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Validation of the Geant4 electromagnetic photon cross-sections for elements and compounds

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ABSTRACT

The Geant4 toolkit provides a wide set of alternative models to describe the electromagnetic interaction of photons with matter. The photon cross-sections that are used by the Geant4 electromagnetic models have been compared to external reference libraries (NIST, EPDL97, SANDIA) for several elements and compounds. The agreement of the Geant4 cross-section with the reference data has been quantified by means of statistical analysis. In particular, the cross-sections of all the Geant4 photon models are in statistical agreement with the NIST database, with the exception of Rayleigh scattering. A critical discussion is presented for those cases where a disagreement is found.

1. Introduction

Geant4 is an object-oriented (OO) toolkit for the simulation of the passage of particles through matter [1,2]. Geant4 offers an ample set of complementary and alternative physics models (electromagnetic, hadronic and optical) to describe the interaction of particles with matter over a wide range of energy, based either on theory, experimental data or parameterizations.

In the old versions of Geant4, up to version 9.2, multiple independent versions of the same electromagnetic (EM) processes were provided, which were included in different Geant4 Electromagnetic Packages: (1) Standard EM Package [3–6]; (2) LowEnergy EM Package [7–9], based on the Livermore data libraries [10–12]; (3) LowEnergy EM Package, based on Penelope analytical approach [13,14]. For example, three Geant4 different processes were available to describe photoelectric effect: `G4PhotoElectricEffect` (from the Standard EM package), `G4LowEnergyPhotoElectric` (from the LowEnergy-Livermore package) and `G4PenelopePhotoElectric` (LowEnergy Penelope package), respectively.

From version 9.3 of Geant4, a model approach has been implemented for the LowEnergy EM processes: in fact, all LowEnergy EM processes have been migrated to follow the same software interface which had been developed for the Standard EM package [3]. In the new approach there is only one process (e.g. `G4PhotoElectricEffect`) and multiple independent models that can be registered to the process, possibly in different energy ranges, e.g. `G4PEEffectModel` (Standard), `G4LivermorePhotoElectricModel` (Livermore) and `G4PenelopePhotoElectricModel` (Penelope). The usage of a unique design and of common interfaces makes much easier to carry on extensive comparisons and cross-checks of the models.

Indeed, the extensive validation of the physics models is fundamental in order to guarantee the accuracy and reliability of Geant4-based simulations. This paper describes the validation of the EM cross-sections for photons provided by the Geant4 models against public libraries based on experimental data. The work presented here is a follow-up which extends the comparison effort published in Ref. [15], since it takes into account experimental databases other than NIST (see Section 3) and has been performed on the most recent Geant4 version, including several updates and fixes.

Fig. 1 shows the 15 elements, spanning the range of atomic number Z from 1 to 82, that have been selected for validation. Also three compounds, namely Air, Water and NaI, have been taken into account in order to validate the algorithms that are used in the Geant4 models to calculate the cross-sections for composite materials starting from the building elements. The electromagnetic processes of photons include: photoelectric effect, Compton scattering, gamma conversion and Rayleigh scattering. The aim of the comparison is to test whether the cross-sections calculated by the Geant4 EM models agree with the data libraries all over the range of energies. The relevant class methods of the Geant4 models are used to retrieve the

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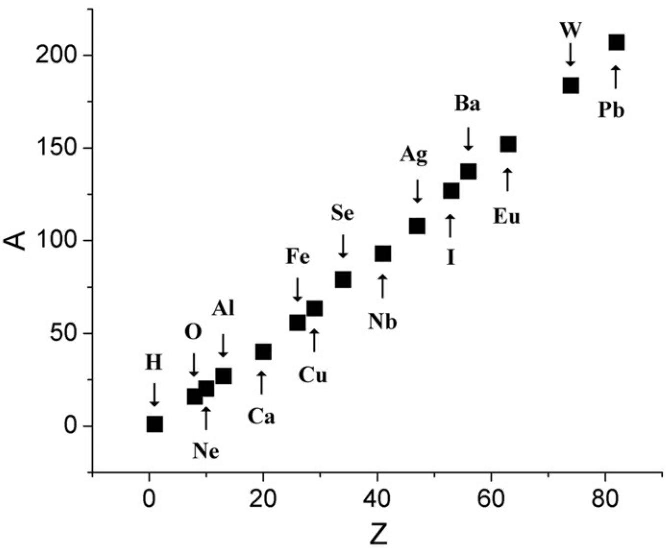

Fig. 1. Elements that are considered in this work for the cross-section validation.

cross-section for the materials listed above in the energy range from a few hundreds eV to 100 GeV. The cross-sections are hence compared against the data libraries.

