Benchmarking GEANT4 nuclear models for light fragments of 80.5 MeV/u carbon ions bombarding heavy-metal targets

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In recent years, with the wide use of carbon beams, in order to verify the predictive ability of Monte Carlo programs to simulate nuclear reactions, researchers around the world have done many benchmark tests on simulations of outgoing fragments of ^{12}C beam bombarding light target materials such as hydrogen, carbon, oxygen, and water targets. With the increase of target mass number, the fragmentation reaction will become more complex, and the applicability of the GEANT4 nuclear reaction models for this aspect is still unknown. In this paper, the simulation results of emitted light fragments using three hadronic reaction models embedded in the GEANT4 toolkit are compared with experimental measurements of Cu, W, Au, and Pb targets. The three models are G4BinaryLightIonReaction, G4QMDReaction, and INCL++. This paper discusses the performance of these models in reproducing the energy spectra and angular distributions of the secondary light charged particles, and the results with different targets are shown.

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I. INTRODUCTION

Recently, simulations of heavy ion induced nuclear reactions using Monte Carlo programs have a wide range of applications in research fields such as heavy ion therapy, accelerator driven system, accelerator physics, space missions, and radiation protection. At present, FLUKA [1,2], MCNPX [3], GEANT4 [4,5], PHITS [6], and other Monte Carlo programs are commonly used to simulate the interactions of particles through matter. To verify the accuracy of the nuclear reaction model simulations in these Monte Carlo programs, researchers from many countries have conducted benchmark tests on these programs over the past decade or two.

The ability of these Monte Carlo codes to reproduce experimental data of charge-changing cross sections and integral and differential yields of secondary charged fragments has been evaluated by Böhlen *et al.* [7]. The experimental data of double differential carbon fragmentation cross sections obtained at intermediate energy was compared with GEANT4 nuclear models by Dudouet *et al.* [8]. Bolst *et al.* benchmarked GEANT4 nuclear models against experimental data for a 400 MeV/u ^{12}C beam incident upon a water phantom [9]. And GEANT4 hadronic models were also tested with a focus on applications in space radiation environments by Ivantchenko *et al.* [10]. Due to space limitations, many other excellent benchmark articles are not covered here. The degree of agreement between the predictions of the nuclear model and the experimental data of these studies is encouraging, but there is still much room for improvement.

However, these tests rarely mention the predictive ability of these nuclear reaction models for the products of ^{12}C bombardment of heavy targets, which is what we are studying in this paper. In addition, the recoil angle particles are also taken into account. This is a nice addition to the previous work. Tungsten and lead are commonly used materials for spallation targets, and copper is an important material for accelerators. This study is also of great significance for the engineering design of accelerator-driven systems. The GEANT4 toolkit is used to simulate the secondary light charged particles produced by an 80.5 MeV/u ^{12}C beam hitting the targets, and the energy spectra and angular distributions obtained from the simulations are compared with the experimental results. The GEANT4 built-in nuclear reaction models [11] used in the study are G4BinaryLightIonReaction, G4QMDReaction, and INCL++. The advantages and disadvantages of these three models in reproducing the energy spectra and angular distributions of secondary light charged particles, as well as their dependence on the target materials, are discussed in the paper.

II. EXPERIMENTAL REVIEW

The results of the simulations were compared with experimental data obtained from the experiment conducted at the Radioactive Ion Beam Line (RIBLL) [12] of the Institute of Modern Physics (IMP) in Lanzhou. The experiment involved an 80.5 MeV/u $^{12}C^{6+}$ beam inducing reactions on Cu, W, Au, and Pb targets. The experimental setup and the electronics

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TABLE I. The energy threshold for going through one set of telescope detectors.

Particle	^{1}H	^{2}H	^{3}H	^{3}He	^{4}He
Energy (MeV/u)	132.4	88.5	70.0	157.2	133.1

were thoroughly described in the previous paper [13]. The double differential cross sections of secondary light charged particles were detected at 30°, 60°, and 120° relative to the beam. The experimental data were compared with the Monte Carlo simulation results to benchmark the reaction models embedded in GEANT4.

