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Simulation of Auger electron emission from nanometer-size gold targets using the Geant4 Monte Carlo simulation toolkit

S. Incerti [a,b,c,d,*], B. Suerfu [e], J. Xu [e,1], V. Ivantchenko [f,g], A. Mantero [h], J.M.C. Brown [i], M.A. Bernal [j], Z. Francis [k], M. Karamitros [l], H.N. Tran [a,b]

[a] Division of Nuclear Physics, Ton Duc Thang University, Tan Phong Ward, District 7, Ho Chi Minh City, Viet Nam
[b] Faculty of Applied Sciences, Ton Duc Thang University, Tan Phong Ward, District 7, Ho Chi Minh City, Viet Nam
[c] Univ. Bordeaux, CENBG, UMR 5797, F-33170 Gradignan, France
[d] CNRS, IN2P3, CENBG, UMR 5797, F-33170 Gradignan, France
[e] Department of Physics, Princeton University, Princeton, NJ, United States
[f] Ecoanalytica, Moscow, Russia
[g] Geant4 Associates International Ltd, Hebden Bridge, UK
[h] SWHARD srl, via Greto di Cornigliano 6r, 16152 Genova, Italy
[i] School of Mathematics and Physics, Queen's University Belfast, Belfast, Northern Ireland, UK
[j] Instituto de Física Gleb Wataghin, Universidade Estadual de Campinas, SP, Brazil
[k] Université Saint Joseph, Faculty of Sciences, Department of Physics, Beirut, Lebanon
[l] Notre Dame Radiation Laboratory, University of Notre Dame, Notre Dame, IN, United States

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ABSTRACT

A revised atomic deexcitation framework for the Geant4 general purpose Monte Carlo toolkit capable of simulating full Auger deexcitation cascades was implemented in June 2015 release (version 10.2 Beta). An overview of this refined framework and testing of its capabilities is presented for the irradiation of gold nanoparticles (NP) with keV photon and MeV proton beams. The resultant energy spectra of secondary particles created within and that escape the NP are analyzed and discussed. It is anticipated that this new functionality will improve and increase the use of Geant4 in the medical physics, radiobiology, nanomedicine research and other low energy physics fields.

1. Introduction

The general purpose Geant4 simulation toolkit [1,2] is capable of simulating the radiative and non-radiative atomic relaxation processes of ionized atoms. This feature was first made available for both the "Low energy" and "Standard" electromagnetic physics processes of Geant4 in December 2011 (version 9.5) via the development of a unified general interface for both physics categories [3] and a common software interface for atomic deexcitation [4]. Evaluation of this atomic deexcitation interface has been undertaken in two independent studies utilizing fluorescence spectra measured from the MeV proton irradiation of simple and complex samples at different research facilities: the Ion Beam Analysis Laboratory of the Lebanese Atomic Energy Commission (Beirut, Lebanon) [5] and the Centre d'Etudes Nucléaires de Bordeaux-Gradignan (Bordeaux, France) [6]. Geant4's ability to simulate atomic deexcitation and, in turn, these two independent comparisons, are of particular interest in the in-silico exploration of the use of high-Z nanoparticles (NP) as radiosensitizers in healthcare and medical physics. The potential benefits of NPs in clinical practice are a relatively young field of research and are still undergoing intense investigation via many groups around the world. Monte Carlo simulation toolkits such as Geant4 serve as key research platforms for exploring the fundamental mechanisms involved in physics, physico-chemistry and chemistry of high-Z NPs that impact cellular function and survival probability after irradiation [6]. This work presents a new capability of Geant4 version 10.2 Beta and above to support this highly active research field: the full simulation of atomic deexcitation cascades of ionized atoms. Whilst this capability is available for all atom species for

* Corresponding author at: Univ. Bordeaux, CENBG, UMR 5797, F-33170 Gradignan, France.
E-mail addresses: sebastien.incerti@tdt.edu.vn, incerti@cenbg.in2p3.fr (S. Incerti).
[1] Now at Lawrence Livermore National Laboratory, 7000 East Avenue, Livermore, CA 94550, United States.

