Study of Double Differential Cross Sections and Angular Distributions of Secondary Neutrons from Medium- and High-Energy Heavy-Ion Induced Reactions Using GEANT4

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Abstract

The double differential cross sections and angular distributions of secondary neutrons from heavy-ion-induced reactions are of significant importance for heavy-ion-driven inertial confinement fusion and high-energy-density physics research. Given the wide variety of heavy ions and the lack of experimental data, calculations must rely on reliable physical models. Using the GEANT4 program combined with the BIC, G4QMD, and LIQMD models incorporating nuclear interaction potential parameters of SLy4, SIII, and SkM*, calculations were performed for the double differential cross sections and angular distributions of secondary neutrons at various emission angles ranging from 5° to 80° for 400 MeV/u ^{84}Kr and ^{132}Xe interacting with Al, Cu, and Pb targets. Comparative analysis with experimental data reveals that for double differential cross sections, the BIC model exhibits significant discrepancies with experimental values in the high-energy region at large angles; the G4QMD model demonstrates reasonable agreement with experimental values for Al, Cu, and Pb targets; and the LIQMD model yields essentially consistent results across different nuclear interaction potential parameters. Regarding angular distributions, the BIC model underestimates experimental values for Al and Cu targets while overestimating those for Pb targets at an emission angle of 80°; simulation results from both G4QMD and LIQMD models reproduce the experimental data reasonably well.

Full Text

Study of Secondary Neutron Double Differential Cross Sections and Angular Distributions for Medium and High Energy Heavy Ion Induced Reactions Using GEANT4

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Abstract

The secondary neutron double differential cross sections and angular distributions from heavy ion induced reactions are crucial for heavy ion beam driven inertial confinement fusion and high energy density physics research. Given the wide variety of heavy ion species and the scarcity of relevant experimental data, reliable physical models are required for accurate calculations. Using the GEANT4 code coupled with the BIC, G4QMD, and LIQMD models (which include the SLy4, SIII, and SkM* nuclear interaction potential parameters), we calculated the secondary neutron double differential cross sections and angular distributions for 400 MeV/u ^{84}Kr and ^{132}Xe projectiles interacting with Al, Cu, and Pb targets at emission angles ranging from 5° to 80°. Comparison with experimental data reveals that for double differential cross sections, the BIC model shows significant discrepancies with experimental values in the high-energy region at large angles, while the G4QMD model demonstrates good agreement with experimental data for all targets. The LIQMD model yields essentially consistent results across different nuclear interaction potential parameters. For angular distributions, the BIC model underestimates experimental values at 80° for Al and Cu targets but overestimates them for Pb targets. Both G4QMD and LIQMD models reproduce experimental data well.

Keywords: GEANT4; Heavy ion; Secondary neutron double differential cross section; Angular distribution; Physical model

1 Introduction

Heavy ion beams exhibit excellent energy deposition characteristics and can produce high energy density matter under extreme densities and pressures, making them a novel tool for driving inertial confinement fusion and studying high energy density physics [1]. The High Intensity heavy-ion Accelerator Facility (HIAF), constructed by the Institute of Modern Physics, Chinese Academy of

Sciences, can generate intense ion beams ranging from hydrogen to uranium with energies from MeV/u to GeV/u, providing an advanced platform for heavy ion driven high energy density physics research [2]. In conceptual designs of heavy ion driven inertial confinement fusion devices, the fusion capsule typically has a spherical structure with an outer layer of materials such as lead and aluminum and an inner layer of deuterium-tritium fuel [3]. Heavy ions interact with the outer layer materials to generate shock waves that compress the deuterium-tritium fuel to achieve ignition, while simultaneously producing numerous secondary particles. Due to their strong penetrating ability, neutrons represent a key factor that must be considered in fusion capsule design, experimental parameter optimization, and radiation protection. Therefore, studying the secondary neutron double differential cross sections from heavy ion induced reactions is of great significance.

Iwata [4] and Heilbronn [5] et al. measured the secondary neutron double differential cross sections for reactions induced by heavy ions such as C, Ne, Ar at 290-600 MeV/u and Fe, Kr, Xe at 230-600 MeV/u using the time-of-flight method. However, given the vast variety of heavy ion species, existing experimental data remain insufficient, making theoretical calculations using Monte Carlo simulation programs with reliable physical models an important approach for obtaining required data. Currently, heavy ion transport programs such as GEANT4 [6], FLUKA [7], PHITS [8], and MCNP [9] are widely used internationally for such calculations. Tsai [10] et al. used MCNP, FLUKA, and PHITS to calculate the secondary neutron double differential cross sections from reactions of C, Ne, Ar ions with various energies interacting with C, Al, Cu, and other materials, systematically evaluating the accuracy of relevant physical models in each Monte Carlo transport program through comparison with experimental data. As an open-source program, GEANT4 has become increasingly widely used in scientific research due to its stability, reliability, and flexibility. However, previous studies using GEANT4 to investigate secondary neutron double differential cross sections have primarily focused on lighter particles such as protons, neutrons, and ^{12}C, with relatively few studies on heavier ions [11-13].

