generated beams is carried out by the requirement for momentum and energy conservation and relies on the refractive indices of the material, the propagation angles of the beams and their photon energies.

Frequency conversion can be achieved when the phase matching condition is fulfilled. This means that both energy and momentum should be conserved:

$$\omega_p = \omega_s + \omega_i,$$
$$\vec{k_p} + \vec{G} = \vec{k_s} + \vec{k_i}.$$

Here, ω_p, ω_s and ω_i represent the frequencies and k_p, k_s and k_i the wave-vectors for pump, signal and idler photons, respectively. G denotes the reciprocal lattice vector which directs the diffraction process [4].

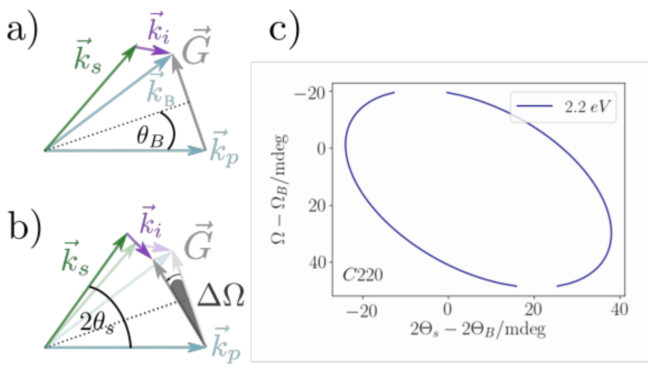

Figure 2: Figure was taken from ref. [4]. The incident pump beam k_p is nonlinearly scattered on the reciprocal lattice G into the down-converted photon pair k_s, k_i (a). As sample is rotated through a rocking angle $\Delta\Omega$ the involved momenta are reoriented (b). A scan of the phase-matching condition yields the characteristic scattering signature (c).

XPDC can be observed for a broad (compared to Bragg reflection) range of incident angles under which a pump photon incises to the lattice plane. This is due to the additional degrees of freedom provided by the idler photon momentum. By tilting the sample by the rocking angle $\Delta\Omega$, the involved momenta are reoriented.

2.2 X-ray tracing software

For the simulations during the project the XRayTracer software (XRT) [5] was used. The X-ray tracing program has a well-documented online manual [6] and some example scripts. Within a python environment the software allows to perform start-to-end modeling of x-ray scattering experiments. It is extremely useful for implementing an experimental setup as it has beamline components with various properties included to adjust for one's specific problem. A graphical user interface (GUI) of XRT — xrtQook is designed for assembling beamlines by combining the xrt modules and beamline parts. It generates ready-to-use script which can be ran within a tool or used in an external python editor. An interactive window xrtGlow provides with a 3D visualization of created beamline. It is a helpful tool to check the alignment of beamline components.

3 Implementation

To simulate XPDC within the ray tracing framework, we had to construct a beam object which resembles the emission cone of the XPDC effect. To create a cone, we first arranged a round aperture and a beam-stop in XRTQook, as shown in Figure 3.

The configuration above is a very simple approximation that was done to get the view of a beam passing through apertures and get understanding on distances between elements of the beamline. But to have a possibility to fully mimic a behaviour of a beam in the experiment, we need to make it possible to adjust the cone by its parameters, such as size and direction of propagation.

To achieve this, we used XRT package for python to construct a desired cone. The simulated experimental setup consists of a geometrical beam source, a round aperture, a round beamstop and a screen. First, the alignment of the cone was done. The direction of propagation of the cone is dependent on the Bragg angle of a crystal it is generated from. The size of the cone, meaning its divergence and resulting radius, is shaped by the radius

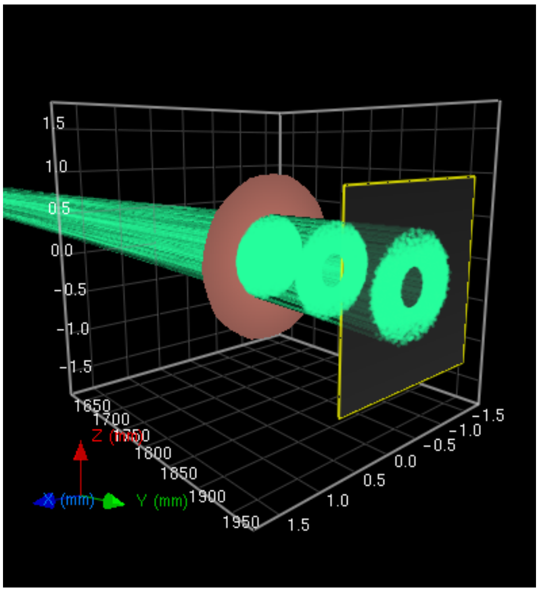

Figure 3: This image from xrtGlow depicts the X-ray divergent monochromatic beam coming from the geometrical source (in the background), impinging on a round aperture (brown) and a round beamstop (in the center of the aperture, not seen here), followed by the screen on which the ring-shaped image of the beam is formed.

of the round aperture. To have an ability to control the radius we connected it to the value of the opening angle of the cone, calculated from the phase-matching condition.

