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DEVELOPMENT OF PHYSICAL PROCESSES IN GEANT4 FOR SIMULATION OF ISOL TARGET-ION-SOURCE SYSTEM

Pilsoo Lee*, Jeong-Jeung Dang, Han-Sung Kim, Hyeok-Jung Kwon, Seunghyun Lee, Young-Gi Song, Sang-Pil Yun and Yong-Sub Cho,
Korea Multi-purpose Accelerator Complex, Korea Atomic Energy Research Institute, 38180 Gyeongju-si, Republic of Korea

Abstract

Geant4 physical processes for simulating diffusion and effusion of radioactive ions in matter have been developed for optimizing ISOL target-ion-source (TIS) system. The developed processes simulate motions of radioactive ions with sub-eV kinetic energy in the TIS geometry. The processes consist of diffusion, effusion, and radioactive decay modules, and they are designed to work seamlessly with other implemented physics lists, extending capability of the Geant4 toolkit to more complicated applications in the field of nuclear physics. The diffusion probability is analytically calculated by using the well-known Fick's formula. The effusive flow of neutral atoms is interpreted in terms of kinetic molecular theory of gases, where the interaction between atoms and the wall of a target container is described by employing Lorentz-Lambert model. By the help of newly implemented processes, it is able to simulate the release of radioactive ions from the irradiation of a proton beam on the TIS system with different geometrical parameters in a single environment. Here, we present the status of the development and plans for further improvements.

INTRODUCTION

In the present manuscript, a Monte-Carlo code for simulating isotope separation on-line (ISOL) target-ion-source (TIS) system [1], which is being developed at the Korea Multi-purpose Accelerator Complex (KOMAC) of Korea Atomic Energy Research Institute (KAERI), will be described. The ISOL TIS is being developed for the production of secondary short-lived radioactive isotope beams with a primary pulsed proton beam, The aim of TIS simulations is to find optimized physical parameters of TIS parts that may show the best performance and to calculate the releases of short-lived nuclides of interest, which can be compared directly with experimental data. In this endeavor, simulation codes for the ISOL TIS were written in the framework of the well-developed general particle tracking codes, Geant4 [2]. The implementation was done by adding new physics models for dynamics of radioactive isotopes in thermal-energy domain and modifying already existing Geant4 physics models.

GEANT4 SIMULATIONS FOR ISOL TARGET-ION-SOURCE SYSTEM

For numerically simulating the dynamics of short-lived radioactive isotopes with sub-eV kinetic energy in the TIS, various physics models imitating the production of isotopes induced by protons in intermediate energy and transportation of the ions in an arbitrary geometry need to be written in computational codes. The exact geometry of the TIS system can be imported into Geant4 directly using CAD files with the help of CAD file interface library for Geant4, CADMesh [3], though simple objects still can be generated by using native geometries of Geant4 (Fig. 1). Therefore, the present work basically focuses attention on creating new physics models that can work seamlessly with other physics processes implemented in Geant4.

The new physics consists of diffusion and effusion modules, and an assistive radioactive decay process. In addition, a messenger module for managing the physics in a consistent way is included. In the following sections, functionality of those new physical processes will be briefly described.

The physical processes have been implemented based on 10.03.p02 version, though they do not work with official Geant4 releases for now because of the required modifications to core sources.

Radioactive Isotope Production

In the simulations of releases of radioactive ions out of the TIS, the spatial distribution of produced radioactive nuclei among target disks inside the TIS is one of important factors that affect overall efficiency, therefore, simulating RI production reactions is a critical issue in the simulations. For the simulation of radioactive isotope production, a data-driven inelastic model, G4ParticleHPInelastic class, in Geant4 has been employed. The physics model employs TALYS-based

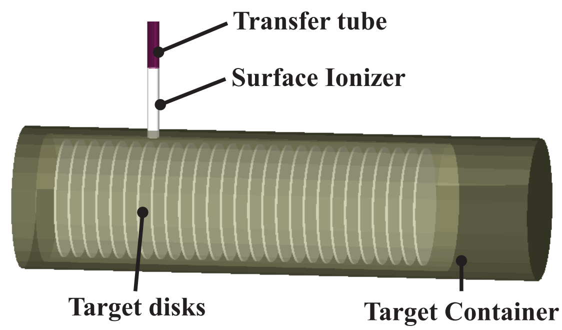

Figure 1: Three-dimensional rendering of four parts, which are directly related to the production of radioactive ions, of the present target-ion-source design in Geant4.