The particle identification was carried out by three sets of telescope detectors, each consisting of two thin silicon detectors and one 5-cm-long CsI detector. As the CsI detectors were not long enough to stop the outgoing fragments of all energies, emitted particles with energies above 150 MeV/u would go through the detectors. For particles of high energy, one part of the energy was deposited in the detector, and the other part left as the particles flew away. The high-energy outgoing fragments would be counted into yields of lower energy. As shown in Table I, the energies at which different particles just cross one set of telescope detectors were calculated by LISE++ [14]. Particles above the threshold energy do not show up on the energy spectra, resulting in a sudden drop in the energy spectra of ^{1}H, ^{2}H, ^{3}H, and ^{4}He. The reason why the drop is not visible in the ^{3}He experimental data is that the double differential cross sections become too low (i.e., out of the range of measurement) at the cutoff energy. Therefore, the double differential cross sections of the high energy segment have little reference value. Since the particle yield of high energy is small compared to that of low energy, and the single differential cross sections are the integral of the double differential cross sections with respect to energy, the data of the single differential cross sections at a specific angle is reliable.

III. SIMULATION INTRODUCTION

A. Reaction mechanism

According to [15], a nucleon-nucleus or pion-nucleus or nucleus-nucleus reaction, in which the incident energy exceeds some tenth of MeV per a.m.u. is referred to as spallation reaction.

There are three stages that can be distinguished in a spallation reaction according to a certain time scale: The intranuclear cascade (INC) phase, the pre-equilibrium phase, and the evaporation and high-energy fission phase. In the first stage, the intranuclear cascade stage, which occurs in about 10^{-22} s, the energy of the primary incident particles is converted into the energy of the nucleons in the target nucleus. The secondary particles produced in this phase are of higher energy, from about 20 MeV to the energy of the incident particles. The low-energy pre-equilibrium particles are then emitted from the nucleus in a highly excited state. In the case of heavy targets, evaporation competes with high-energy fission in the final stage, which occurs within a time frame of about 10^{-18} s. Particles emitted during the evaporation phase are of low energies (<20 MeV) and have isotropic angular distributions. The nucleus that remains may become radioactive and may emit γs.

In addition to the INC models, an alternative model for the first stage is the quantum molecular dynamics (QMD) model which is an n-body theory simulating ion reactions at intermediate energies on an event-by-event basis. The details the INC models and the QMD model used in this paper are introduced in Sec. III C.

B. Simulation condition setup

The energy spectra and angular distributions of light charged particles produced by ^{12}C ions incident on Cu, W, Au, and Pb targets are simulated and calculated using the 11.0.2 version of GEANT4. The number of incident particles is set to 10^{10} for the simulation of the W target and 10^9 for the simulations of other target materials. The statistical error for the angular distributions of the W target ranges from 0.04% to 2.75%, with the yield of ^{3}He fragments emitted at 170° using the QMD model having the largest statistical error of 2.7%. The primary incident particle is set as $^{12}C^{6+}$. The target is set as a round sheet, and the material used is the built-in material of GEANT4. The size, shape, and placement of the detectors during the calculation of secondary particle energy spectra are consistent with those in the experiment.

C. Simulation model

The simulations of nuclear reactions at intermediate energies in GEANT4 are handled by a dynamical model coupled with a set of statistical de-excitation models. The BIC and INCL++ models are variants of the standard INC model, while the QMD model is a quantum molecular dynamics model. The BIC, INCL++, and QMD models are used as the main dynamical models to describe the first stage of the reaction.

The GEANT4 binary cascade model (BIC) [16] is implemented by G4BinaryLightIonReaction using G4BinaryCascade. It is an intranuclear cascade model designed to deal with the interaction between a light nucleus and the individual nucleons of the target nucleus. The participant nucleus is described by a three-dimensional model and the propagation of the particle is done by numerically solving the equation of motion. The cascade will break down when there is no particle with kinetic energy above the threshold energy of 75 MeV or the mean kinetic energy of all the participants is below 15 MeV. The remaining prefragment will be passed on to the G4PreCompoundModel.