In this study, we used multiple physical models in the GEANT4 program to simulate the secondary neutron double differential cross sections and angular distributions for 400 MeV/u ^{84}Kr and ^{132}Xe interacting with Al, Cu, and Pb targets, comparing the results with experimental data to evaluate the reliability of different physical models. The experimental data were measured by Heilbronn et al. [5] at the Heavy Ion Medical Accelerator in Chiba (HIMAC), Japan. The statistical errors of these data are primarily in the range of 5%-30%, with some data points having errors greater than 30%. Systematic errors arising from detection efficiency and solid angle are between 14%-18%. This dataset has been included in the EXFOR database.

2.1 GEANT4 Program

GEANT4 is a Monte Carlo program for simulating particle interactions with matter, capable of constructing experimental geometries and material properties, and simulating various particle types including electrons, gamma rays, hadrons, and ions, along with their physical interactions. It is widely used in high-energy physics experiments, neutron shielding, and medical physics. Users can track particles in materials and visualize particle trajectories, with calculation results stored in multiple formats according to subsequent analysis requirements.

2.2 Calculation Methods

The GEANT4 simulation process primarily includes detector construction, particle source definition, physics process selection, and data recording. Each step is described in detail below:

(1) Detector Construction: To ensure comparability between simulation and experimental results, the geometry, dimensions, and materials of the targets in this simulation were identical to those used in the experimental setup described in reference [5], as shown in Table 1 . Sensitive detectors were placed around the target to record information on neutrons emitted from the target, including energy and angle.

(2) Particle Source Definition: GEANT4 provides two methods for defining particle sources: G4GeneralParticleSource and G4ParticleGun. This simulation used G4ParticleGun to set the particle type, energy, position, and emission direction. The particle types and energies are listed in Table 1. In the simulation, the particle source was a point source located on the same horizontal line as the target center, emitting particles horizontally toward the target center.

Table 1 Beam species, energies, and target types and dimensions

Beam (Energy)	^{84}Kr (400 MeV/u)	^{132}Xe (400 MeV/u)
Al target	10 cm × 10 cm × 0.2 cm	10 cm × 10 cm × 0.1 cm
Cu target	10 cm × 10 cm × 0.09 cm	10 cm × 10 cm × 0.095 cm
Pb target	10 cm × 10 cm × 0.05 cm	10 cm × 10 cm × 0.05 cm

(3) Physics Process Selection: The GEANT4 PhysicsLists file provides a series of hadronic physics models, such as BIC [14], QMD [15], and LIQMD [16] models. The BIC model is suitable for simulating interactions of nucleons, mesons, and ions with nuclei across an energy range from MeV to GeV. Participating nucleons are described using Gaussian wave functions, with particle propagation in the nuclear field determined by solving equations of motion. When the average energy of participating nucleons falls below a given threshold, the cascade terminates, and the remaining fragments are processed by pre-equilibrium decay and de-excitation models. QMD is a semi-classical microscopic dynamics transport model that uses Gaussian wave packets to describe nucleons in nuclei. All nucleons in the target and projectile are treated as participating particles in the collision process, with the potential energy evolving dynamically over time. Sato et al. [16] improved the QMD model in GEANT4 (G4QMD) by introducing a surface symmetry energy term to the potential energy component based on Skyrme interactions and adding three nuclear interaction potential parameters (SLy4, SIII, and SkM*), forming the LIQMD model. This work used the QGSP_{{{BIC}}_{{HP}}} physics list from GEANT4-v11.2.1 to invoke the BIC model and the Shielding physics list to invoke the QMD and LIQMD models.

(4) Data Recording: When neutron information was recorded by the sensitive detectors, the double differential cross sections were calculated using the following formula, with results stored as ROOT format data files for subsequent analysis. For calculated data in the 10-500 MeV energy range, statistical errors were less than 1%.

$$\frac{d^2\sigma}{dEd\Omega} = \frac{n_N}{\mathrm{ion}_N \times N_V \times x \times \Delta E \times \Delta\Omega}$$

where n_N is the number of detected neutrons, ion_N is the number of incident particles, N_V is the number density of target nuclei per unit volume, x is the target thickness, ΔE is the energy bin width, and $\Delta\Omega$ is the detector solid angle.

Integrating the double differential cross section over energy yields the neutron angular distribution:

$$\frac{d\sigma}{d\Omega} = \int \frac{d^2\sigma}{dEd\Omega} dE$$

3 Calculation Results

Kr Beam Results Analysis

Using the GEANT4 simulation program, we calculated the secondary neutron double differential cross sections for 400 MeV/u ^{84}Kr interacting with Al, Cu, and Pb targets at emission angles ranging from 5° to 80°, with results shown in Figures 1 [Figure 1: see original paper]-3. Comparison with experimental data reveals that calculations from the BIC, G4QMD, and LIQMD models all reproduce the broad peak near 400 MeV formed by projectile fragmentation in the forward angular region. In the LIQMD model, calculations using the SLy4, SIII, and SkM* nuclear interaction potential parameters show no significant differences. For neutron energies below 40 MeV, the BIC model significantly underestimates experimental values for Al and Cu targets at small angles, while slightly overestimating experimental values for Pb targets. The

G4QMD and LIQMD models show good agreement with experimental data for Al, Cu, and Pb targets. For neutron energies between 40-400 MeV, the BIC model shows significant deviations from experimental values at 80° for Al and Cu targets. The G4QMD model reproduces experimental values well for Al, Cu, and Pb targets. The LIQMD model generally underestimates experimental values at 20° for all three targets. For neutron energies above 400 MeV, all physics models underestimate experimental data for Al and Cu targets at large angles, while G4QMD and LIQMD models maintain high consistency with Pb target experimental data.