* pilsoolee@kaeri.re.kr

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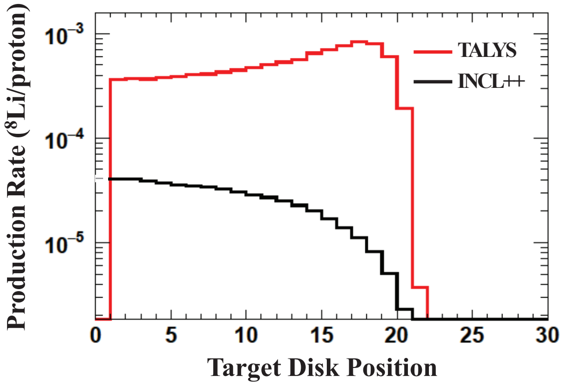

Figure 2: Simulated distributions of ^{8}Li nuclei among BeO target disks inside the TIS. The incident beam is a 100-MeV protons with a uniform profile. The two production curves are obtained with cross sections calculated in the Liege intranuclear cascade model and TALYS.

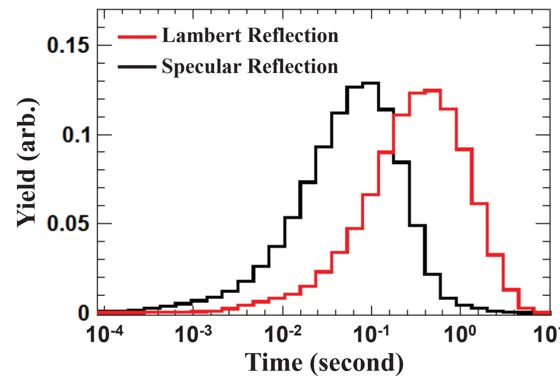

Figure 3: Time distribution of effusive flows of neutral ^{8}Li atoms in pure (black) specular and (red) Lambert reflection modes. In above plots, diffusion is not considered and observed delay results entirely from effusion. The mean values for specular and Lambert reflections correspond to 51 ms and 290 ms, respectively.

nuclear data library (TENDL) for the reaction cross sections by default, while the data could be replaced by experimental data in later. The TENDL provided with standard Geant4 releases has limited data table for cross sections for production reactions of interest, such as ^{9}Be(p, 2p)^{8}Li or ^{nat}B(p,$xnyp$)^{8}Li, therefore, the cross section table was substituted with new one which was recalculated by using TALYS [4] and transformed into G4NDL format for being used in the G4ParticleHPInelastic process. Moreover, the original source code for the G4ParticleHPInelastic was modified so as to add certain nuclear reaction channels, which are required to populate the final states in nuclides of interest. The G4ParticleHPInelastic process has missing reaction channels, which are defined in the ENDF-6 format [5] and required to populate the final state of ^{8}Li from the initial states of ^{nat}B: (p, 3p), (p, n3p), (p, 2pd), or (p, p^{3}He). These undefined reaction channels are additionally implemented in the modified G4ParticleHPInelastic process. Simulated production rates of ^{8}Li nuclei for a BeO target disk array in a target container bombarded with a 100-MeV proton beam are shown in Fig. 2. The two production curves are obtained employing cross sections calculated respectively in the Liege intranuclear cascade (INCL++) model and TALYS.

Diffusion

For the sake of simplicity, the diffusion of atoms in a thin film is implemented based on the analytic form of Fick's equation [6], assuming diffusion coefficient for ^{8}Li to be 10^{-8} cm^2/s. Using the analytic formula for calculation of diffusion probability makes the diffusion algorithms run faster, saving computational time. It was found that the release curve of short-lived radioactive ion, i.e. ^{8}Li, showed lack of sensitivity on the diffusion coefficient [6], though choosing exact diffusion coefficient is not a critical matter in the phase of code development.

Effusion

When radioactive atoms diffuse out from the target disks, the particles freely move inside the target container until they escape through the extraction hole of the TIS or disappear because of radioactive decay. The effusive flow of neutral atoms in the enclosed space is interpreted in terms of kinetic molecular theory of gases, where interaction between atoms and objects in the volume is described by elastic and inelastic scatterings. Elastic scattering (or equivalently specular reflection) assumes that, at the moment of collision, perpendicular component of momentum is inverted while tangential component is conserved. On the other hand, for handling inelastic scattering, Lorentz-Lambert model was employed. Kinetic energy of a particle in the specular reflection is always conserved, whereas, in case of Lambert reflection, it is assumed that particles transfer heat energy with objects in successive collisions and establish thermal equilibrium with objects at temperature T.