Following the approach described in Ref. [15], quantitative comparisons have been performed by means of a Goodness-of-Fit Statistical Toolkit [16], specialized in the comparison of data distributions. Among the ones available in the Goodness-of-Fit Statistical Toolkit, the χ^2 test has been selected as statistical analysis tool, because it can take into account data uncertainties in the computation of the test statistics. The Goodness-of-Fit Statistical Toolkit returns the computed χ^2 value together with the number of degrees of freedom and the p-value of the comparison. P-values higher than the chosen confidence level $\alpha = 0.05$ lead to the acceptance of the null hypothesis, namely the statistical agreement between reference data and Geant4 models.

2. The Geant4 electromagnetic models

The three EM packages available in Geant4 employ different cross-section models and final state sampling algorithms. Details are available in the Geant4 Physics Reference Manual [17]. The models in the Standard package [3–6] use analytical approaches to describe the interactions in the energy range from 1 keV up to about 100 TeV, that are relevant for accelerator and cosmic-ray experiments. In general, the Standard models employ simpler transport algorithms and are more computationally efficient.

The Livermore models [7–9] in the LowEnergy package extend the range of accuracy for the simulation of EM interactions down to 250 eV. They include atomic and shell effects, that are commonly required for space science, medical and astroparticle physics applications. The Livermore approach exploits evaluated libraries (EPDL97 [10], EEDL [11] and EADL [12]) that provide data for the calculation of the cross-section and for the sampling of the final state for the interactions of photons, electrons and ions with matter.

The physics models originally developed for the PENELOPE (PENetration and Energy Loss of Positrons and Electrons) Monte Carlo code [13,14] have been implemented in Geant4 by re-engineering the code as a complete and independent set of models. The Penelope models are based on an approach which combines numerical databases with analytical cross-sections for the different interactions. They are applicable for energies ranging from a few hundreds eV to about 1 GeV. The Geant4-Penelope models are based on the version 2001 of PENELOPE.

The models in the LowEnergy EM package (Livermore and Penelope) have been migrated to Standard EM design starting from version Geant4 9.3. The new design of Geant4 allows a given physical process, which is described by a process class (inheriting from `G4VEmProcess` or `G4VEnergyLossProcess`), to be simulated according to several models, each one implemented in a model class (inheriting from `G4VEmModel`). For example, `G4ComptonScattering` is a physical process which can be described by several models, e.g. `G4KleinNishinaCompton` (from the Standard package), `G4LivermoreComptonModel` (Livermore) and `G4PenelopeComptonModel` (Penelope). Notice that a polarized version for the LowEnergy Livermore models is also available [18,19], which accounts for photon polarization in the sampling of the final state (e.g. `G4LivermorePolarized-ComptonModel`). Since cross-sections of polarized models are tabulated from EPDL97, as in the non-polarized Livermore models, they are not explicitly considered in this work. Models can be alternative and/or complementary in certain energy ranges. When no models are explicitly registered to a process, the model from the Standard EM package is taken as the default.

The migration of the former LowEnergy EM processes allowed also—as a side effect—to fix a few known bugs. In the original approach of the LowEnergy package, the process itself takes care of building the cross-section vs. energy table, which is loaded in memory and internally used for tracking. The table is made of 200 points with uniform logarithmic spacing in energy. Cross-section for energies not included in the grid are calculated by log–log interpolation on the existing table [15,17]. For the migrated models, a dedicated method is available which computes the cross-section (or the mean free path for compound materials) at any specific energy for the model applicability range. For some models—e.g. the Livermore ones—an interpolation is performed on an external cross-section database (instead of an analytical approach). However, the number of points in the energy grid of the original datasets is usually much larger than the one implemented in the Geant4 internal tables. For this reason, one can see some shell-structures in the mean free path (MFP) profile of photoelectric effect that are present in the migrated model but not visible in the original process, because of the insufficient grid spacing (see Fig. 2a). Fig. 2b shows a difference in migrated vs. non migrated Penelope Compton scattering models for very low energies. The change is due to a recent bug fix in the migrated Penelope model, which is giving now the same results as the original Penelope 2001 FORTRAN code. The bug is still present in the original `G4PenelopeCompton` process, which is not going to be maintained or updated.[1]

3. Identification of data libraries for validation

Since the aim of this work is the validation of the Geant4 EM photon models, the identification of suitable and reliable data libraries is a crucial issue. The following evaluated photon data libraries are taken into account:

- SANDIA [20]. The Sandia National Laboratories provide analytical approximations of the cross-sections for photo-electric absorption and Compton scattering of photons by atoms. The SANDIA representation is convenient for use in computer programs to evaluate these cross-sections

[1] Nevertheless, the bug is irrelevant for most practical applications, since it affects the Compton cross-sections only at very low energy (< 10 keV), where the photon interaction is largely dominated by photoelectric effect.

