WEB OF SCIENTIST: INTERNATIONAL SCIENTIFIC RESEARCH JOURNAL
ISSN: 2776-0979, Volume 5, Issue 3, March - 2024

ATOMIC RELAXATION SIMULATION IN GEANT4: EXPANDING THE POSSIBILITIES

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Abstract
The low-energy electromagnetic package Geant4 includes a component for modeling atomic relaxation of elements with atomic numbers ranging from 6 to 100. This process is initiated by creating a vacancy in the filled atomic shell as a result of the interaction between the incident particle and the target material atom. X-ray fluorescence and emission of Auger electrons are the results of the relaxation cascade. The integration of an atomic relaxation model within Geant4 significantly broadens the utility of the modeling toolkit, particularly in experimental scenarios linked to the subsequent examination of material properties via characteristic X-ray emission or Auger emission. This enhancement holds relevance for precision modeling applications, including microdosimetry, and the design and optimization of detectors rooted in nanotechnologies. The article delves into key aspects of the software development process, software architecture and design, providing comprehensive details about the implementation of the physical model.

Keywords: Monte Carlo, Geant4, Modeling, X-ray Fluorescence, Auger Electron.

Introduction:

Accurate modeling of electromagnetic interactions between particles and matter is a crucial requirement in various experimental fields. The Geant4 toolkit [1] encompasses numerous packages tailored for this purpose, specialized for different types of particles, energy ranges, or employing various approaches to physical modeling. Among them, the low-energy electromagnetic package of Geant4 includes models of physical processes for electrons, photons, charged hadrons, and ions, extending to energies below 1 keV. It is characterized by a detailed description of particle interactions, taking into account the atomic structure of matter, and a

thoughtful design based on object-oriented technology supported by a rigorous software development process. The modeling of atomic relaxation falls within the scope of this package; a specific component simulates effects related to physical processes that induce the ionization of atoms: X-ray fluorescence and Auger electron emission.

Development of the atomic relaxation reactions in Geant4 aligns with the requirements of various experimental applications. Motivations for modeling this physical domain can be categorized into two main groups: experimental studies based on specific features of atomic relaxation, i.e., X-ray fluorescence and Auger electron emission as indicators of material composition through measured spectra. Additionally, in the case of microdosimetry or other precise investigations of detector characteristics, detailed descriptions of secondary effects arising from ionization of atoms during primary interactions are required. Recent projects involving the development of particle detectors based on nanotechnologies have spurred further interest in modeling low-energy electrons for the design and optimization of detectors.

Software Implementation Features: The low-energy electromagnetic package of Geant4 manages the physical processes of photons (photoelectric effect, Compton scattering, Rayleigh scattering, and pair production), electrons (ionization and bremsstrahlung), and positrons (annihilation, along with the same processes as electrons), as well as the process of ionization for hadrons and ions. Two different physical approaches are employed for electron and photon processes: models based on evaluated data libraries and analytical models initially developed for Monte Carlo codes. Positrons are only handled using analytical models. Various models are employed for hadronic and ionization processes, depending on the energy and charge of the incident particle [2].

The code handles the creation of secondary particles (photons and electrons) that arise from transitions between bound atomic states. Transitions from the continuum to bound states are not considered. To complete the atomic relaxation process while maintaining energy balance, the energy equivalent to transitions from the continuum to bound states is calculated. This is done as the difference between the binding energy of the ejected primary electron and the sum of the energies of all secondary relaxation products. It is assumed that this energy is deposited locally where the primary process occurs.

For the radiative transition between subshells i and j, the energy E_γ of the emitted photon is calculated as the difference between the binding energies E_i and E_j of the two subshells:

WEB OF SCIENTIST: INTERNATIONAL SCIENTIFIC RESEARCH JOURNAL
ISSN: 2776-0979, Volume 5, Issue 3, March - 2024

$$E_\gamma = E_i - E_j \quad (1)$$

On Figure 1, the distribution of X-ray energy generated by transitions originating from vacancies in the K, L, M, N, and O shells is illustrated.