The time distribution of effusive flows of neutral ^{8}Li atoms is shown in Fig. 3, illustrating that the pure Lambert reflection has longer delay than the pure specular reflection. In the plots, diffusion is not considered and observed delay results entirely from effusion. The mean values for effusive delay are found to be 51 ms for specular and 290 ms for Lambert reflections, respectively. In reality, reflection could be combination of the two modes with a weighting factor, which significantly depends on the degree of surface polishing. The weighting factor may vary even for materials with the same physical compositions. Therefore, it may need to search an appropriate weighting factor for experimental data with the TIS.

Radioactive Decay

Although Geant4 has a well-developed physical process for radioactive decay, called G4RadioactiveDecay, a new code for handling radioactive decay was written, being more

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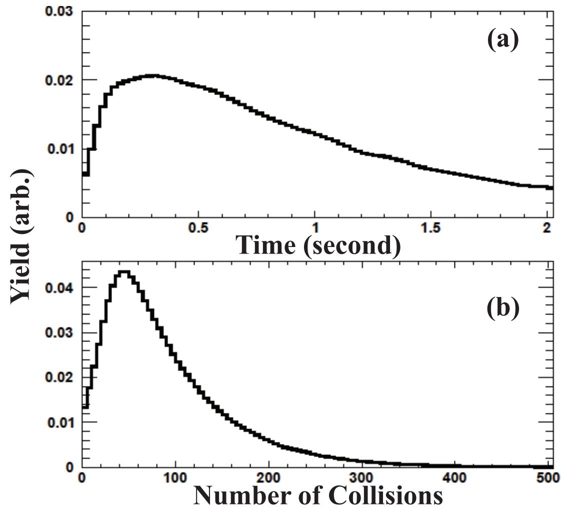

Figure 4: Resulting plots for (a) a ^{8}Li release curve with one shot of a 100-MeV proton at $t = 0$ and (b) the number of collisions of atoms with wall within a surface ionizer.

appropriate for the transportation of nuclei in the thermal-energy domain. Geant4 basically determines the priority of a physical process based on estimated mean free path of the process. In case of a radioactive nucleus with a sub-second half-life, the mean free path of the effusive flow of atoms generally is longer than that of the radioactive decay. As a result, the tracking of the particle is terminated in a single step by the G4RadioactiveDecay process. Moreover, the G4RadioactiveDecay process determines the life-time of a nucleus at the end point of each step, and such a decay scheme is not adequate for multiple-step processes like the effusion process. Instead of the G4RadioactiveDecay process, a new decay process, which still uses the evaluated nuclear structure data file (ENSDF) included in standard Geant4 releases, is implemented.

The new decay process randomly determines the life-time of every nucleus according to the general decay law at the beginning of heavy-ion transportation, and it keeps the nucleus alive until the actual tracking time reaches the predetermined life-time.

Surface Ionization

An ionizer part is the last stage that determines the efficiency of the TIS design. The extraction-hole position could be determined in a way that maximize the flux at the hole becomes maximum for the given beam and target conditions. On the other hand, as for ionization efficiency, an ionizer model was established based on the Saha-Langmuir equation [7]. For saving the cost of CPU time for Monte-Carlo simulations, ionization efficiency is calculated by analytic formula, and then multiplied by the number of collisions of target atoms with the wall of surface ionizer to obtain the number of ions at the transfer tube.

Results

Simulation results specifically for ^{8}Li produced by one shot of 100-MeV protons at $t = 0$ are shown in Fig. 4. Simulated release curve having the mean value of 795 ms for the total delay time indicates that the temporal distribution of extracted ions could be extended for a few second even for a pulsed beam. On the other hand, the mean number of collisions of the atoms with wall within a surface ionizer, whose diameter and length are correspond respectively to 3 mm and 30 mm, is found to be 91.

CONCLUSION

In the present paper, new Geant4 physical processes developed for simulating the ISOL TIS at KOMAC is briefly described. Using the code, it is able to simulate the thermal motions of gaseous atoms in a complicated geometry and estimate the characteristics of radioactive ions at the exit of the TIS in a single environment. The developed code will be utilized to evaluate the overall efficiency and to enhance the performance of the TIS at KOMAC. Because the code is still in a development phase, functionality will be improved further in the near future with verification of the code by experimental data.

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