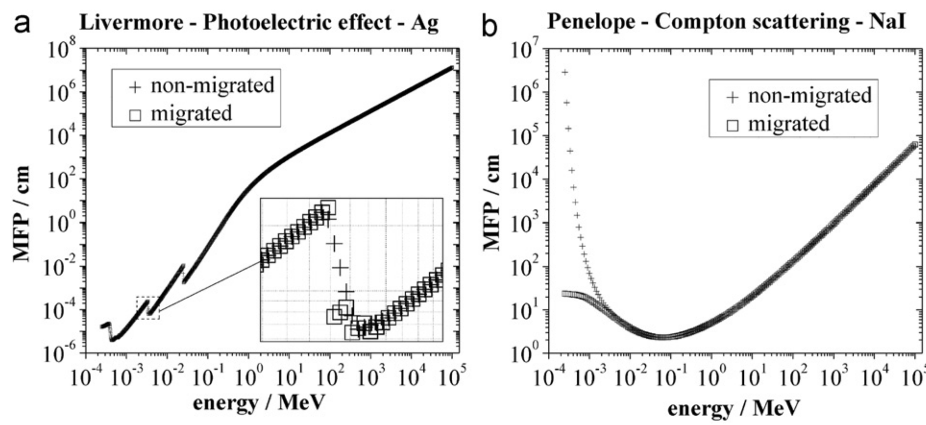

Fig. 2. Mean free path (MFP) for the original EM processes vs. the new migrated models. (a) Livermore photoelectric effect in Silver; (b) Penelope Compton scattering in NaI.

numerically. The results apply to atoms of atomic number between 1 and 100 and for photon energies $>10\,\text{keV}$. The library provides the relative root-mean-square uncertainty for photoelectric cross-sections for every element. Uncertainties are typically within 10%.

- Evaluated Photon Data Library (EPDL97) [10]. It has been developed by the Lawrence Livermore National Laboratory for use in photon transport calculations. The library includes photon interaction data for all elements with atomic number from $Z=1$ (hydrogen) to 100 (fermium) and provides cross-section data over the energy range from 1 eV to 100 GeV. The uncertainty quoted in the library documentation depends on energy, varying typically from 10% to 20% at low energy ($<1\,\text{keV}$) to less than 5% for energies above 1 keV. Nevertheless, uncertainty can be up to a factor of 10 for solids in the energy range below 1 keV. Furthermore, uncertainties are typically larger in proximity of the edge energies of atomic shells.
  The EPDL97 cross-section data are used by the Geant4 Livermore models, which encompass: photoelectric effect, Rayleigh and Compton scattering, and gamma conversion. Therefore, the comparison of the cross-sections calculated by the Livermore models with the EPDL97 database should be regarded as an internal cross-check of the models, rather than as a real validation. The same applies to the Penelope photoelectric and gamma conversion models, although they use an older version of the EPDL library (EPDL89) [21].
- NIST [22]. The National Institute of Standards and Technologies (NIST) maintains the XCOM library. It includes a computer code and a database which can be used to compute photon cross-sections for Compton and Rayleigh scattering, photoelectric absorption and gamma conversion, in any element, compound or mixture, at energies from 1 keV to 100 GeV. The quoted uncertainty is about 1% at high energy and away from the atomic edges, while it can be substantially larger, up to 10–20%, for energies close to the atomic absorption edges.

The uncertainties reported in the documentation of the libraries are taken into account for the evaluation of the χ^2 statistics for the comparison with the Geant4 models. Notice that the Geant4 models are able to deliver a cross-section value (by direct computation from an analytical model, or by interpolation from an external database), without the need to run a real Monte Carlo simulation (namely, no random numbers are involved). Therefore, cross-sections derived by the Geant4 models are free from statistical errors.

As shown in Fig. 3, the photoelectric cross-sections reported by the three databases are not mutually consistent close to the absorption edge energies. Furthermore, the Compton cross-sections from the SANDIA library are substantially higher than the other two databases at low energy ($<1\,\text{keV}$). The cross-section data of EPDL97 for gamma conversion are very close to NIST, because the two datasets are based on the same data source [23]. Rayleigh scattering cross-sections reported by the EPDL97 library are not consistent with NIST database for energies close to the absorption edges (see also discussion in Section 4.4).

4. Validation of the Geant4 photon processes with respect to the experimental data libraries

4.1. Photoelectric effect

The cross-section in the Standard package for the photoelectric effect is computed from the parameterized formula developed by SANDIA [20], which is made of fourth-degree polynomials in reciprocal powers of the photon energy. The Livermore and Penelope cross-sections are tabulated according to EPDL97 and EPDL89, respectively.

The sources of EPDL97 data include data calculated using Scofield's subshell cross-sections by a phase-shift calculation for a central potential and a Hartree–Slater atomic model [24] from the edge energy up to 1 MeV and Hubbell's total photoelectric cross-sections [25–27] from 1 keV to 100 GeV. These two sets of data have been combined to compute the total cross-section: from the edge to 1 MeV, the cross-section, defined as the sum of the subshells, is based on Scofield's data. From 1 MeV to 100 GeV, the cross-section is based on Hubbell's data. NIST employs the same data obtained by Scofield, extended up to 1.5 MeV. At higher energies, where the photoelectric cross-section is relatively small, a semi-empirical formula from Ref. [28] connects the Scofield's values to the asymptotic high energy limit calculated by Pratt [29].