For a non-radiative transition between subshells i and j, where an electron is emitted from subshell h, the energy E_e of the emitted electron is calculated as follows:

$$E_e = E_j - (E_h + E_i) \quad (2)$$

Where E_j, E_h, and E_i are the binding energies of the respective subshells involved. The energy distributions of electrons from Auger and Coster-Kronig transitions generated by the initial vacancy in the K, L, M, N, and O shells are shown in Figure 2.

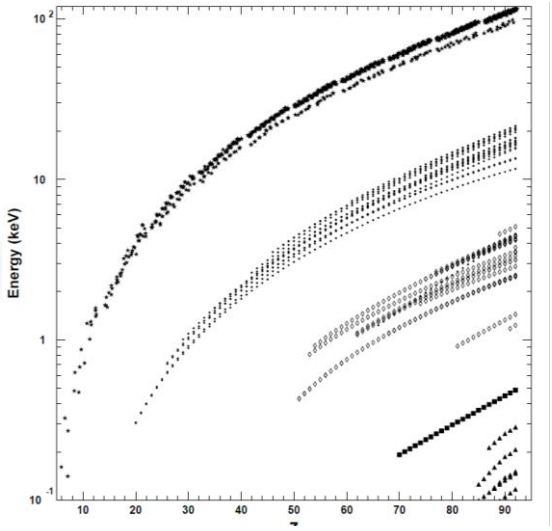

Fig. 1. Photon energy of fluorescence generated by atomic relaxation in Geant4 as a function of atomic number Z; symbols represent transitions originating from vacancies in the K-shell (stars), L-shell (dots), M-shell (diamonds), N-shell (squares), and O-shell (triangles); for better readability, transitions from K, L, and M shells with a probability > 10^{-3}, N-shell transitions with a probability > $5 \cdot 10^{-4}$, and O-shell transitions with a probability > 10^{-6} are shown on the graph.

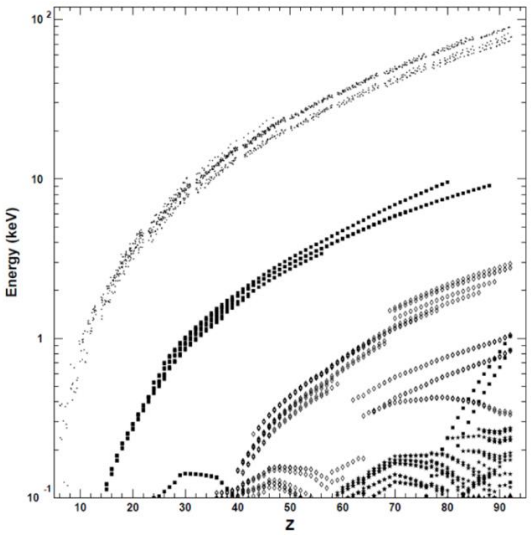

Fig. 2. Electron energy generated by atomic relaxation in Geant4 as a function of atomic number Z; symbols represent Auger and Coster-Kronig transitions originating from vacancies in the K-shell (dots), L-shell (squares), M-shell (diamonds), N-shell (stars), and O-shell (triangles); for better readability, K-shell transitions with a probability > 10^{-3}, and L, M, N, and O-shell transitions with a probability > 0.1 are shown on the graph.

Conclusion:

A component for modeling atomic relaxation of elements with atomic numbers ranging from 6 to 100 has been developed and integrated into the low-energy electromagnetic package of Geant4. It simulates both radiative and non-radiative atomic transitions that occur due to the formation of a vacancy in the atomic shell, producing X-ray fluorescence and Auger electrons as secondary particles. The presence of this component in Geant4 expands the functionality of the toolkit for precise modeling, particularly relevant for experimental applications sensitive to the accurate spatial distribution of energy deposited in detectors or the generation of low-energy secondary particles. This tool also allows the use of Geant4 as a simulation

system for physical studies related to the emission of characteristic X-rays and Auger electrons from materials. The development and implementation of Geant4 Atomic Relaxation have reached a mature stage, with current efforts focused on the experimental validation of the software [3,4].

Literature:

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