LATEST GEANT4 DEVELOPMENTS FOR PIXE APPLICATIONS

S. Bakr[1], D. Cohen[2], R. Siegele[2], S. Incerti[3,4], V. Ivanchenko[5,6], A. Mantero[7], A. Rosenfeld[1], S. Guatelli[1,8]

[1] CMRP, University of Wollongong, Wollongong, NSW, Australia sb759@uowmail.edu.au
[2] Australian Nuclear Science and Technology Organization, Lucas Heights, NSW, Australia
[3] CNRS/IN2P3, Centre d'Etudes Nucléaires de Bordeaux-Gradignan, Bordeaux, France
[4] Université de Bordeaux, Centre d'Etudes Nucléaires de Bordeaux-Gradignan, Bordeaux, France
[5] Geant4 Associates International Ltd
[6] Tomsk State University, Russian Federation
[7] SWHARD s.r.l.
[8] Illawarra Health and Medical Research Institute, University of Wollongong, Wollongong, NSW, Australia

Introduction: In Geant4, atomic relaxation simulation is articulated through two stages:

1) The creation of a vacancy by a primary process e.g. photoelectric effect, Compton scattering and ionisation. For the ionization process an additional particle induced X-ray emission (PIXE) cross section is used.

2) The relaxation cascade is triggered, starting from the vacancy created by the primary process. Fluorescence X-ray or Auger electrons and Coster Kronig transitions are generated through radiative and non-radiative transitions, based on the respective transition probabilities and tracked in the simulation.

The goal of this project is to improve the set of shell cross sections for PIXE, based on the state of the art recommendations documented in [1]. In particular the cross section of protons and α particles we propose are based on [2], [3], providing the excitation of the K, L and M shells.

The novel shell cross sections, called ANSTO ECPSSR, will have important implications in Nano-medicine where high atomic number nanoparticles (NPs) are internalized in cancerous cells. McMahon et al demonstrated that Auger electrons play a crucial role in the deposition of energy close the NP [4]. The accuracy of the Auger electron and Coster-Kronig transition are strongly connected to the precision of the X-ray fluorescence modelling as its yield is 1 minus the fluorescence yield ω. Besides X-rays deriving from K, L and M shells can deposit energy in the cell as well therefore an accurate prediction of Auger electrons and Coster-Kronig transitions and fluorescence X-rays, together with specialized models for nanoscales such as the Geant4-DNA, are crucial to characterise this novel radiotherapy technique.

Methods: ANSTO ECPSSR shell cross sections have been included in the G4EMLOW6.50 library and can be selected in a Geant4 user application by means of interactive commands.

In the first part of the project, the ANSTO ECPSSR cross sections have been compared directly to the alternative data sets already available in Geant4 to quantify the agreement of the different approaches. In the second part of the project, the X-ray emission generated by using the novel ANSTO ECPSSR cross sections has been compared to the other available approaches.

The default atomic de-excitation library of Geant4, based on the EADL, has been used to calculate the emission rates of the fluorescence X-ray, once the vacancy has been generated. The fluorescence X-rays have been counted once they are generated in the target.

Results: The ionisation cross sections: for K shell, an agreement within 10% was observed for protons energies below 2.5 MeV for low Z sample materials. However, larger differences (~25%) are observed for high Z sample materials for proton energies below 1.5 MeV. Differences up to ~10% are observed for incident α particles of all considered energies, for all sample materials. For L sub-shells, the differences are less than 5% for the entire proton energy range for low Z targets. For high Z (e. g. Au) materials differences are up to ~10% in the range 2 – 5.2 MeV for protons and α particles. For M sub-shells, the differences are less than 10% for the entire proton energy range. Differences up to ~25% and ~15% have been found for α particles with energy (0.2 – 3 MeV) and (3 – 10 MeV), respectively.

The number of X-ray emitted per initial particle calculated via ECPSSR Form Factor cross section is higher than the one calculated with ANSTO ECPSSR.

Conclusion: ANSTO ECPSSR cross sections for proton and α particles have been integrated in Geant4 for PIXE simulation. This study showed that all the available Geant4 alternative PIXE cross sections provide similar results for K and L shells (and sub-shells). The ECPSSR Form Factor and ANSTO ECPSSR approaches handle the M sub-shell de-excitations. The two alternative sets, while providing more similar results for K and L shell, show significant differences when modelling the M shell. The novel ANSTO ECPSSR cross sections will be released publicly within Geant4 in the next future.

The next step of the project is to compare systematically the alternative approaches to shell ionization cross sections to be used in Geant4 for PIXE applications with respect to the energy of the incident particle and of the target material. We will also validate the application of Geant4 for PIXE simulation capabilities and atomic relaxation against original experimental measurements performed at ANSTO.

References:

[1] D. D. Cohen, J. Crawford, and R. Siegele, "K, L, and M shell datasets for PIXE spectrum fitting and analysis," *Nucl. Instruments Methods Phys. Res. Sect. B Beam Interact. with Mater. Atoms*, vol. 363, pp. 7–18, 2015.

[2] D. D. Cohen and M. Harrigan, "K- and L-shell ionization cross sections for protons and helium ions calculated in the ecpssr theory," *At. Data Nucl. Data Tables*, vol. 33, no. 2, pp. 255–343, 1985.

[3] D. D. Cohen and M. Harrigan, "L shell line intensities for light ion induced X-ray emission," *Nucl. Instruments Methods Phys. Res. Sect. B Beam Interact. with Mater. Atoms*, vol. 15, no. 1, pp. 576–580, 1986.

[4] S. J. McMahon *et al.*, "Biological consequences of nanoscale energy deposition near irradiated heavy atom nanoparticles," *Sci. Rep.*, vol. 1, p. 18, 2011.