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Comparison of scattering experiments using synchrotron radiation with Monte Carlo simulations using Geant4

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ABSTRACT

Monte Carlo techniques are powerful tools to simulate the interaction of electromagnetic radiation with matter. One of the most widespread simulation program packages is Geant4. Almost all physical interaction processes can be included. However, it is not evident what accuracy can be obtained by a simulation. In this work, results of scattering experiments using monochromatized synchrotron radiation in the X-ray regime are quantitatively compared to the results of simulations using Geant4. Experiments were performed for various scattering foils made of different materials such as copper and gold. For energy-dispersive measurements of the scattered radiation, a cadmium telluride detector was used. The detector was fully characterized and calibrated with calculable undispersed as well as monochromatized synchrotron radiation. The obtained quantum efficiency and the response functions are in very good agreement with the corresponding Geant4 simulations. At the electron storage ring BESSY II the number of incident photons in the scattering experiments was measured with a photodiode that had been calibrated against a cryogenic radiometer, so that a direct comparison of scattering experiments with Monte Carlo simulations using Geant4 was possible. It was shown that Geant4 describes the photoeffect, including fluorescence as well as the Compton and Rayleigh scattering, with high accuracy, resulting in a deviation of typically less than 20%. Even polarization effects are widely covered by Geant4, and for Doppler broadening of Compton-scattered radiation the extension G4LECS can be included, but the fact that both features cannot be combined is a limitation. For most polarization-dependent simulations, good agreement with the experimental results was found, except for some orientations where Rayleigh scattering was overestimated in the simulation.

1. Introduction

Using a Monte Carlo simulation code such as Geant4 [1], the complete interaction processes of X-rays with matter can be simulated. The accuracy of electromagnetic processes within Geant4 has already been investigated by several authors [2,3], but mainly in comparison to other simulation codes, usually based on the same cross section. For a really quantitative validation, a direct comparison to absolute experimental data has to be accomplished, requiring a known incident photon flux and a calibrated detection system in a well-defined geometry. The photon flux of monochromatized synchrotron radiation that is available in a wide photon energy range at an electron storage ring like BESSY II can be determined by photodiodes, calibrated against a cryogenic radiometer [4]. Furthermore, the calculable undispersed synchrotron radiation of BESSY II can be used to calibrate and fully characterize an energy-dispersive detector [5]. In this paper, Geant4 simulations and absolute measurements of scattered and fluorescence radiation are compared for different materials, geometries, and polarization directions.

2. Instrumentation

The Physikalisch-Technische Bundesanstalt (PTB), Germany's national metrology institute, operates a laboratory at the electron storage ring BESSY II [6]. Monochromatized synchrotron radiation of high spectral purity is available at different beamlines in the PTB laboratory and at a wavelength shifter beamline in the photon energy range from the UV up to above 100 keV.

2.1. Radiation sources and beamlines

The X-ray range is covered by two beamlines: the four-crystal monochromator (FCM) beamline from 1.75 keV to 10 keV [7] and above 8 keV up to 120 keV, the BAMline, a 7 T wavelength shifter beamline [8]. At the BAMline, which is jointly operated by PTB and BAM (Bundesanstalt für Materialforschung und–prüfung, a double-crystal monochromator with high spectral resolving power

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and a double multilayer monochromator with efficient suppression of higher-order radiation can be used in series to combine both advantages. The higher-order contributions obtained are typically below 2×10^{-5}. Additionally, the BAMline can be used without monochromators to provide calculable undispersed synchrotron radiation for the calibration of energy-dispersive detectors [7,9].

2.2. Energy-dispersive CdTe detector

For the measurements described in this work, an energy-dispersive cadmium telluride (CdTe) detector was used, which has been the subject of Monte Carlo simulations for medical [10] and space-based X-ray detection applications [11,12]. The detector (XR-100T-CdTe, Amptek Inc., USA) [13] has a sensitive area of 3 mm × 3 mm and a CdTe thickness of 1 mm. This type of detector is especially convenient for angle-dependent experiments because of its compact size and Peltier cooling, in contrast to the LN_2 cooling of conventional germanium detectors. For the measurements in this work, the detector was used without applying the so-called "rise time discrimination" (RTD), resulting in an absolute photon-counting capability but with a pronounced tailing at higher photon energies. The detector was used with a collimator consisting of two apertures measuring 2 mm in diameter, and was attached to a goniometer, keeping the collimator at a fixed distance of 73.9 mm from the center of the foil under investigation. The detector was modeled in detail using the Monte Carlo simulation code Geant4. To achieve absolute measurement capabilities, the detector in turn had to be calibrated in undispersed synchrotron radiation and be fully characterized. The response function and the charge transport of cadmium telluride detectors have been the subject of several previous works on simulations using Geant4 [11,12], also in combination with a comparison to experimental results [14,15].