As shown in Fig. 4, the deviation of the Geant4 Standard model with respect to NIST and EPDL97 is within 10%. The two Geant4 LowEnergy models exhibit a very close agreement with these libraries, as it is expected, because both NIST and EPDL97 use the same data source below 1 MeV. The agreement of the Livermore and Penelope photoelectric models with the SANDIA database is within 10%. Of course, no deviation between the Standard EM package and SANDIA is observed, since cross-sections are computed according to the same parameterization.

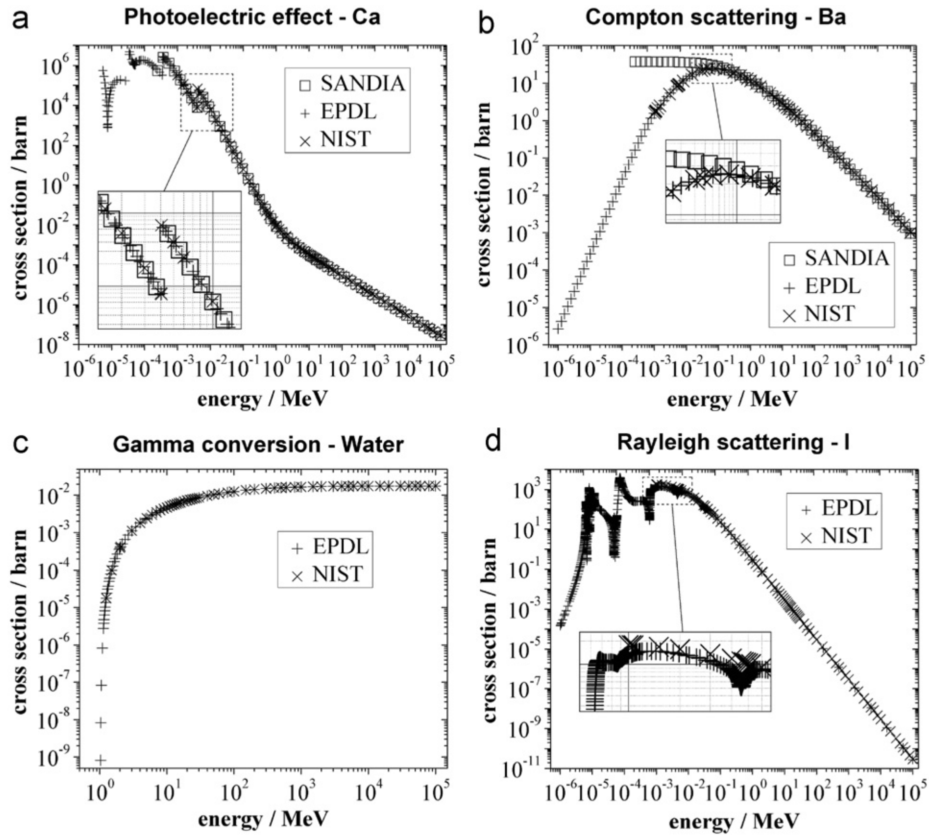

Fig. 3. Comparison of cross-sections for the three databases: (a) photoelectric effect for Ca; (b) Compton scattering for Ba; (c) gamma conversion for Water; (d) Rayleigh scattering for I.

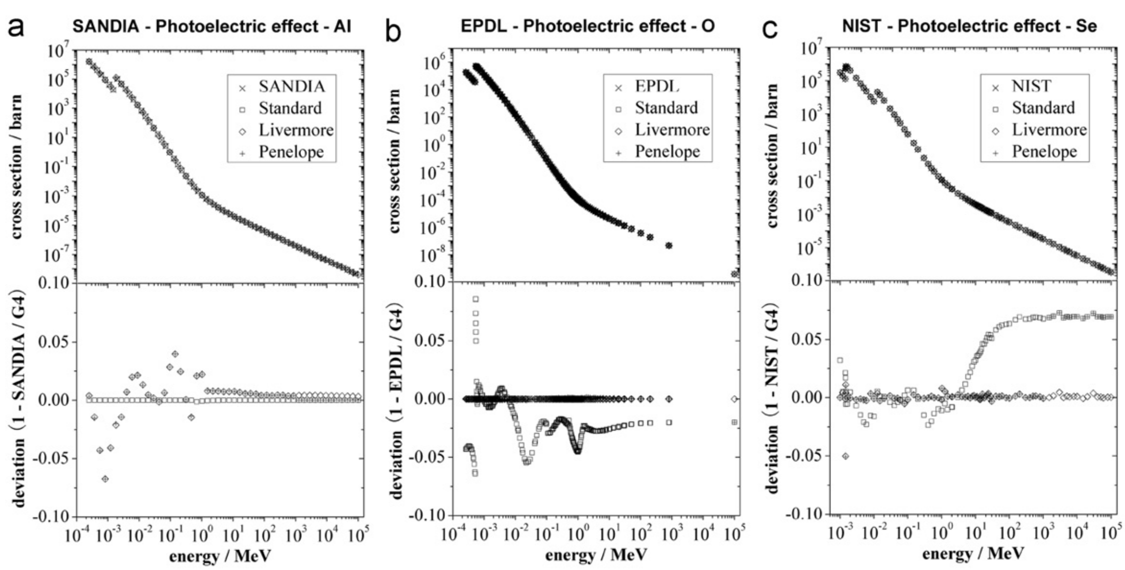

Fig. 4. Photoelectric effect cross-sections for the three EM models compared to data libraries. (a) SANDIA for Al; (b) EPDL97 for O; (c) NIST for Se.

