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SIMULATING MATTER INTERACTIONS OF PARTIALLY STRIPPED IONS IN BDSIM*

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Abstract

Acceleration and storage of beams of relativistic partially stripped ions is more challenging than in the case of fully stripped ions because the interactions with matter, such as those with residual gas and collimators can strip electrons via ionisation. BDSIM is a code for the simulation of energy deposition and charged particle backgrounds in accelerators that uses the Geant4 physics library. Geant4 includes a broad range of ion elastic and inelastic interactions and allows the definition of partially stripped ion beams. However, no models are currently available to handle in-flight interactions involving the bound electrons. In this paper we present a semi-empirical model of beam ion stripping by material atoms that is implemented in BDSIM as an extension of Geant4's existing physics processes and is fully integrated into a comprehensive set of matter interactions for partially stripped ions. The stripping cross-section for select cases and results from comprehensive simulations are presented.

INTRODUCTION

In recent years, partially stripped ions (PSI) have been a topic of increasing interest in accelerator physics. Large projects such as the Facility for Antiproton and Ion Research (FAIR) at GSI (Germany) [1] or the Gamma Factory initiative at CERN (Switzerland) [2] motivate studies into the aspects of accelerating and storing of PSI beams. In contrast to the fully-stripped ions that have been used in nucleus-nucleus colliders and in other applications, PSI are incompletely ionised and retain some of their bound electrons. The presence of the bound electrons enables processes of interest like laser excitation of atomic states, but also makes accelerator operation with PSI beams more challenging. The interactions between PSI and matter like residual gas or beam-intercepting devices can change the charge state of the ions by means of electron loss and reduce the beam lifetime [3]. For example, during the first PSI beam tests at the Large Hadron Collider (LHC), the secondary beams produced by stripping of beam ions by the primary collimators was found to be one of the limiting factors for the beam intensity [4, 5]. There has been a significant effort to improve the understanding PSI interactions with matter and the charge-changing processes involved and to benchmark the theoretical results with measurements [6]. Dedicated simulation tools have been developed to calculate charge-changing cross-sections for different ion species traversing a variety of materials [7]. Semi-empirical cross-section formulae have been derived from the results of these simulations, including an electron stripping cross-section formula. The aim of this work is to integrate an electron stripping physics process, based on a semi-empirical model, into Beam Delivery Simulation (BDSIM) [8–10] in order to allow for comprehensive radiation transport studies with arbitrary one-electron and many-electron PSI species traversing arbitrary materials and material mixtures.

BDSIM is a program that combines particle tracking routines and radiation transport to simulate energy deposition and charged particle background in a 3D beamline model. It uses the Geant4 [11–13] physics library, which includes a large selection of physical interaction models. Geant4 currently allows PSI beams to be defined, but does not have processes that handle in-flight interactions involving the bound electrons. BDSIM is chosen for the process implementation because it is an integrated tool that provides an interface to the Geant4 library. BDSIM features a build system, modular physics lists and model design utilities that help the development and testing of new physics processes. The PSI stripping process is built upon the Geant4's physics processes interfaces, ensuring that the implementation is consistent and the model can potentially be a candidate feature for a later Geant4 release.

INTERACTIONS OF PARTIALLY STRIPPED IONS WITH MATTER

When traversing a target of neutral atoms, ions can undergo charge-changing interactions - electron capture or electron loss. The rate of those interactions depends on the projectile ion species and energy, as well as on the target material. In general, electron loss and electron capture compete with each other and eventually form an equilibrium of charge state fractions. This study is primarily interested on the ultra-relativistic regime (E > 10 GeV/u), where the electron capture and multi-electron capture and ionisation processes are suppressed [6], meaning that the equilibrium charge state is a bare nucleus and the dominant charge-changing process is single electron loss. The semi-empirical formula used to obtain the electron loss cross sectionis [14] is:

$$\sigma\left[\frac{\mathrm{cm}^2}{\mathrm{atom}}\right] = 0.88\times10^{-16}(Z_T+1)^2\frac{u}{u^2+3.5} \times\left(\frac{Ry}{I_1}\right)^{1+0.01q}\left(4+\frac{1.31}{n_0}\ln\left(4u+1\right)\right), \tag{1}$$

$$u = \frac{(\beta c)^2}{I_1/Ry}, \tag{2}$$

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where q and β are the projectile charge and relativistic factor, $c = 137$ is the speed of light in atomic units, I_1 is the projectile first ionisation energy in units of Ry units, u is the reduced projectile energy, n_0 is the principal quantum number of the outermost shell and Z_T is the atomic number of the target.

The above formula is appilcable over a broad energy range, including the relativistic domain. In solid targets the electron loss cross-section is further enhanced (the so-called target density effect) and this is currently not taken into account for cross-section calculations.