The second model, the Liège Intranuclear Cascade Model (INCL++) [17,18] is available through the G4INCLXXInterface. The latest version of INCL++ implemented in GEANT4 is v6.0. It is another INC model for simulating reactions induced by protons, neutrons, pions, kaons, and light ions ($A \leqslant 18$). Any particles heavier than deuterium can be used as the target nucleus. The cascade stops when there are no participants left in the nucleus or the time reaches $70 \times (A_{\text{target}}/208)^{0.16}\text{fm}/c$. GEANT4 uses

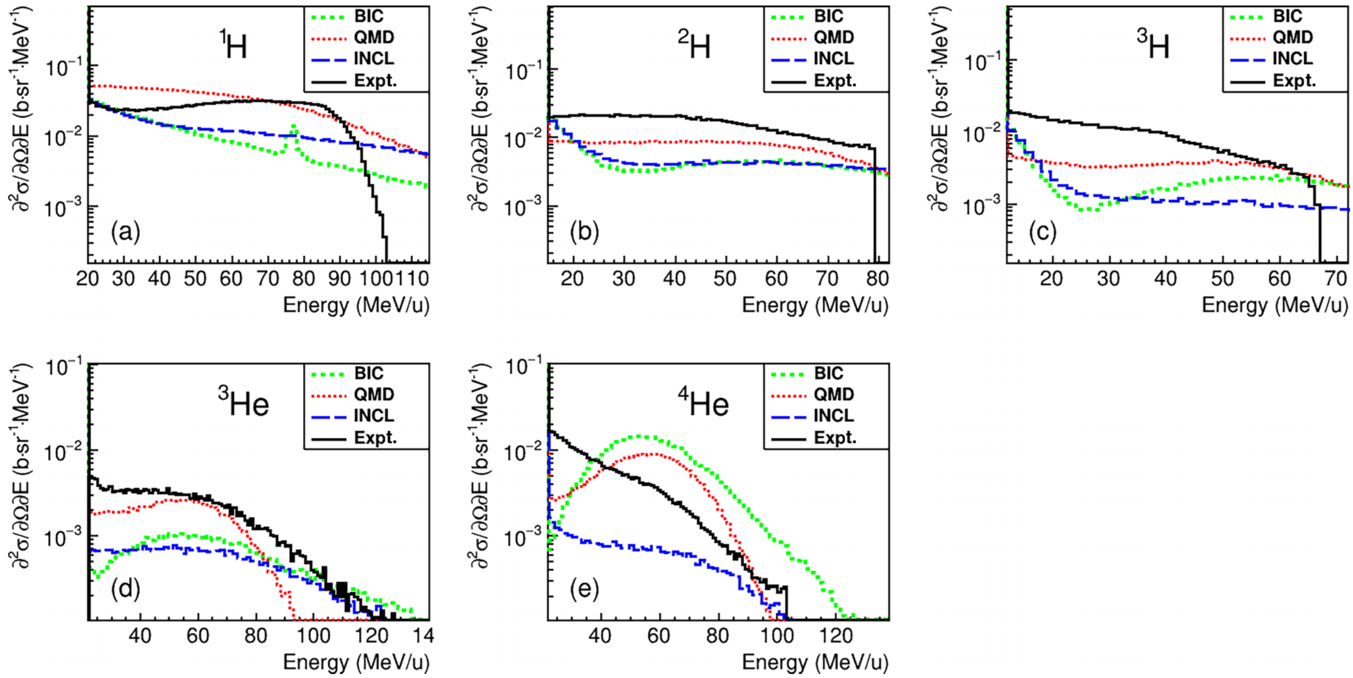

FIG. 1. Energy distributions of ^{1}H (a), ^{2}H (b), ^{3}H (c),^{3} He (d), and ^{4}He (e) fragments out of tungsten target at 30°. The colored lines represent the GEANT4 simulation results with BIC, QMD, and INCL++ models. The black lines are experimental data.

G4ExcitationHandler to deal with the de-excitation of the remnants by default. The INCL++ model has advantages for complex particle emission due to its dynamical phase-space coalescence algorithm for cluster formation in the cascade phase.

The QMD model in GEANT4 is implemented through G4QMDReaction. The JAERI QMD (JQMD) model [19,20] is the basis of the GEANT4 QMD model. As the participant particles contain the nucleons in both the projectile nucleus and the target nucleus, the wave function of the whole system is defined to be the product of the Gaussian wave function of each nucleon. This model requires more computing resources because participant-participant scattering is also included in the calculation, resulting in the QMD model being about 20 times slower than other models. The system evolves and the potential changes dynamically in the QMD model. This time evolution will terminate when 100 fm/c is reached. The generalized evaporation model (GEM) is used as the default de-excitation model of the QMD model.

