X-ray Rayleigh scattering model for GEANT4 standard electromagnetic package

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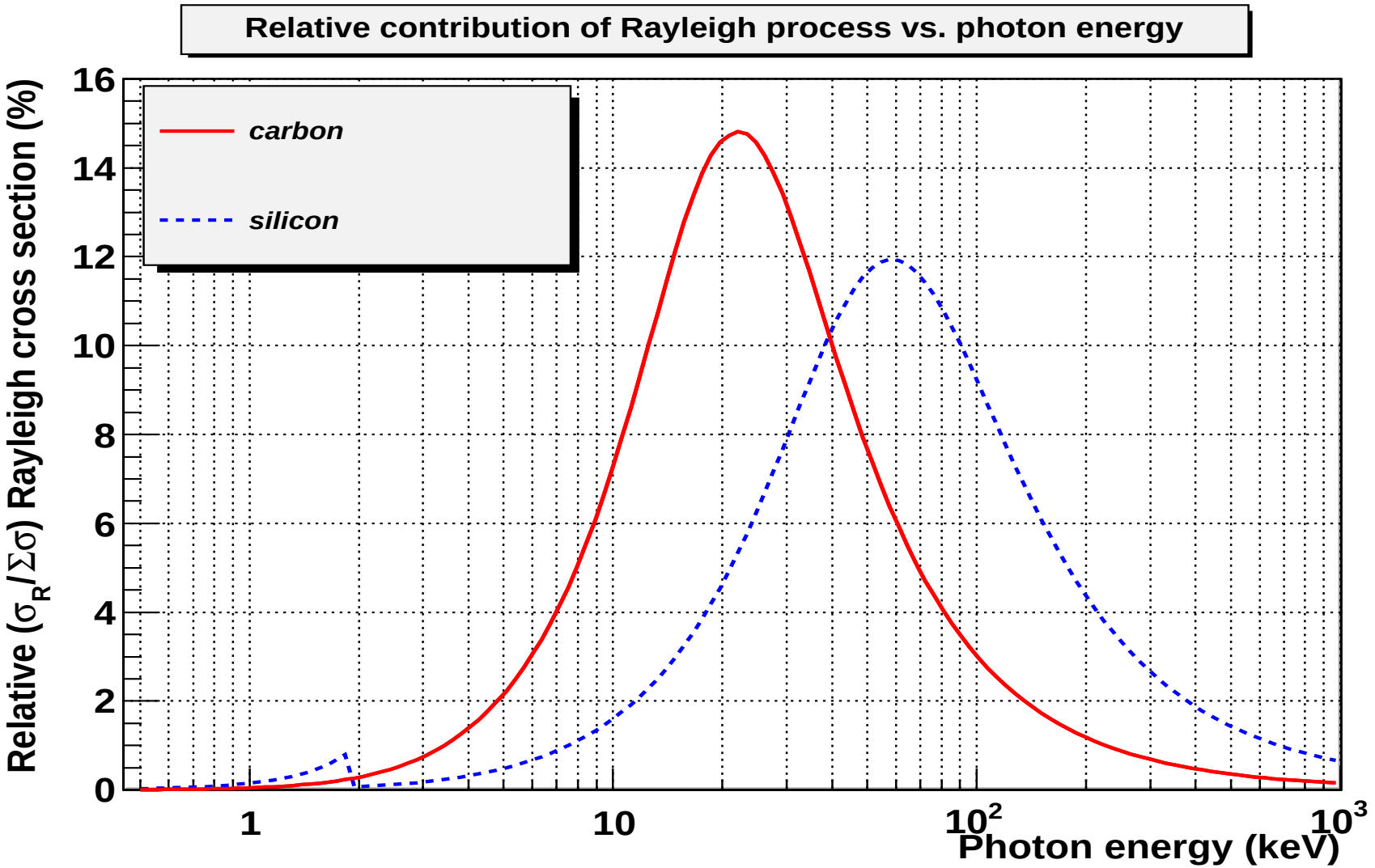
Abstract

A simplified version of X-ray Rayleigh scattering process is discussed. The model is in satisfactory agreement with experimental data. It can be recommended for an implementation for GEANT4 electromagnetic standard package.

1 Outline

1. Motivation.
2. GEANT4 simplified X-ray Rayleigh scattering model.
3. Comparison with experimental data for the Rayleigh scattering cross section and angular distribution.
4. Conclusions.