PROCESS IMPLEMENTATION IN BDSIM

The electron stripping process is implemented as a discrete process in BDSIM by inheriting *G4VDiscreteProcess* and a dedicated modular physics list is created as a user interface. Currently, the ionisation model in Geant4 enforces a charge equilibrium between the projectile ion and the traversed medium by re-setting all ions to bare nuclei. In order to retain the electron occupancy when target ionisation is enabled, the *G4IonIonisation* process was wrapped in a BDSIM process that re-assigns the electrons in the final state. In the future, it would be of interest to explore more advanced methods of handling ionisation for PSI in Geant4.

The beam ion definition only requires the atomic number (Z), the atomic mass number (A) and the charge (Q). The difference between the Z and Q is used to determine the electron occupancy. Ion parameters such as mass, ionisation energy and electron shell configuration are dynamically evaluated using internal tables in Geant4. Equation 1 is used to calculate the cross-section for all materials in the model. In the case of mixture material, the Bragg additivity rule [15] is used to combine the cross-sections for different elements in the mixture. An example of the cross-section calculated by the process is shown in Fig. 1. Good agreement is observed with the results for the same case found in [14], showing that the model implementation produces the expected results.

A mean free path for the beam ion in the material is calculated from the cross-section and the standard Geant4 Monte-Carlo routines use it to compute interaction distances for individual particles. The process is registered with the Geant4 process manager for ions, ensuring correct ordering of processes (e.g multiple scattering must aways happen second to last) and the correct Monte-Carlo process selection. This integration into the Geant4 process workflow enables the stripping process to work with any combination of other physics processes. It also opens the possibility to make use of Geant4 and BDISM biasing tools to study low-rate interactions such as stripping by residual gas.

When the process is triggered, a single electron is removed from the outermost filled shell. Within the scope of this work the, only the charge change of the projectile ion is of interest and the process is simplified by disregarding the kinematics of the interaction. The interacted ion is emitted with the same momentum as the incident ion and no electron is produced. In future developments, the kinematics will be included in order to enable studies involving the secondary electrons.

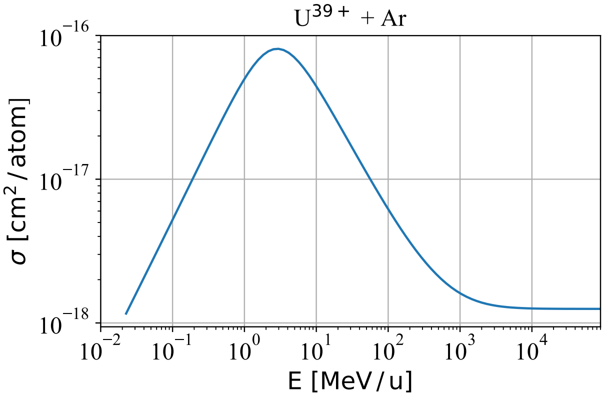

Figure 1: Cross-section of uranium ions with 53 electrons on an argon target obtained from the electron stripping model. The ion parameters such as charge, mass and electron binding energies are obtained from internal tables in Geant4. The material is from the Geant4 predefined material database. The cross-section estimation agrees well with the one shown for the same case in [14], showing the consistency of the model implementation.

RESULTS

In order to test the stripping process, a simple toy-model beamline made up of two 3 m long, −1 rad bending angle dipoles, separated by a drift is prepared. In the middle of the drift is a 50 µm-thick carbon foil ($\rho = 2\,\mathrm{g\,cm^{-3}}$). A beam of 450 GeV/Z $^{208}\mathrm{Pb}^{79+}$ ions on the ideal orbit is fired into the model. The visualisation of the model shown in Fig. 2 demonstrates the effect of the stripping. For the visualisation only the stripping physics processes is enabled. The action of the foil produces a distribution of charge states in the emerging beam. The different charge states have different magnetic rigidities and the downstream dipole separates out their trajectories, demonstrating the tracking of different PSI species.