IV. RESULTS

To verify the ability of the nuclear models in GEANT4 to reproduce the products of a carbon beam bombarding heavy metal targets, the simulation results are compared with the experimental data.

A. Energy spectra

Figures 1–3 show the comparison between the energy spectra of light charged particles (p, d, t, ^{3}He, and ^{4}He) ejected from the tungsten target at 30°, 60°, and 120°, as simulated by GEANT4 and the experimental results, where the black solid lines represent the experimental results.

Figure 1 shows that the simulation results of the INCL++ model for protons, deuterons, and tritons at 30° in the low energy range (about 20 MeV/u below) are in good agreement with experimental results, however there is a significant underestimation in the higher energy part of the spectrum. This phenomenon is also clearly observed at higher energy, when comparing INCL simulation results with experimental measurements of 2.5 GeV protons bombarding Au targets [21]. When $Z = 1$ of the outgoing light particle, the larger A is, the greater the difference between the simulation results and the experimental measurements. This may be due to when a nucleon hits the nucleus surface and satisfies successfully the test for emission, it is tested to see whether it belongs to a possible cluster. Actually, the candidate cluster is constructed, starting from the considered nucleon, by finding a second, then a third, etc., nucleon fulfilling the condition to form a cluster. The following light clusters are considered: d, t, ^{3}He, ^{4}He. Also, this is one of the reasons why ^{3}He and ^{4}He have been underestimated. Another reason is that the INC procedure, originally used for nucleon-nucleus reactions, is now being used for nucleus-nucleus reactions, and the model ignores the clusters present in the structures of incident particles.

The energy spectra simulations of the QMD model for three kinds of outgoing light charged particles (p, d, and t) in high energy part at 30° are generally in better agreement with the experimental results than those of the BIC and INCL++ models. For the outgoing ^{3}He fragments, the QMD model reproduces the double differential cross section at the low energy end better, but there is an obvious underestimation at $E > 75$ MeV/u. In this case, the BIC and INCL++ models

