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GEANT4 Spectroscopy of Heavy and Superheavy Atomic Nuclei: Element 115

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A high-resolution α, electron, X-ray and γ-ray coincidence experiment was conducted at the GSI Helmholtzzentrum für Schwerionenforschung GmbH in Darmstadt, Germany. It aimed to identify and study α-decay chains of isotopes of element $Z = 115$. Experimental data, including the 30 identified chains, were analyzed self-consistently with a virtually constructed spectroscopic set-up using GEANT4. A workaround which allows for the use of this simulation toolkit for elements $Z > 100$ is presented. The interpretation of the real experimental data, i.e. the derived decay schemes of some of heaviest man-made atomic nuclei, crucially depends on the cross check with the virtual "GEANT4 spectroscopy" experiment.

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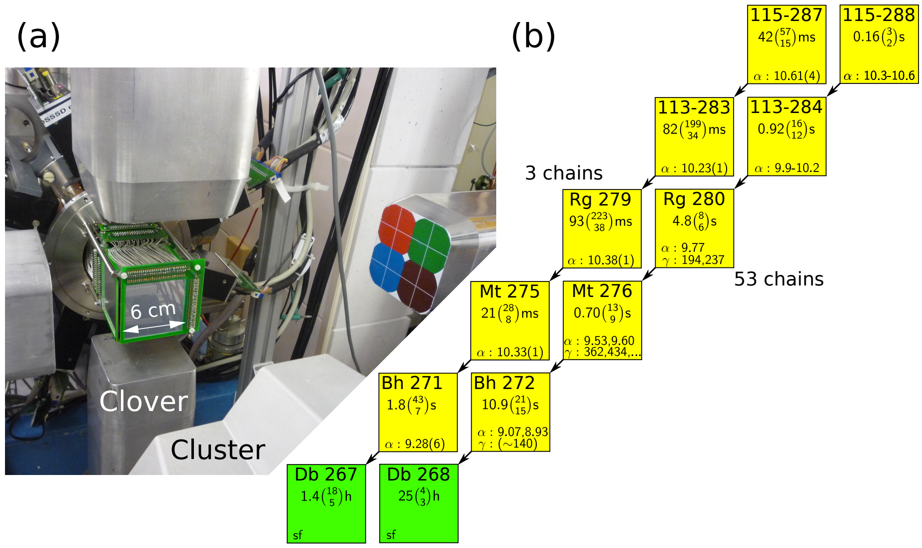

Figure 1: (a) Photograph of the TASISpec α-photon coincidence set-up [4] in the focal plane of the TASCA gas-filled separator at GSI [5, 6]. See text for details. (b) Proposed decay chains of $^{287,288}115$ based on the combined data and assignments of Refs. [2, 7, 8].

1. Introduction

During the past decade, ^{48}Ca-induced fusion-evaporation reactions on radioactive actinide targets have been the driving force behind the observations of several correlated α-decay chains, which all terminate by spontaneous fission. These decay chains are interpreted to originate from the production of atomic nuclei with proton numbers $Z = 113 - 118$ [1]. However, neither their mass, A, nor their atomic number, Z, have been measured directly thus far.

In November 2012, a three-week experiment was conducted at the GSI Helmholtzzentrum für Schwerionenforschung GmbH in Darmstadt, Germany [2, 3]. The reaction ^{48}Ca+^{243}Am was used, with fusion-evaporation products being focused into the TASISpec set-up [4], which was coupled to the gas-filled separator TASCA [5, 6]. The proposed decay chains of $^{287,288}115$ based on the combined data and assignments of Refs. [2, 7, 8] can be found in Fig. 1. The analysis of the seemingly scarce decay chains is a probe for direct nuclear structure insights at the upper extreme of the nuclear landscape.

Monte Carlo simulations are already an established method to assess various aspects of experiments in nuclear and particle physics among many others. Packages such as the GEANT4 simulation toolkit [9] have been used systematically to benchmark and characterize complete experimental set-ups. More recently, GEANT4 has also been used to verify the coherence and consistency of decay schemes of heavy and superheavy elements [10, 11].