3. Monte Carlo simulations using Geant4 and scattering experiments

While transmittance and energy absorption in matter can be calculated with various programs, the angle and polarization dependence of electromagnetic radiation interacting with a scattering foil can only be fully characterized with Monte Carlo techniques that also cover scattering processes as well as fluorescence. The Monte Carlo simulation code Geant4, in combination with its low-energy extension, *G4LowEnergyPolarizedCompton*, *G4LowEnergyPolarizedRayleigh* and *G4LECS* [16], which also takes the Doppler broadening of scattered photons into account, was applied to the simulations of the detector and the experimental set-up. For data analysis and visualization of detector components (Fig. 1) the programs AIDA, JAS3 [17] and WIRED4 [18] were used. The scattering experiments were performed at the BAMline, and the power of the incident radiation was measured with a calibrated photodiode so that simulations could be compared directly to the experimental results, both normalized to the same number of incident photons.

3.1. Calibration of an energy-dispersive CdTe detector

Response functions of an energy-dispersive CdTe detector were measured with monochromatic radiation in the photon energy range from 2 keV up to 110 keV at the FCM beamline and the BAMline. A typical response function for 50 keV radiation is shown in Fig. 2, consisting of the photopeak, the Kα and Kβ escape peaks of Cd and Te as well as the Compton backscattering edge at

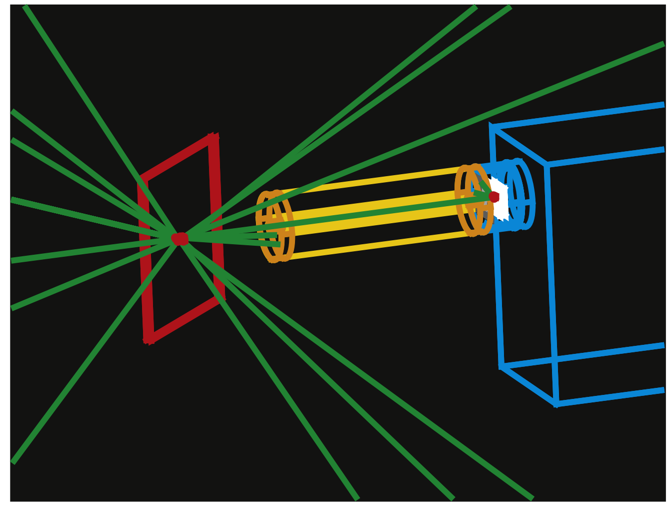

Fig. 1. The energy-dispersive CdTe detector with its collimator, including a scattering foil and the trajectories of the particles, modeled with Geant4 and visualized with the program WIRED4.

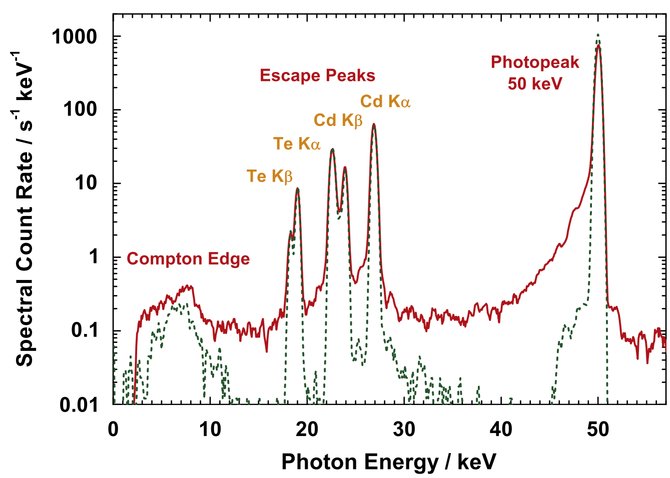

Fig. 2. Measured response function of a CdTe detector for monochromatic radiation of 50 keV (solid line) and simulation with Geant4 (dashed).

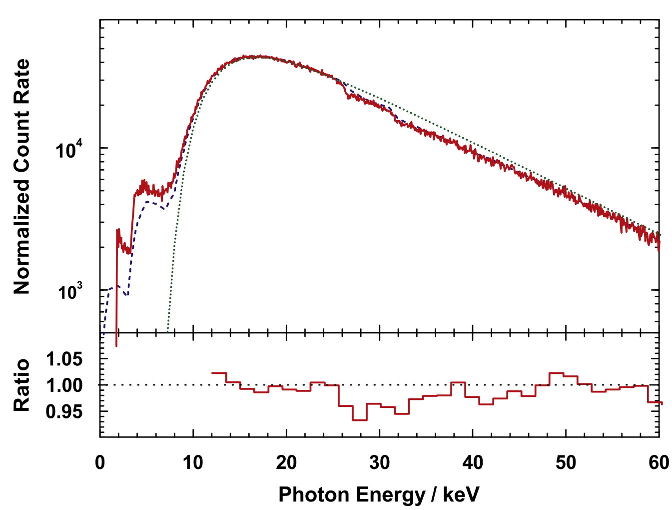

Fig. 3. Spectra of a CdTe detector exposed to undispersed synchrotron radiation behind a 0.21 mm Al filter: Geant4 simulation (dashed) and measurement at the BAMline (solid line), together with the calculated spectral distribution of the primary photons (dotted). The ratio of the measured and simulated spectra is shown in the lower part.