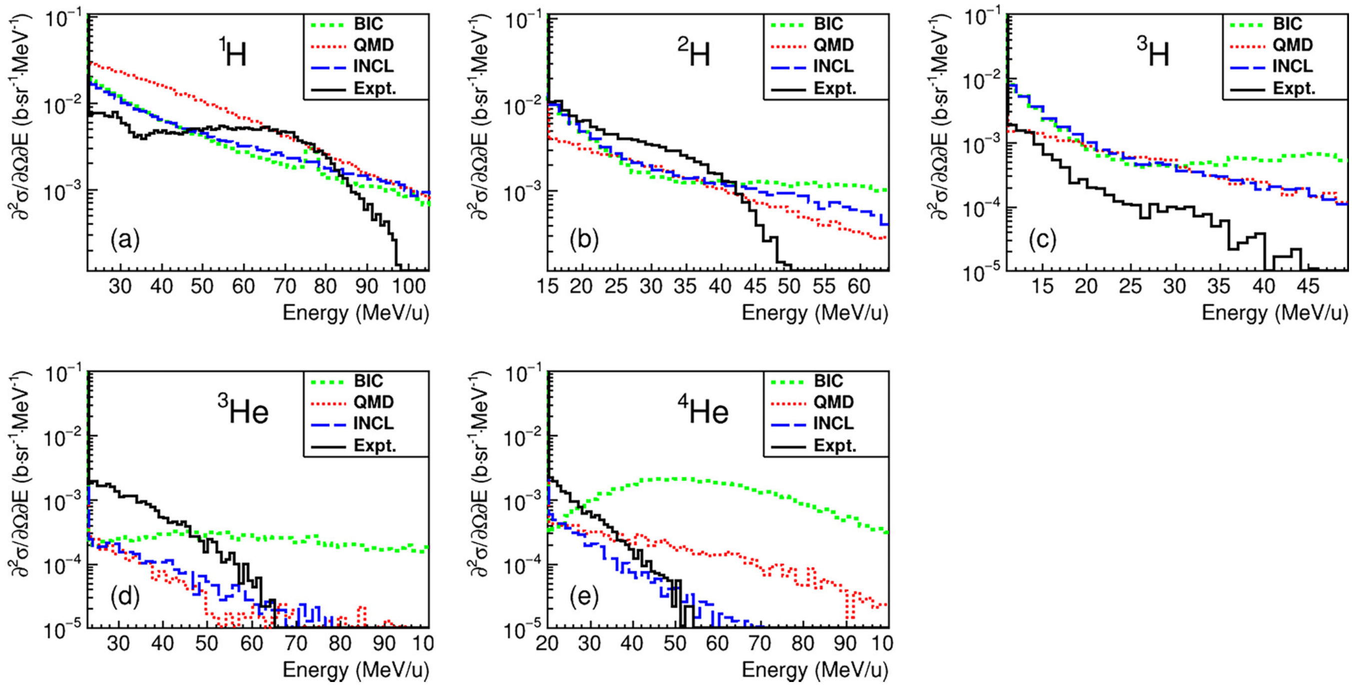

FIG. 2. Energy distributions of ^{1}H (a), ^{2}H (b), ^{3}H (c),^{3} He (d), and ^{4}He (e) fragments out of tungsten target at 60°. The colored lines represent the GEANT4 simulation results with BIC, QMD, and INCL++ models. The black lines are experimental data.

can predict the ^{3}He of the high energy segment slightly better than the QMD model. For ^{4}He particles, the BIC and QMD models poorly predict the energy spectrum trend compared to experimental measurements, and there is a peak not observed in the experiment. The INCL++ model is in better agreement with the experimental results in terms of the overall trend, although there is still a significant underestimation in the low-energy range. Figure 2 shows the results of the energy distributions of light charged particles at an exit angle of 60°. For protons, the double differential cross sections obtained by the QMD model is slightly larger than that obtained by the other two models. When $E < 80$ MeV/u, the difference between the simulation results and the experimental results is not more than 30%. For ^{2}H, all three models underestimate the experimental results at less than 45 MeV/u and overestimate them at greater than 45 MeV/u. For ^{3}H, ^{3}He, and ^{4}He, all three models fail to reproduce the experimental results, and the energy trends obtained from the BIC model are completely different from the experimental measurements. Only the INCL++ model has a better description of the trend of the energy distributions. This may be due to the simulation of composite particle emission in the INCL++ model for the cascade phase. When a nucleon is about to leave the system, the clustering algorithm will look for other nucleons that are very close together in phase space to form candidate clusters. Then, the algorithm selects the one with the least excitation to carry out the penetration test of the Coulomb barrier. The cluster will be emitted if the penetration is successful. This also explains why the INCL++ model has better prediction in general for ^{3}He and ^{4}He fragments.

Figure 3 shows the results at 120°. In the experiment, since the outgoing light charged particles are mostly emitted at forward angles, the number of particles detected at 120° is small and the statistics become poor. The number of ^{3}He and ^{4}He obtained in the experiment is too small to be distinguished, so the experimental energy spectra of these

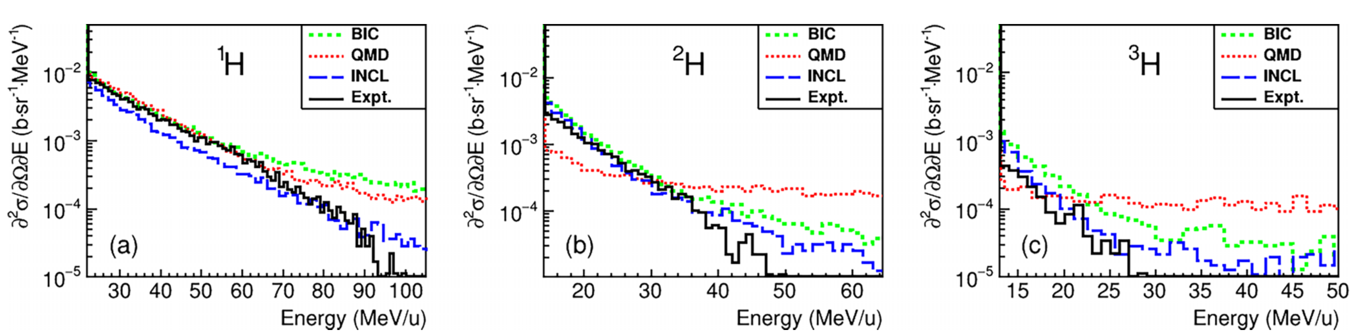

FIG. 3. Energy distributions of ^{1}H (a), ^{2}H (b), ^{3}H (c) fragments out of tungsten target at 120°. The colored lines represent the GEANT4 simulation results with BIC, QMD, and INCL++ models. The black lines are experimental data.