Fig. 5 displays the results of the χ^2 test for the photoelectric effect: the *p*-values are plotted as a function of the atomic number *Z* of the selected elements. The *p*-values of the three Geant4 packages with respect to the NIST data are higher than the acceptance level for all *Z*. Similar results are found for the three compounds. This leads to the conclusion that there is no difference between NIST and Geant4 cross-sections.

4.2. Compton scattering

The cross-section of the Standard package model (`G4KleinNishinaCompton`) is derived from an empirical parameterized approach [23,30], whose accuracy is estimated to be 10% between 10 and 20 keV, and 5–6% above 20 keV [17]. The cross-sections of the Geant4 Livermore model are tabulated according to the EPDL97

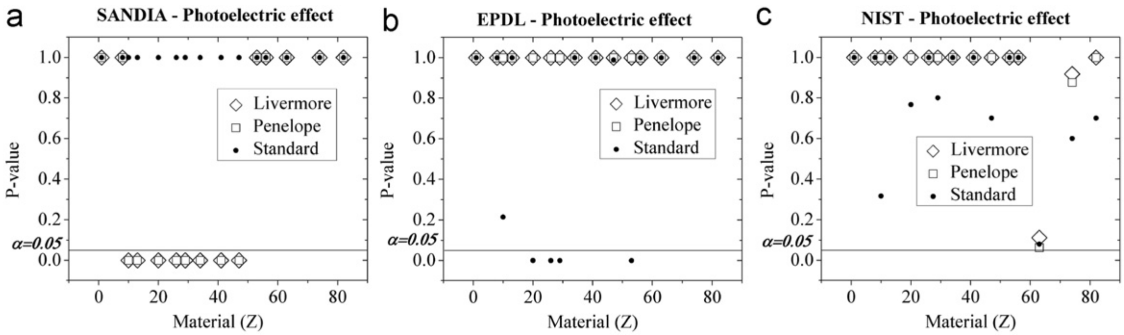

Fig. 5. χ^2 test results of the three EM models against data libraries for photoelectric cross-sections. (a) SANDIA; (b) EPDL97; (c) NIST.

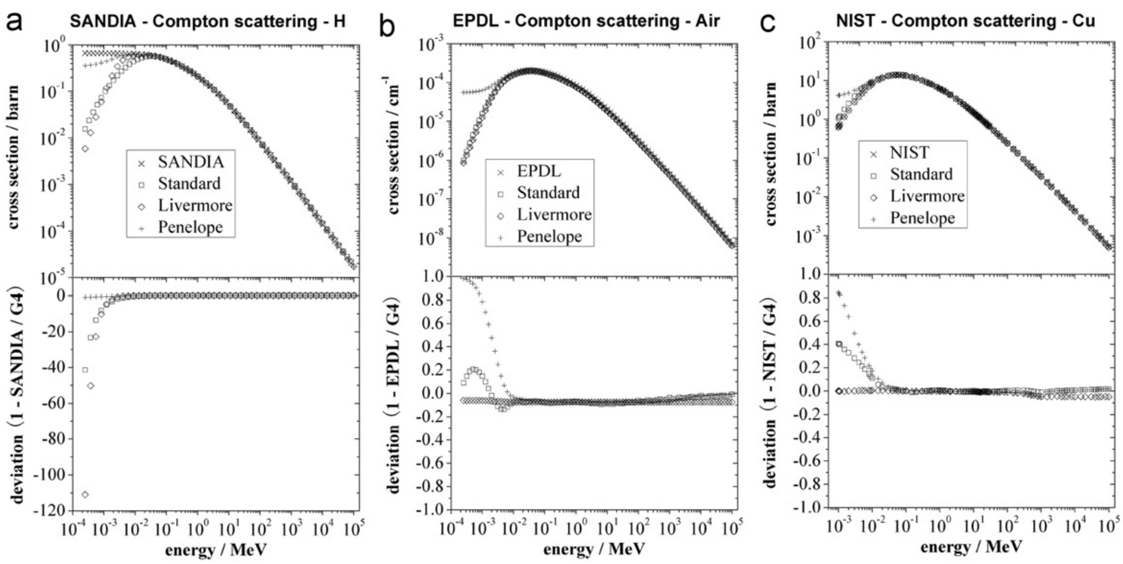

Fig. 6. Compton scattering cross-sections for the three EM models compared to data libraries. (a) SANDIA for H; (b) EPDL97 for Air; (c) NIST for Cu.

library, while for the Penelope model they are determined from an analytical parameterization [31]. The Penelope parameterization uses the Klein–Nishina formula [32] for energy >5 MeV. Below 5 MeV, a more accurate function is considered, which takes into account atomic binding effects and Doppler broadening.