The cone radius is dependent on the characteristic scattering signature, so the opening angle has to be reassigned to the difference of total scattering angles belonging to the upper and lower arc of the ellipse, shown in Figure 2 for varying values of rocking angle $\Delta\Omega$.

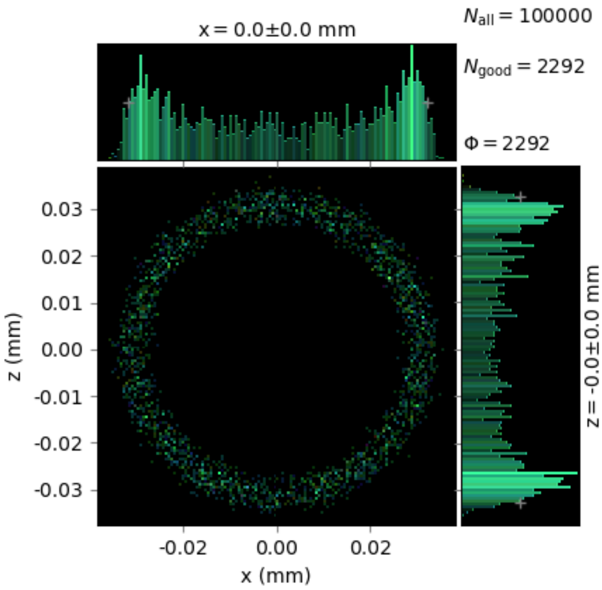

Figure 4: The 2D positional diagram (in the center) shows the obtained beam, as depicted in Figure 2, disposition on the screen. 1D histograms on the top and on the right, show the beam distribution in x and z directions, respectively. Input parameters for this configuration are signal energy, $\omega_s = 9690eV$, idler energy, $\omega_i = 5eV$, $\Delta\Omega = -50$ mdeg.

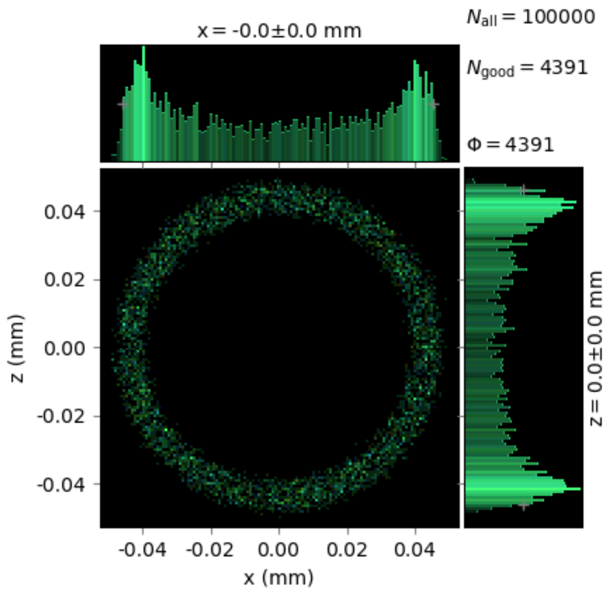

Figure 5: The similar diagrams as in Figure 4 for input parameters $\omega_s = 9690eV$, $\omega_i = 5eV$, $\Delta\Omega = -0.5mdeg$. As the rocking angle gets bigger, an increase in the cone diameter is observed.

The resulting code is dependent on signal and idler energies, material of the crystal, and its Miller indices for the lattice plane on which the diffraction process takes place, Bragg angle of the crystal, and rotation angles to align all the elements of the setup.

4 Conclusion

X-ray parametric down conversion has a great potential in providing applications for valence electron specific imaging. Despite the fact that this effect has been known and studied for a long time, its detection still remains challenging in certain regimes.
The initial intent of the project was to build a a bent-analyzer setup to resolve x-ray-to-visible XPDC, but we mainly focused on the setting of the cone object.
As a result of this work, the code that simulates the propagation of the cone, which can be obtained after interacting with a diamond crystal, was written. The resulting cone, which can be easily adjusted to the required parameters, can be used as a beam object within a simulation.

References

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