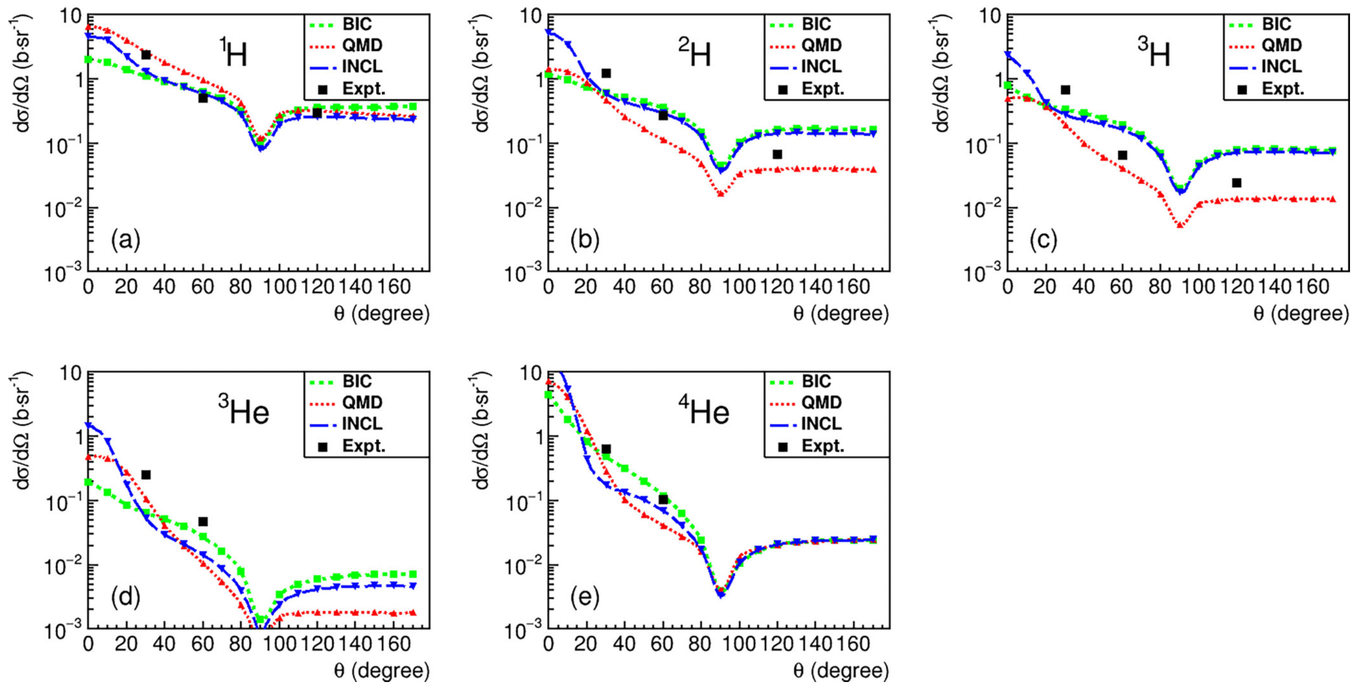

FIG. 4. Angular distributions of ^{1}H (a), ^{2}H (b), ^{3}H (c),^{3} He (d), and ^{4}He (e) fragments out of tungsten target. The colored lines represent the GEANT4 simulation results with BIC, QMD, and INCL++ models. The black lines are experimental data.

two particles are missing and cannot be compared here. The INCL++ predictions for the recoiling light charged particles are in good agreement with the experimental data, except for the overestimation of the high-energy tail. The deviation from experimental data at large angles shows that the projectile nucleons lose too little transverse momentum during the INC collision. Although the INCL++ model is superior to other models in reproducing the experimental data at 120°, it lacks accuracy in describing projectile fragmentation in some aspects. The BIC's results, which have the same problem of projectilelike fragments, are slightly worse than INCL++ but acceptable. The simulation results of the QMD model deviate the most from the experimental measurements among the three models.