Figure 1 (color online) Secondary neutron double differential cross sections at different emission angles for 400 MeV/u ^{84}Kr bombarding Al target
Figure 2 [Figure 2: see original paper] (color online) Secondary neutron double differential cross sections at different emission angles for 400 MeV/u ^{84}Kr bombarding Cu target
Figure 3 [Figure 3: see original paper] (color online) Secondary neutron double differential cross sections at different emission angles for 400 MeV/u ^{84}Kr bombarding Pb target

Integrating the double differential cross sections over neutron energies above 10 MeV yields the emitted neutron angular distributions, shown in Figure 4 [Figure 4: see original paper]. The secondary neutron angular distributions exhibit strong forward peaking that increases with target mass number. The BIC model significantly underestimates experimental values at 80° for Al and Cu targets, while slightly overestimating experimental values at 60° and 80° for Pb targets. The G4QMD and LIQMD models show good agreement with experimental data for Al and Cu targets, though some deviations exist with Pb target data at small angles, while large-angle data are basically consistent.

Xe Beam Results Analysis

Using the GEANT4 simulation program, we calculated the secondary neutron double differential cross sections for 400 MeV/u ^{132}Xe interacting with Al, Cu, and Pb targets at emission angles ranging from 5° to 80°, with results shown in Figures 5 [Figure 5: see original paper]-7. Comparison with experimental data reveals that for neutron energies below 40 MeV, the BIC model slightly overestimates experimental values for Pb targets, while G4QMD and LIQMD models reproduce experimental values well for Al, Cu, and Pb targets. For neutron energies between 40-400 MeV, the BIC model significantly underestimates experimental values at 80° for Al and Cu targets. The G4QMD model overestimates experimental values at 10° for Al, Cu, and Pb targets. The LIQMD model shows overall consistency with experimental values for all three targets. For neutron energies above 400 MeV, the BIC model underestimates experimental data for all three targets at large angles, while G4QMD and LIQMD models basically reproduce experimental data except at 80° emission angles.

Figure 5 (color online) Secondary neutron double differential cross sections at

different emission angles for 400 MeV/u ^{132}Xe bombarding Al target
Figure 6 [Figure 6: see original paper] (color online) Secondary neutron double differential cross sections at different emission angles for 400 MeV/u ^{132}Xe bombarding Cu target
Figure 7 [Figure 7: see original paper] (color online) Secondary neutron double differential cross sections at different emission angles for 400 MeV/u ^{132}Xe bombarding Pb target

Figure 8 [Figure 8: see original paper] shows the angular distributions of neutrons emitted from ^{132}Xe bombarding Al, Cu, and Pb targets. The BIC model results disagree with experimental data at 10° and 80° emission angles but agree well at other angles. The G4QMD and LIQMD model results are essentially consistent and both reproduce experimental data well.

Figure 8 (color online) Secondary neutron angular distributions for 400 MeV/u ^{132}Xe bombarding Al, Cu, and Pb targets

Overall, the BIC model performs poorly in calculating high-energy neutron cross sections at large angles for Al and Cu targets, likely because it cannot adequately describe collisions between $^{\{84\}\mathrm{Kr}/}${132}Xe nuclei and Al/Cu nuclei. The differences between G4QMD and LIQMD models are mainly observed in the 10-300 MeV energy range in the forward angular region, possibly due to the new nuclear interaction potential parameters used in the LIQMD model. For the ^{84}Kr beam, the G4QMD model provides more accurate results, while for the ^{132}Xe beam, the LIQMD model demonstrates better performance.

4 Conclusion

This study used the GEANT4 simulation program with BIC, G4QMD, and LIQMD models to calculate the secondary neutron double differential cross sections and angular distributions for 400 MeV/u ^{84}Kr and ^{132}Xe interacting with Al, Cu, and Pb targets at emission angles from 5° to 80°. The results show that compared with experimental data, the BIC model exhibits significant deviations, while the G4QMD model demonstrates good agreement. The choice of nuclear interaction potential parameters in the LIQMD model has no significant effect on the results. Overall, the G4QMD and LIQMD models perform better than the BIC model. In general, when using GEANT4 to calculate secondary neutron double differential cross sections and angular distributions from heavy ion induced reactions, the accuracy of different physics models is closely related to the projectile species, energy, and target species. To more accurately predict secondary neutrons from heavy ion interactions with matter and provide reliable data support for heavy ion fusion and high energy density physics research, more high-quality experimental data are needed to further improve the relevant physical models.

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