2. GEANT4 overview

Any GEANT4 simulation requires some basic "ingredients". Fig. 2 cartoons the elements of the simulation of the TASISpec experimental set-up [12]. The geometry was included in the most realistic, yet practical manner (see upper-left of Fig. 2). The other components of the simulation

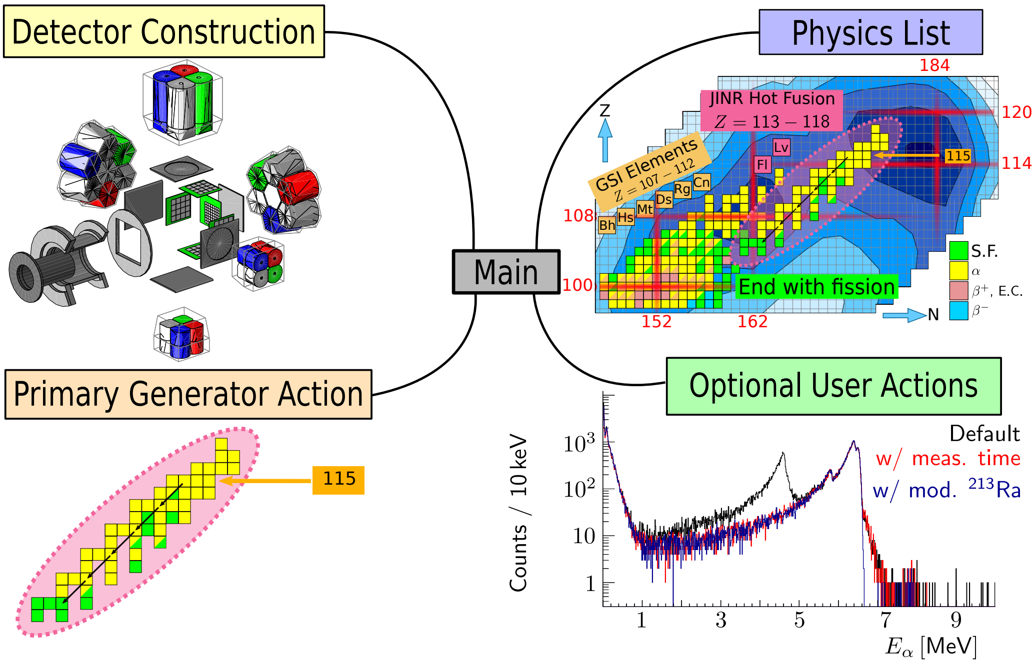

Figure 2: Schematic presentation of the different components of a Monte Carlo simulation using GEANT4. The physical description of the "world" (geometry, materials, positions) are defined in the *Detector Constructor*. The relevant physics to be used (electromagnetic interactions, radioactive decay, etc.) are included in the *Physics List*. In the *Primary Generator Action* the properties and definitions of the initial particles to be simulated are included. On top of these three mandatory components the user has the possibility to use some *Optional User Actions*. See text for details.

have been carefully tailored in such a way that it was even possible to use calibration-source data to determine the experimental thicknesses of the dead layers of the silicon detectors for more than 2000 pixels on a pixel-by-pixel basis [13], and to implement these in the GEANT4 simulated geometry.

To test the performance of the simulation under "in-beam" conditions, i.e. as opposed to point-like calibration sources, the deposition of ^{213}Ra ions into TASISpec was investigated. The deposition profile, rate, and energy of the ions were set to match the experimental conditions after the SHIPTRAP set-up at GSI during an experiment performed in 2009 [14, 15]. The results of the simulation of 15 h of ^{213}Ra deposition at a rate of 2 ions/s can be found in the lower-right part of Fig. 2: By default the simulation includes the α-decay of the long-lived ^{209}Po (102 y at $\sim$4.8 MeV) as a part of the ^{213}Ra decay chain. Using *Optional User Actions* of GEANT4 it is possible to remove the ^{209}Po *artifact* by including a finite maximum "measuring time" of 15 h into the simulation (red curve). This time is being shortened accordingly to the production time and the deposition rate along the real experiment.

In addition, there is a set of tools that allows for the non-intrusive inclusion of user-defined decay schemes into the GEANT4 simulation. It is not necessary to modify the source code or the data files. These tools were used to reconcile the mismatch between the simulated (blue line in lower left of Fig. 2) and experimental spectrum of ^{213}Ra [15].

3. GEANT4 and the decay of heavy and superheavy atomic nuclei

Ideally, to simulate the implantation and decay of heavy and superheavy atomic nuclei, in particular element 115, one should apply the same "recipe" as for the simulation of ^{213}Ra decays. This includes the already included physic cases we are interested in; in particular electromagnetic interactions, atomic relaxation and radioactive decays. As for the *Primary Generator Action*, i.e. an initial nucleus of element 115, it should be a matter of creating the corresponding particle- and electromagnetic decay properties of the full chain and include them in the simulation using the existing tools for it. Unfortunately, the GEANT4 source code in its present version, 9.6.2, has a hard-coded upper limit in the atomic number of $Z \leq 100$. For the time being, this limit prevents the straightforward simulation of the decay of heavy and superheavy atomic nuclei.