From the combination of Figs. 1–3, as the angle increases, the deviation of the calculated results of the INCL++ and BIC models from the experimental results becomes smaller. According to the reaction mechanism, the particles emitted in the intranuclear cascade stage are mostly forward-angled, while the particles emitted by evaporation are isotropic. As the angle increases, the proportion of evaporated particles relative to the total outgoing particles increases. It can be seen that the simulations of the evaporation process are consistent with the experimental data, whereas the simulations of the INC stage are significantly different from the experiment. The INC stage does not take into account the structure of the carbon ion, so most of the predictions are underestimated. Because the residual nucleus in the equilibrium stage have no memory of the projectile, the prediction of the evaporated particles is more accurate than those generated during the INC stage. Especially, given that the target modeling in INCL++ is superior to the projectile preparation, better prediction for targetlike fragments is somewhat expected.

B. Angular distribution

Figure 4 shows the comparison between the simulation results and the experimental results of the angular distributions of light charged particles emitted from a tungsten target bombarded by an 80.5 MeV/u ^{12}C beam. Since the target is set up as a very thin cylinder when the Monte Carlo simulation is carried out, the outgoing particles around 90° have to go through a longer transport path in the target, which is no longer in line with the condition of a thin target. Therefore, the angular distribution curve has an obvious downturn at around 90°. The angular distribution curves of this interval are not of reference value. But the sections of the curves near the experimental points are basically unaffected. It can be seen from the figure that the simulation results of the three models for proton and ^{4}He are in significantly better agreement with the experimental results than other fragments, which may be due to the simpler emission mechanism of these two kinds of particles. The difference between most of the single differential cross sections from the simulations and experimental data is within 50%, among which the INCL++ model gives slightly better results than the other two models, which is consistent with the conclusion of De Napoli *et al.* [22] at lower energy. Although the BIC model's prediction for ^{4}He appears to be in good agreement with the experiment, it still cannot be considered that the BIC model is better than the other two models based on the energy spectra at 30° and 60°.

C. Different targets

Figures 5 and 6 show the energy distributions of protons and α particles obtained by C-beam bombardment of targets of different materials at 30°. In order to have a more

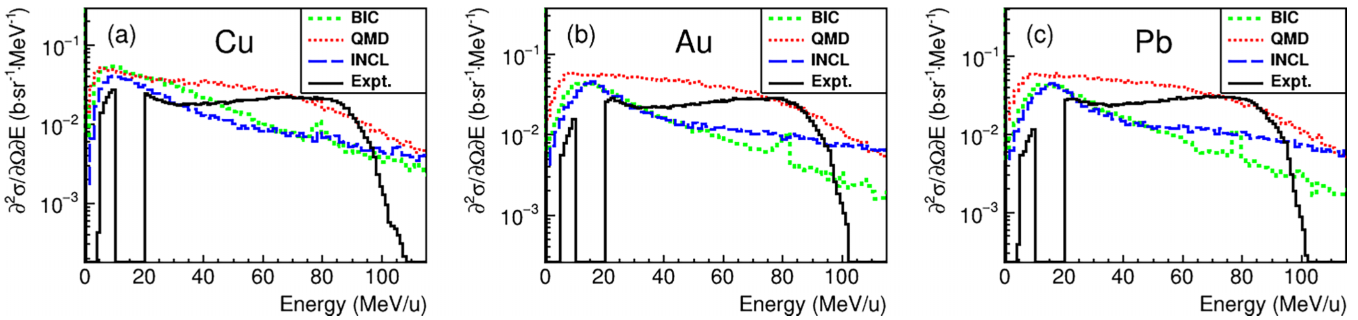

FIG. 5. Energy distributions of protons at 30° for Cu (a), Au (b), and Pb (c) targets. The colored lines represent the GEANT4 simulation results with BIC, QMD, and INCL++ models. The black lines are experimental data.

comprehensive view of the results, the energy spectra below all start at 0 MeV/u. The vacant part of the experimental data is mainly due to the fact that the energy response of the CsI detector does not start from 0.

As can be seen from Fig. 5, for the three different targets, the simulation results of the INCL++ model are closer to the experimental results when $E < 10$ MeV/u, while the results of the QMD model are closer to the experimental measurements for the higher energy part.