2 Motivation



3 GEANT4 simplified X-ray Rayleigh scattering model

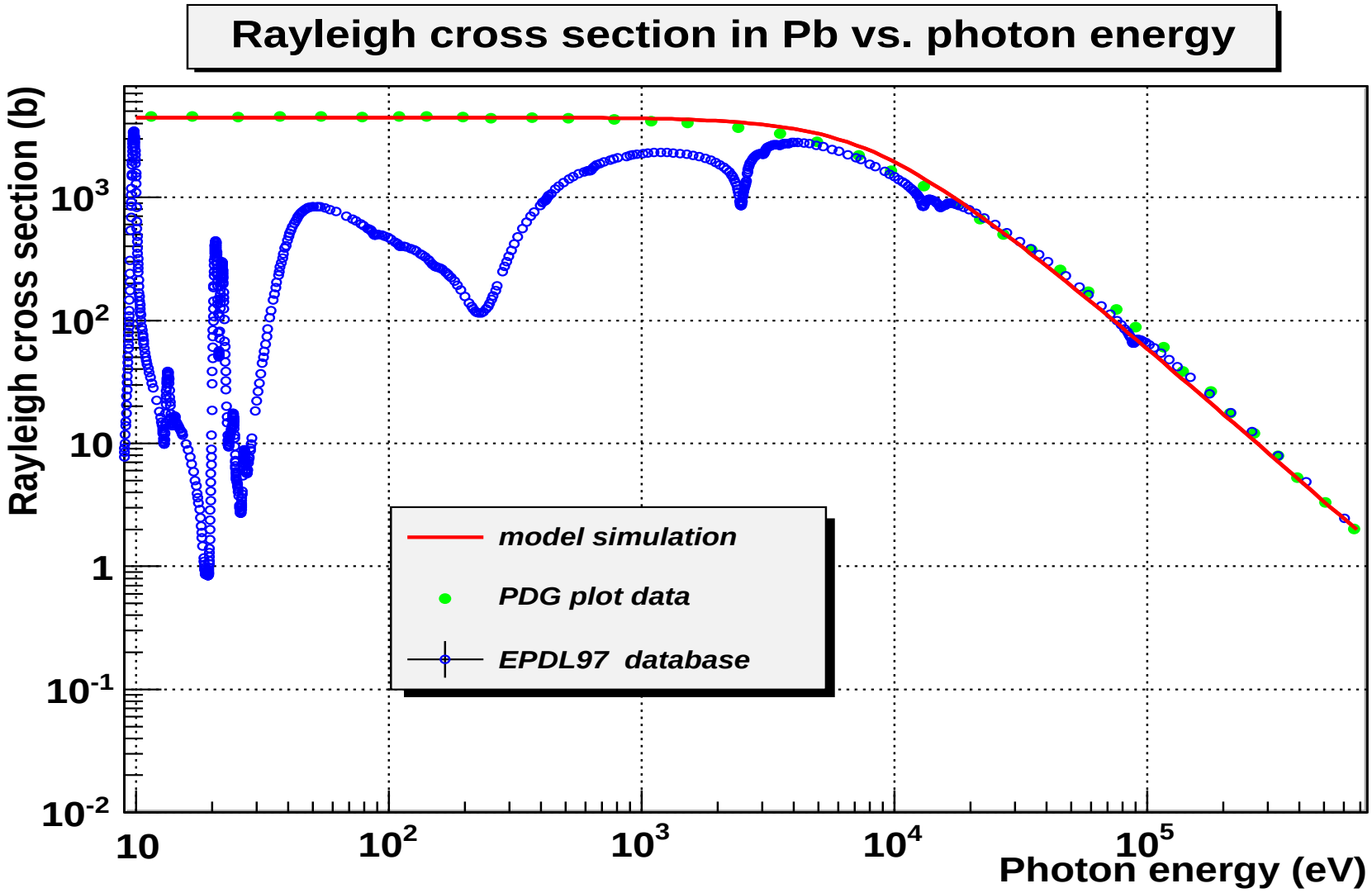
The atomic form-factor is written in the simple closed-form expression based on the calculation for the hydrogen-like atom with the atomic number, Z, dependence in the spirit of the Thomas-Fermi statistical approach. Then the Rayleigh scattering differential cross-section σ_R per unit solid angle Ω for X-ray photon with the energy E_γ reads:

$$\frac{d\,\sigma_R}{d\,\Omega} = \frac{r_e^2 Z^2 (1+\cos^2\theta)}{2[1+f(1-\cos\theta)]^4}, \quad f = b(Z)[r_o k]^{a(Z)}, \tag{1}$$

where $d\,\Omega = 2\pi d\,\cos\theta$, θ is the scattering angle, $k = E_\gamma/\hbar c$ is the photon wave vector, $\hbar$ is the Planck constant, c is the speed of light in vacuum, r_e is the classical radius of electron, and r_o is the Bohr radius.

$$\sigma_R(E_\gamma) = \frac{8}{3}\pi r_e^2 Z^2 \frac{f^2+(1+f)^2}{(1+2f)^3}. \tag{2}$$

The correction factors $a(Z)$ and $b(Z)$ are phenomenological functions of the target atomic number Z.