The Klein–Nishina formula [32] is used in SANDIA to evaluate the Compton scattering cross-section. In the same way as NIST, the EPDL97 data are obtained from the combination of the Klein–Nishina formula and of the Hubbell scattering functions [33–35], which neglect atomic binding effects.

As shown in Fig. 6, the Penelope cross-section is higher than the other models in the region <10 keV and has a behaviour closer to the SANDIA library than to EPDL97 and NIST. For energy >100 keV, the agreement of the three EM models with the three data libraries is always within 10%.

Fig. 7 shows the statistical analysis results of three Geant4 Compton scattering models against data libraries. All Geant4 EM packages are in statistical agreement with the three datasets, except the Penelope Compton model which is in disagreement with the EPDL97 library for some materials. This is due to the different behaviour in the low energy region and to the bias observed in the high-energy region (>100 MeV).

4.3. Gamma conversion

The cross-section of the Standard gamma conversion model is parameterized according to the data of Hubbell et al. [23]. The accuracy of the parameterization is estimated to be 5% with a mean value of 2.2%. Above 100 GeV the cross-section is constant. Below 1.5 MeV, the extrapolation scheme described in Ref. [17] is used. The Livermore and Penelope cross-sections are taken from the EPDL97 and EPDL89 libraries, respectively.

While gamma conversion cross-sections are not available in the SANDIA library, EPDL97 and NIST use the same data source [23] and provide separately the cross-sections of pair production and triplet production. Since all the Geant4 gamma conversion models are meant to describe both singlet and triplet production, the cross-sections calculated by them are compared to the sum of the singlet and triplet cross-sections from EPDL97 and NIST. As expected, the Livermore and Penelope models exhibit a very close agreement with EPDL97 and NIST. On the other hand, since the cross-section close to threshold varies very rapidly with energy, the extrapolation algorithm used in the Standard package results to be less accurate. In particular, the deviation of the `G4BetheHeitlerModel` (Standard package) with respect to the data libraries is more than 10% in the energy range between 1.022 (threshold) and 1.5 MeV, as displayed in Fig. 8. Anyway, this is irrelevant for most practical applications, since for photon energy below 1.5 MeV the gamma conversion cross-section is largely negligible with respect to photoelectric effect and Compton scattering. The results of the statistical analysis displayed in Fig. 9 show that the three Geant4 EM packages are in agreement with the data libraries.

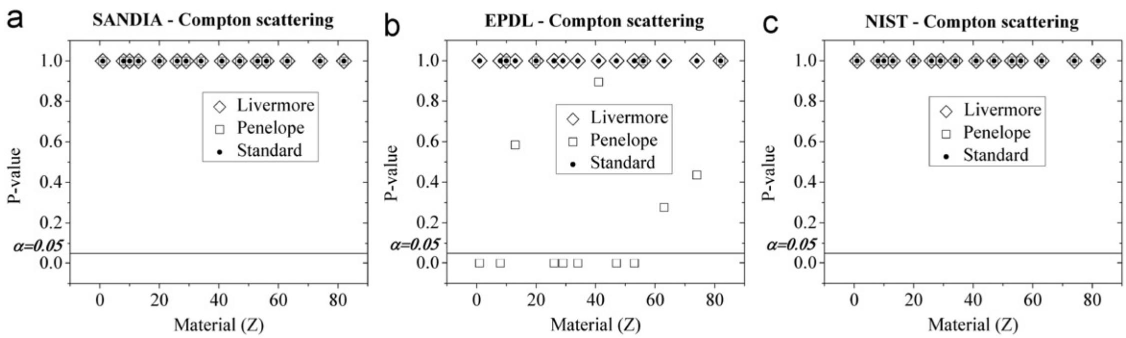

Fig. 7. χ^2 test results of the three EM models against data libraries for Compton cross-sections. (a) SANDIA; (b) EPDL97; (c) NIST.