While it is rather simple to modify the source code to allow the radioactive decay of atoms with $Z > 100$, it is not trivial to fully extend the code to include such ions to other processes than radioactive nuclear decay and relevant atomic relaxation. Particle transport in the simulation is not a problem for those ions. The electron binding energies for elements up to $Z = 120$ are readily found in the literature [16]. Fluorescence and Auger energies and their corresponding transitions probabilities can be obtained using a linear extrapolation of the data files for low energy electromagnetic processes for elements $Z = 95-100$, which are available in GEANT4 [17]. However, proper stopping power tables, bulk density values and many other quantities associated with a properly defined element –or material– are still to be provided.

As a workaround it is possible to *disguise* heavy elements as lighter ones. At a source code level one can modify the atomic properties such as electron binding energies, occupancy, X-ray and Auger energies, etc, of the heaviest odd number element to be taken as the heaviest odd element available in GEANT4, i.e. to convert $Z = 115$ to $Z = 99$ and $Z = 113$ to $Z = 97$, in their atomic properties. Because this has to be a one-step workaround subsequent modifications, such as $Z = 113$ to $Z = 99$ and $Z = 111$ to $Z = 97$ for the second step, are needed to study the different steps of the decay chain from Fig. 1 one by one.

4. Results

Fig. 3(a) shows the experimental (black) and simulated (green) particle and photon spectra of the transfer-reaction background isotope, ^{211}Bi, and its α decay daugther, ^{207}Tl. The simulation comprised 10^5 decays following the decay scheme shown on the left hand side. The experimentally measured energy values, $E_\alpha = 6274(1)$ keV and $E_\gamma = 350.7(1)$ keV, differ slightly from $E_\alpha = 6278.2(7)$ keV and $E_\gamma = 351.07(5)$ keV found in the literature [18], but for the experimental numbers also systematic uncertainties of $E_\alpha \lesssim 10$ keV and $E_\gamma \lesssim 1$ keV need to be considered.

The particle energy spectrum as seen by the simulated set-up was normalized to the number of α particles detected experimentally. The α-photon coincidence efficiency of the simulation is notably very well under control, because the yield of the 351-keV line in the photon energy spectrum is nicely reproduced using a normalization factor identical to the one of the particle spectrum.

The α decay of ^{280}Rg was also simulated. In this case it is necessary to apply the workaround described in the previous section. Fig. 3(b) shows the result of the comparison between the ex-

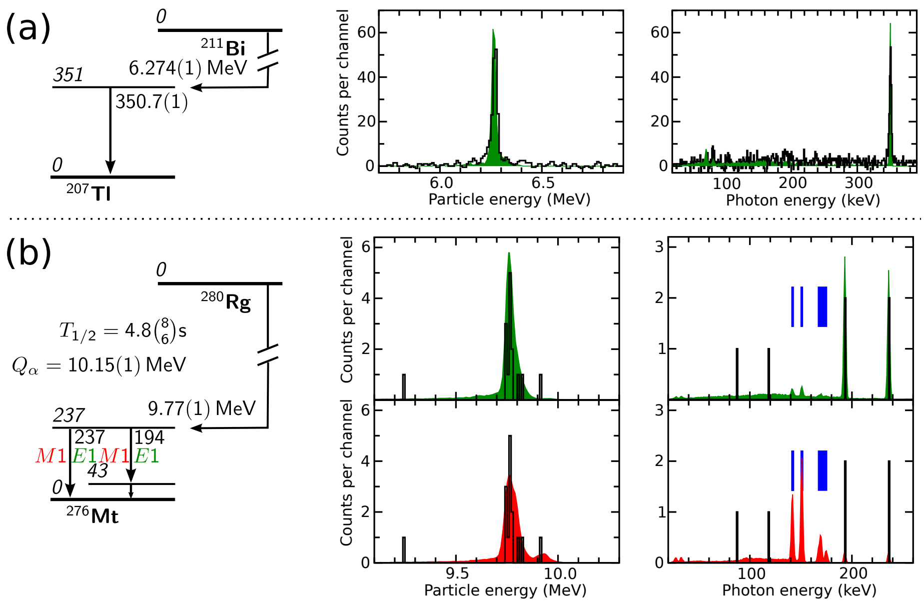

Figure 3: Experimental (black) and simulated (green and red) particle- and photon-energy spectra for the (a) ^{211}Bi $\rightarrow$ ^{207}Tl and (b) ^{280}Rg $\rightarrow$ ^{276}Mt decays. The simulations used 10^5 decays following the schemes shown on the left hand side. The level scheme shown in (a) contains only statistical uncertainties of the peak fit. Level energies and γ-ray energies are in keV. In blue, the K X-ray energies of Mt are indicated in the photon spectra. See text for details.