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0168-583X/

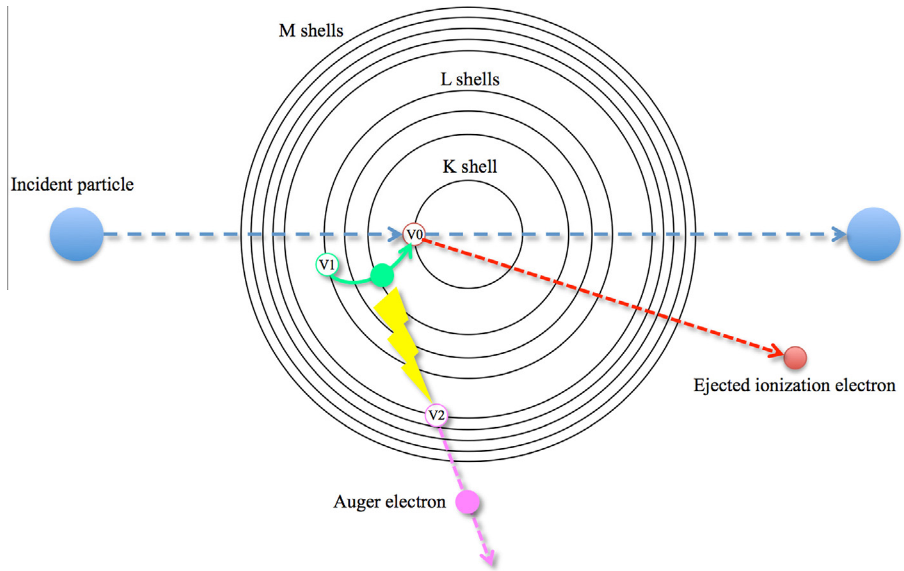

Fig. 1. Illustration of the limitation of Geant4 for the tracking of Auger electron vacancies up to Geant4 release 10.1 (December 2014) (adapted from https://www.ikp.uni-koeln.de/research/pixe/). In this figure corresponding to a hypothetical KL_3M_1 Auger transition, the "V1" vacancy left by the electron (green sphere) filling the vacancy on K shell ("V0") after ionization (the red sphere representing the ejected electron) induced by the incident particle (blue sphere) is taken into account by Geant4, but the "V2" vacancy left by the emitted Auger electron (purple sphere) is neglected. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

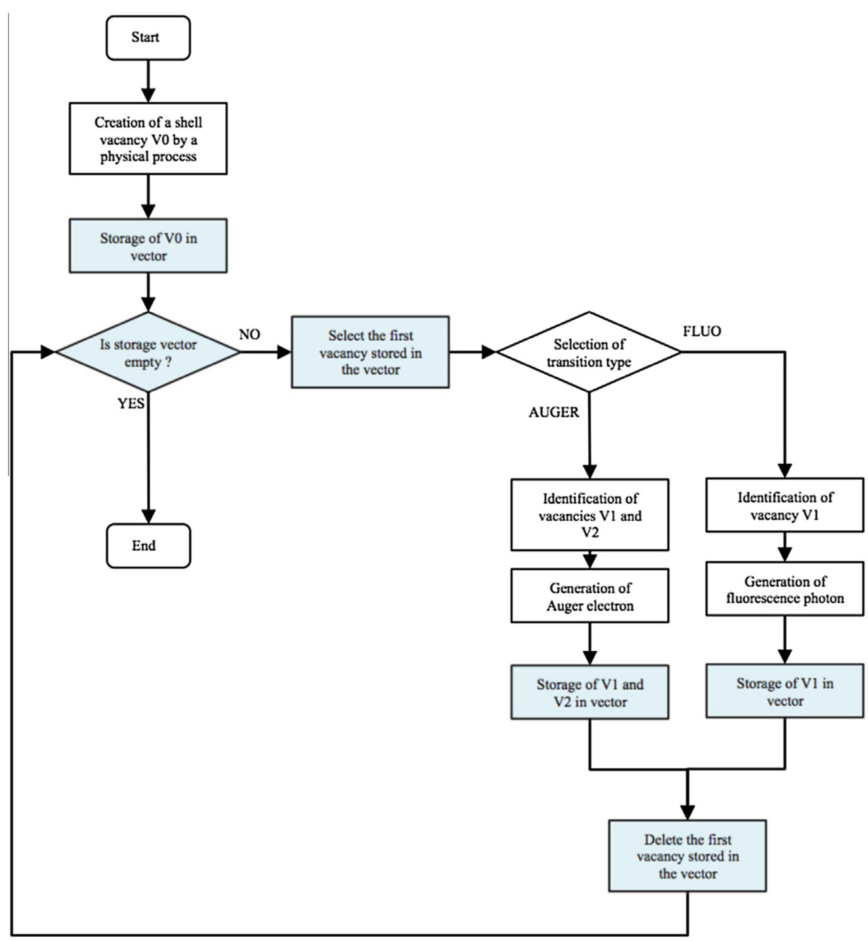

Fig. 2. Diagram describing the algorithm for the simulation of the full deexcitation cascade, as available in Geant4 10.2 Beta release (June 2015). Examples of vacancies denoted as "V0", "V1" and "V2" are shown in Fig. 1. Elements shaded in blue represent new features specifically added for the full simulation. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)