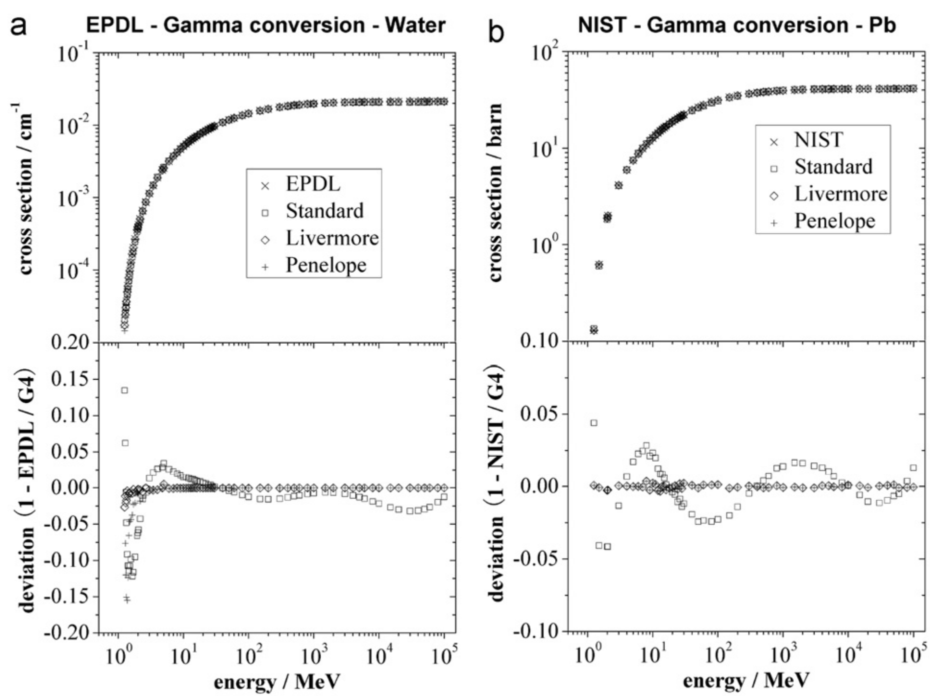

Fig. 8. Gamma conversion cross-sections for the three EM models compared to data libraries. (a) EPDL97 for Water; (b) NIST for Pb.

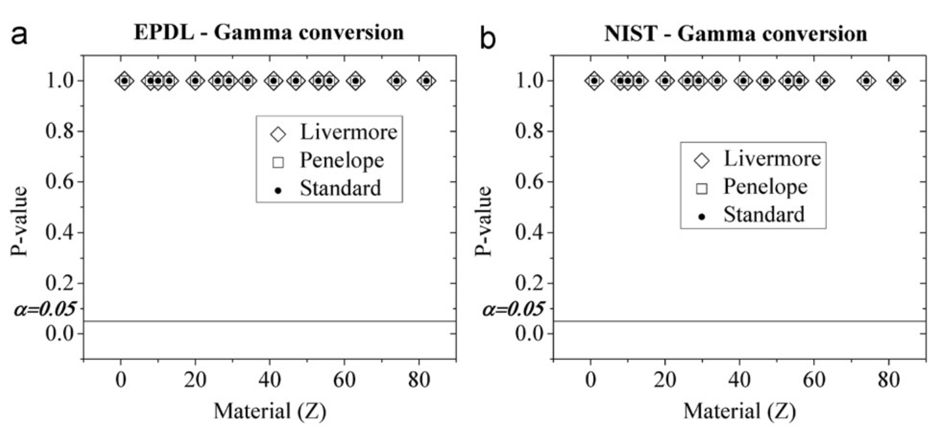

Fig. 9. χ^2 test results of the three EM models against data libraries for gamma conversion cross-sections. (a) EPDL97; (b) NIST.

4.4. *Rayleigh scattering*

The Standard EM package of Geant4 does not contain its own model to describe the Rayleigh scattering. Therefore, only two alternative models are available in Geant4 rather than three: Livermore (default) and Penelope. While the cross-section of `G4LivermoreRayleighModel` is based on the EPDL97 database, the cross-section of the Penelope model is determined by numerical integration from an analytical parameterization [36].