The distribution of secondary particles after the foil was also compared between the case of only stripping processes and the case of a complete set of physics processes. In the later case *G4EmStandardPhysics, G4HadronPhysicsFTFP_BERT, G4DecayPhysics, G4IonPhysics, G4IonElasticPhysics, G4HadronElasticPhysics, G4EMDissociation* are also enabled in addition to the stripping. The comparison results can be seen in Fig. 3. In both cases, different charge states of the primary ion isotope can be observed, with similar fractions. In the multi-process case, a variety of other particle species are also found in the spectrum of secondary particles escaping the foil, showing that stripping process functions as expected on its own, as well as in combination with other processes. A summary of calculated stripping mean free paths inside the foil and charge fractions for

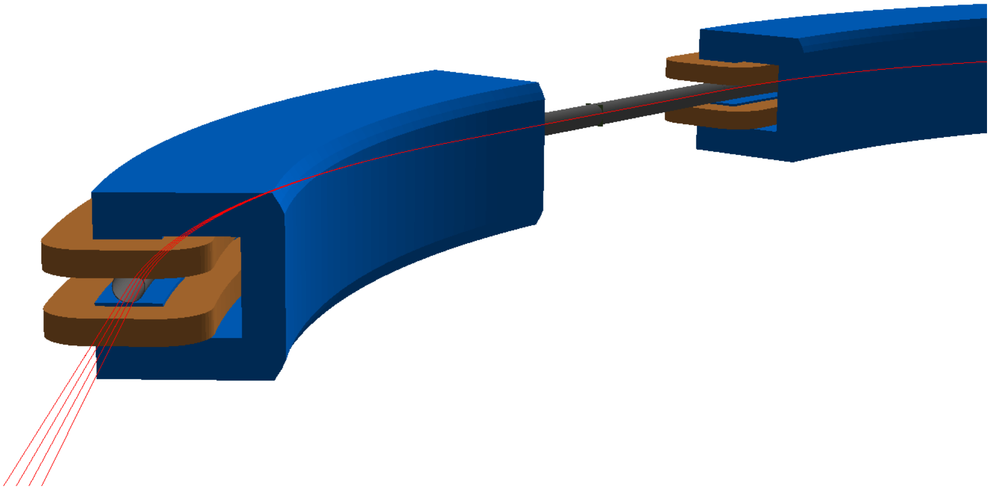

Figure 2: Visualisation of partially stripped ion tracking in bending magnets before and after a stripping foil positioned in the middle of the drift. The beam goes from right to left and it can be observed that after the stripping foil, the emerging trajectories of partially-stripped and fully-stripped ions are separated out by the second dipole.

different charge states of the beam isotope after the foil can be found in Tab. 1.

Table 1: Summary of stripping mean free paths inside the foil and fractions after the foil for different charge states.

Charge state	Mean free path [μm]	Fraction [%]
$^{208}Pb^{79+}$	172	6.00
$^{208}Pb^{80+}$	93	64.75
$^{208}Pb^{81+}$	102	23.45
$^{208}Pb^{82+}$	n/a	5.80

CONCLUSION AND OUTLOOK

An electron stripping model for PSI, based on a semi-empirical cross-section model, has been implemented in BDSIM. The model covers stripping of electrons from relativistic one-electron and multi-electron PSI interacting with neutral atoms in targets made up of arbitrary material mixtures. In the relativistic regime, this process alone is expected to be a good approximation to the all charge-changing interactions for PSI. The model is fully integrated into the Geant4's tracking and physics process frameworks. The results from preliminary tests carried out agree with expectations previous results from using the same model, but additional tests and validation are necessary. Proposed future developments are integration of the target density effect, including correct kinematics with secondary electron emission and adding a semi-empirical model of electron capture.

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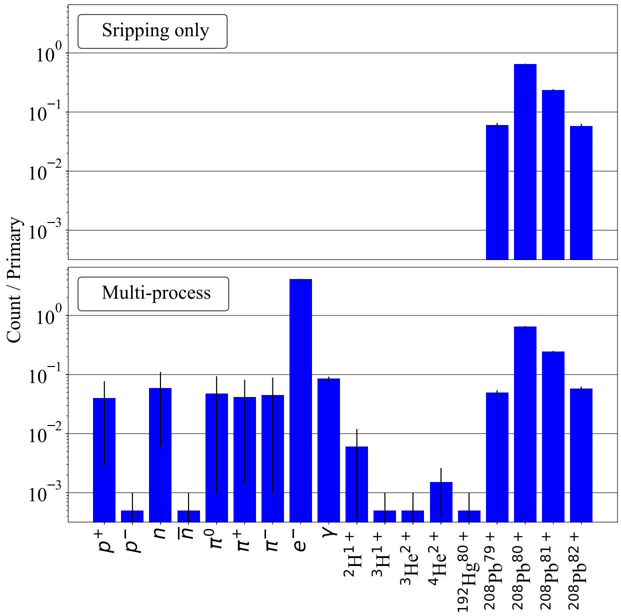

Figure 3: Populations of secondary particle species coming from a beam of $^{208}Pb^{79+}$ impinging on a 50 μm thick carbon foil. The top plot shows the species produced when only the stripping process is enabled, while the bottom plot includes a comprehensive set of physics processes. A beam of 2000 primary ions is used in both cases.

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