Figure 6 shows the energy spectra of the emitted α particles. The same with Fig. 5, the simulation results of the INCL++ model are closer to the experimental results. In the low-energy part, unlike the simulation of the outgoing proton energy spectra, the GEANT4 simulations of the Au target and the Pb target have a better agreement with the experimental results than the energy spectrum of the lighter Cu target. In the higher energy part, the simulated results of all three models deviate from the experimental results. Here is an explanation of why the INCL++ model gives good results for the parts of the energy spectra below 10 MeV/u, but seriously underestimates the parts of the energy spectra above 20 MeV/u: The α particles in the high-energy part are emitted in the INC phase, where the INCL++ model does not take into account the structure of the incident particles themselves, whereas the α particles in the low-energy part are emitted in the evaporation phase. The de-excitation of the target remnant is unrelated to the projectile, so the prediction of the evaporated particles is more accurate. Generally speaking, the simulated energy distribution trends of the INCL++ model are in better agreement with the experimental measurements.

V. DISCUSSION

In this paper, Monte Carlo simulations of the nuclear reactions induced by an 80.5 MeV/u ^{12}C beam on Cu, W, Au, and Pb targets are performed using the GEANT4 toolkit to obtain the energy spectra and angular distributions of the outgoing light charged particles, and the simulation results are compared with previous experimental measurements. Three major nuclear reaction models are used in the simulations: G4BinaryLightIonReaction, G4QMDReaction, and INCL++, and the agreement between the calculated results of these three models and the experimental measurements is analyzed.

For the energy distributions, the INCL++ model describes the trend of the double differential cross section with the energy better. The emitted light charged particles predicted by QMD at 30° are in better agreement with the experimental measurement in the high-energy part of the energy spectra (except for ^{3}He), and the simulation results of the BIC model have the lowest agreement with the experimental results. In addition, the INCL++ model better reproduces the energy spectra of the fragments at 60° and 120°.

For the angular distributions, the difference between the single differential cross sections of most fragments and the experimental data is less than 50%, and in particular, the simulations for protons and α particles are in good agreement with the experimental results. The results of the BIC and the INCL++ models are slightly better than those of the QMD model. However, the three models do not differ much in their ability to reproduce the angular distribution of outgoing light charged particles.

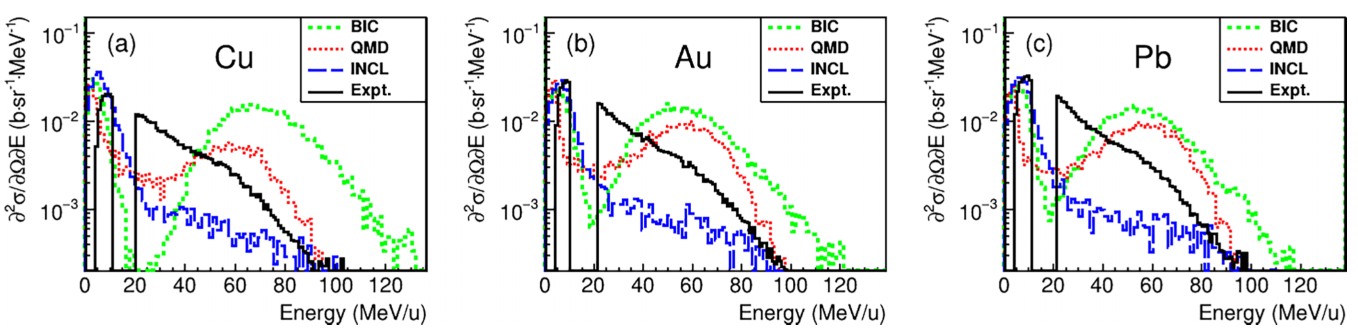

FIG. 6. Energy distributions of α particles at 30° for Cu (a), Au (b), and Pb (c) targets. The colored lines represent the GEANT4 simulation results with BIC, QMD, and INCL++ models. The black lines are experimental data.

For the outgoing light charged particles of different target materials, the INCL++ model has good prediction results for the protons and α particles with $E < 10$ MeV/u at 30Â°, but none of the three models is accurate enough for the higher energy fractions.

In summary, the study shows that none of the three GEANT4 built-in hadronic physics models (BIC, QMD, and INCL) can accurately reproduce the experimental results, including energy spectra and angular distributions of secondary light charged particles. And some reasons for the disagreement between the simulation results and the experimental measurements are analyzed. The models still have opportunities for improvement in predicting the forward-angle emitted particles in the intermediate-energy nucleus-nucleus reactions.

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