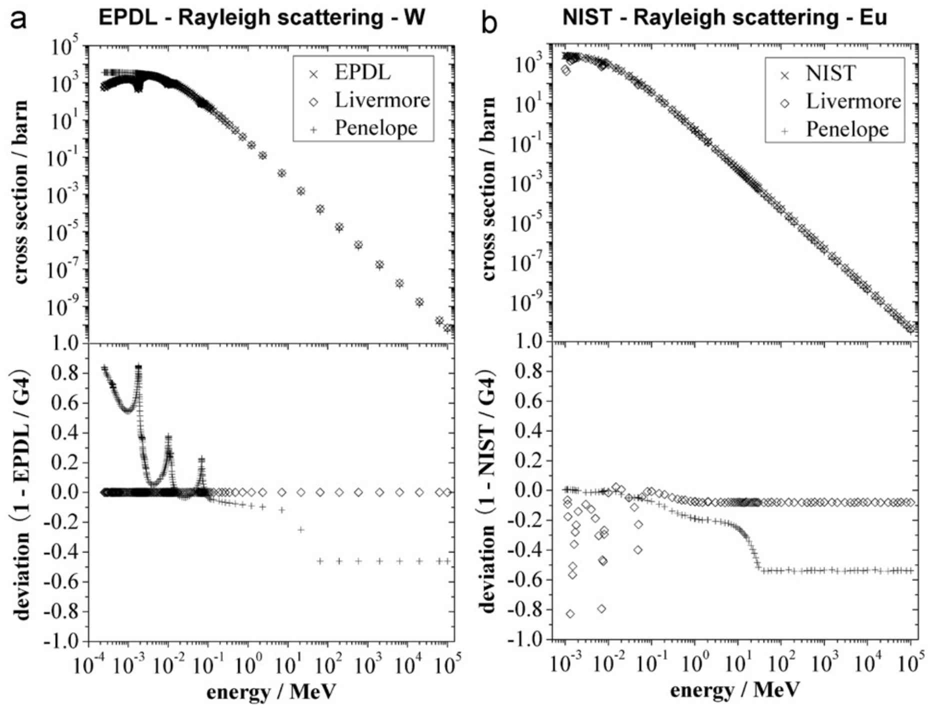

Fig. 10. Rayleigh scattering cross-sections for the Geant4 EM models compared to data libraries. (a) EPDL97 for W; (b) NIST for Eu.

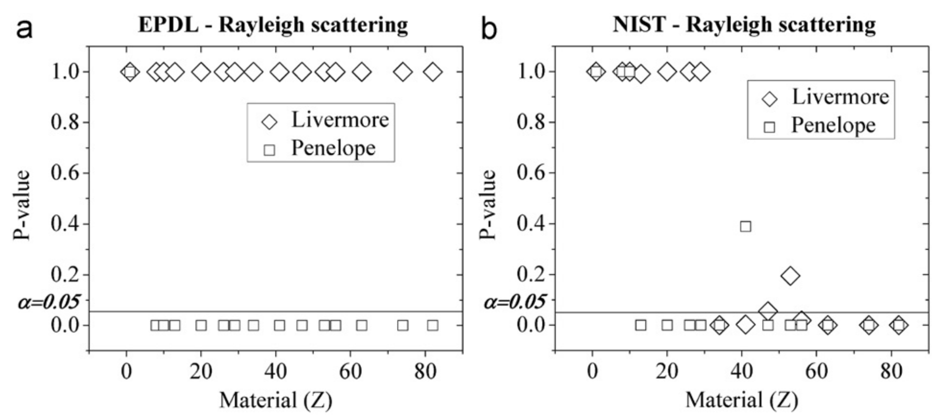

Fig. 11. χ^2 test results of the Geant4 EM models against data libraries for Rayleigh scattering cross-sections. (a) EPDL97; (b) NIST.

The EPDL97 database for the Rayleigh scattering cross-section is a combination of the Thomson formula, the Hubbell non-relativistic form factor [33–35], and the anomalous scattering factors [37], which were numerically integrated. The Rayleigh scattering cross-sections in NIST are calculated from the Thomson formula and the relativistic Hartree–Fock atomic form factor [34]. Data for Rayleigh scattering are not available in the SANDIA library.

As visible in Fig. 10, the Livermore package (and then the EPDL97 database) is largely different from the NIST database for energies close to the atomic absorption edges. This is due to the fact that the latter uses different form factors and neglects the anomalous scattering functions.

The Penelope Rayleigh cross-section is not consistent with neither EPDL97 nor the NIST datasets. In fact, in the version 2001 of the original PENELOPE code, which is the one implemented in Geant4-Penelope, the cross-section is calculated according to a parameterization [36] which does not account for the atomic form factors and for the anomalous scattering functions. Therefore, `G4PenelopeRayleighModel` is unable to properly reproduce the oscillating structures of cross-section vs. energy reported in the EPDL97 database. Furthermore, the underestimation of the Rayleigh cross-section by the Penelope model above a few MeV is not relevant for most applications, since the absolute cross-section is $<10^{-5}$ barn. Notice that in the most recent version of the PENELOPE code (namely, Penelope2008) the Rayleigh cross-section is derived from the EPDL97 database. It is actually planned to upgrade in the near future the Penelope models implemented in Geant4 from the PENELOPE version 2001 to the version 2008. Fig. 11 shows the results of the χ^2 test.

5. Conclusions

The Geant4 toolkit includes a wide set of physics models, specialized for particle type, energy range and detector applications, and is being currently used in many physics domains for simulations of numerous interaction types. A systematic validation of the cross-sections provided by the Geant4 electromagnetic photon models has been performed comparing the three EM packages available in Geant4 against the SANDIA, EPDL97 and NIST data libraries for several elements and compounds.

Geant4 includes a set of electromagnetic models (the Livermore package) that are actually based upon the EPDL97 data libraries; therefore, the agreement of the G4Livermore models with the EPDL97 data is simply a software verification. In fact, the deviation between the EPDL97 library and the Geant4-Livermore cross-sections is below 0.2% for all models and all materials. This is consistent with the accuracy of the interpolation algorithms.

It is shown that all the Geant4 photon models are in statistical agreement with the NIST datasets, with the exception of Rayleigh scattering. The disagreement for `G4LivermoreRayleighModel` is due to the fact that the NIST and the EPDL97 libraries are mutually inconsistent at low energy.

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