Rayleigh cross section in Pb vs. photon energy
Rayleigh cross section (b)
Photon energy (eV)
model simulation
PDG plot data
EPDL97 database

The simulation of the X-ray Rayleigh angular distribution is started with sampling of $\cos\theta^{'}$ according to the dipole distribution:

$$\cos\theta^{'} = A - \frac{1}{A}, \quad A = -\mathrm{sign}(d)\sqrt[3]{\frac{|d| + \sqrt{d^2+4}}{2}},$$

where $d = 4 - 8r$, and $r \in (0,1)$ is the uniform random value. Since

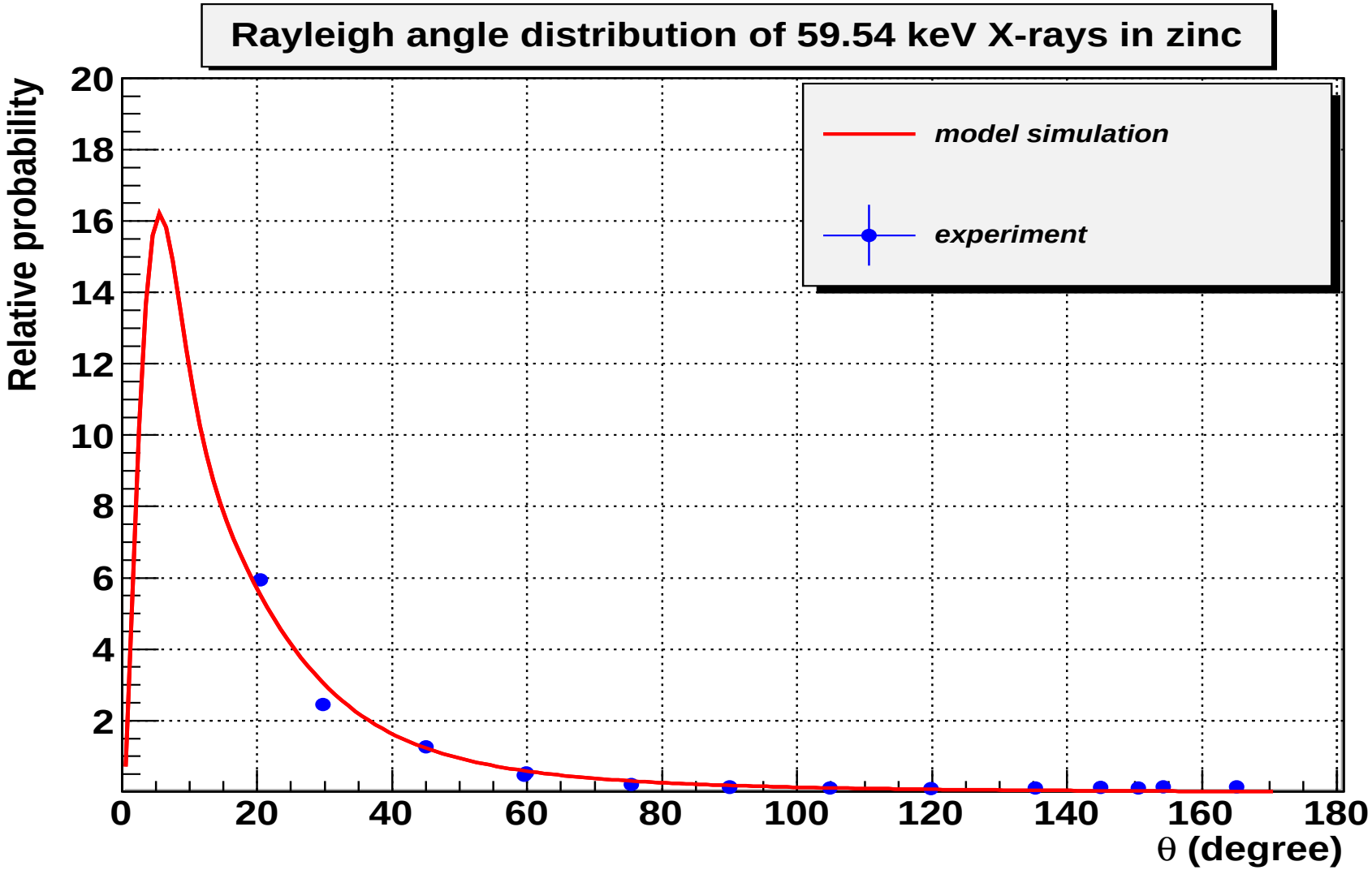
$$1 + f(1 - \cos\theta) \sim (1 - \beta^{'}\cos\theta), \quad \beta^{'} = \frac{f}{1+f},$$

we boost $\cos\theta^{'}$ with the velocity:

$$\beta = \frac{gf}{1+gf},$$

where the phenomenological factor $g \sim 3$ is defined from comparison of the model calculation with experimental data for the angular distribution of the X-ray Rayleigh scattering. The final cosine of the scattering angle reads:

$$\cos\theta = \frac{\cos\theta^{'} + \beta}{1 + \beta\cos\theta^{'}}.$$


Rayleigh angle distribution of 59.54 keV X-rays in zinc
model simulation
experiment
Relative probability
20
18
16
14
12
10
8
6
4
2
0
20
40
60
80
100
120
140
160
180
θ (degree)

4 Conclusions

1. Simplified X-ray Rayleigh scattering model was developed for the GEANT4 em standard package (class G4XrayRayleighModel).
2. The model is in satisfactory agreement with experimental data in the range where the relative X-ray Rayleigh scattering contribution is high.
3. The model is under verification and validation before it'll be included in GEANT4 physics lists.