perimental data and the simulation for two cases, namely varying the electromagnetic character of the simulated 194-keV and 237-keV γ-ray transitions: either $E1$ (green) or $M1$ (red). Just like for the ^{211}Bi α decay, the photon spectra were normalized to the number of α particles detected experimentally. Low-statistics simulations (see Fig. 4) prove that the experimental appearance of two-counts within 1 keV constitute a *peak*. Two or more counts only occur in the simulated spectra when there are corresponding γ-ray transitions in the decay scheme!

Combining the accuracy at which the α-photon coincidence efficiency of the ^{211}Bi $\rightarrow$ ^{207}Tl decay is described by the simulation, and the argument proposed with the Fig. 4, it is possible to assign the 194-keV and 237-keV transitions as $E1$ transitions in the decay scheme of Fig. 3(b). If the γ-ray transitions had $M1$ character instead, the simulation would suggest the detection of K_α X rays, because $M1$ transitions with energies just above the K-binding energy are highly converted. This, in turn, would have been the ideal case for X-ray fingerprinting of superheavy elements, while the proposed $E1$ character implies very interesting nuclear structure physics [2, 19, 20].

5. Conclusions

It is shown that it is possible to tune the "ingredients" of a GEANT4 simulation to provide a self-consistent cross check of the interpretation of the sometimes very scarce experimental data. Even though quantities such as implantation depth or recoil energy of the nuclei after the α decay are not *strictly* correct they do not alter the validity of the spectroscopic results as long as the relevant atomic decay information is properly accounted for. The use of a high-resolution spectro-

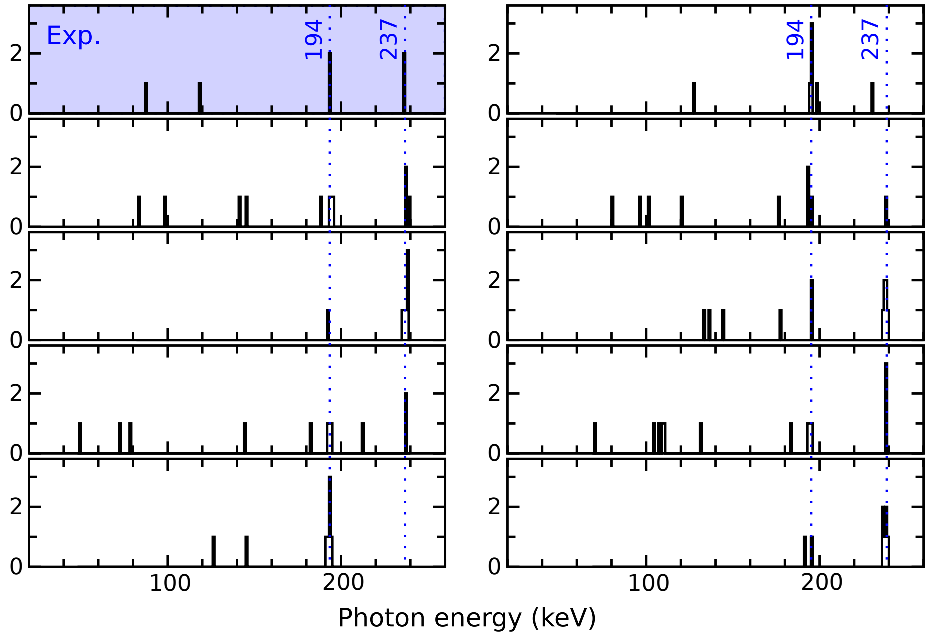

Figure 4: Ten photon spectra corresponding to ^{280}Rg $\rightarrow$ ^{276}Mt decays. All simulated photon spectra are based on 22 α-decay events. The left uppermost spectrum corresponds to the experimental data. Dotted lines are included to guide the eye. See text for details.

scopic set-up in conjunction with comprehensive Monte Carlo simulations proves to be an effective probe to study the nuclear structure properties of heavy and superheavy man-made elements.

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