PRIMARY ISOTOPIC YIELDS FOR MSDM CALCULATIONS OF SPALLATION REACTIONS ON ²⁰⁸Pb WITH PROTON ENERGY OF 1 GeV

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Introduction

Spallation reactions have recently attracted considerable attention due to their importance in technical applications and fundamental physics. For example, they can act as intense neutron sources for accelerator-driven radiologically clean nuclear systems (ADS) [1,2] for energy generation and nuclear waste transmutation. In this system, lead constitutes an ideal spallation target since its neutron yield is high and it is very transparent to neutrons of energies below 1 MeV. Isotopic production data from proton-induced reactions with energies up to 5 GeV are of great importance for understanding the reaction mechanisms of intermediate nuclear reactions. Recently, precise and numerous measurements of elements produced from proton-induced spallation reactions with energy ranges from 10 MeV to 5 GeV using several target materials were carried out [3-5] due to the interest in a spallation neutron source and ADS. More than 15 000 experimental data points have been obtained. R. Michel [3-5], et al., systematically investigated the data in order to provide a database for model calculations while Yu. E. Titarenko [6] measured the yields of residual product for proton energies from 100 to 2 600 MeV to compare theoretical codes. The target elements were chosen according to their relevance in cosmo chemistry and cosmo physics applications in which the production of cosmogenic nuclides in extraterrestrial matter, the target elements with atomic numbers < 29 and a few high-Z, such as Rb, Sr, Y, Zr, Te, Ba, Nb, etc. are needed. Heavy elements such as Ta, W, Hg, Pb, Bi, Tu and U are under discussion as spallation target materials for spallation neutron source and ADS applications.

However, while these experiments showed the isotopic cross-section of heavy residuals, light residuals were not given. Heavy residual production cross-section relied on mass spectrometry [3-5] and radiochemical methods [7], which only give cumulative yields due to long-lived residuals resulting from short-lived beta decay of primary reaction products. Development of precise spallation reaction models suffered due to lack of primary experimental data. It is hard to systematically compare model calculations with available measured data to investigate the physical reasons for shortcomings of theoretical models. When T. Enqvist [8]/GSI used inverse kinematics by bombarding a liquid hydrogen target with relativistic heavy ions, cross-sections of produced primary residuals from manganese to lead were obtained.

Some theoretical codes (i.e. LAHET [9], quantum molecular dynamics (QMD) [10]) and the semi-empirical method (i.e. Silberberg's YIELDX [11]) can be used to study the isotopic product data from proton-induced spallation reactions with intermediate energies. However, general experience has shown that these models and codes do not satisfy the accuracy requirements of engineering needs for isotopic production [3,6]. S. FAN, one of the authors, introduced a fission model into QMD [12,13] to investigate the mass and charge distribution of residual nuclear fragments from proton-induced reactions with incident energies up to several GeV. The simulation results using QMD plus a fission model were in good agreement with the experimental data; however, the fission model in QMD is only a semi-empirical model. Recently, the cascade exciton model (CEM) was developed to investigate intermediate energy reactions with fission processes and shell corrections introduced into the model [14-18]. The CEM code includes an old cascade code by Toneev and Gudima [19], which models inelastic nucleon/pion nucleus collisions at energies from tens of MeV to 5 GeV, and an exciton/evaporation model, which models the stage following the cascade.

In the present work, the many stage dynamical model (MSDM) [19-21] developed by Russian scientists was adapted to investigate the primary isotopic product cross-section of proton-induced spallation on ²⁰⁸Pb with the energy of 1 GeV. The simple Fermi-gas level density was replaced by the Ignatyuk formula in MSDM to improve the simulations.

MSDM code

The MSDM [19-21] code has been under development since the 1970s by Russian scientists to study intermediate energy nuclear reactions based on well-known Russia nuclear models (e.g. Dubna cascade model, cascade exciton model). MSDM was extended to calculate hadron-induced spallation.

MSDM simulated in an exclusive approach both hadron-nucleus and nucleus-nucleus interactions at energies up to 1 TeV. MSDM was modelled as a three-step process. The first step (the intra-nuclear cascade stage of the reaction below 600 MeV) was treated according to the Dubna cascade model. In this step, the nucleon-nucleon collisions inside the nucleus induced the loss of a few nucleons and led to the formation of an excited pre-fragment. Above 10 GeV, the independent quark-gluon string model (QGSM) [22] was used. In the intermediate area (600 MeV to 10 GeV), an extension QGSM was adopted. A self-consisted description of the cascade stage was provided over a whole energy range of primary hadrons up to 1 TeV. Evolution of the excited residual nucleus to an equilibrium state was described in terms of the pre-equilibrium model based on a Monte Carlo solution of the corresponding master equation (this is the second stage). In the third step of the process, the excited nucleus was de-excited by evaporation of light particles or by fission. Equilibrium de-excitation of the residual nucleus included several mechanisms. For light nuclei (A < 16), the modified Fermi break-up model [23] was used. Medium and heavy nuclei at moderate excitations (E < 2 MeV/nucleon) underwent evaporation, including fission competition for heavy nuclei. Highly excited nuclei (E > 2 MeV/nucleon) could decay into several excited fragments according to the statistical model of multi-fragmentation with consequent particle emission. The equilibrium de-excitation stage completed the run of the MSDM generator.

In the MSDM code, the level density adopted the simple Fermi-gas formula [20]:

$$\rho(E^*) \sim \exp 2\sqrt{aE^*}$$

with the level density parameter $a = (0.1 \text{ to } 0.14) \text{ AMeV}^{-1}$.

To take into account shell effects on level densities and their decrease with increasing excitation energy, the Ignatyuk formula [24] of the level density parameters was adopted:

$$a(Z, N, E^*) = \overline{a}(A)\{1 + \delta W_{gs}(Z, N) \frac{f(E^* - \Delta)}{E^* - \Delta}$$
$$f(E^*) = 1 - \exp(-\gamma E^*)$$

where $\bar{a}(A) = \gamma_1 A + \gamma_2 A^{2/3} B_s$ is the asymptotic Fermi-gas values of the level density parameter at high excitation energies, B_s is the parameter about the surface area of the deformed nucleus. As an approximation, B_s is related to the excitation energy of nuclei in the surface area and can be written as:

$$B_s \propto \frac{E^*}{A} \times A^{2/3} = E^* \times A^{-1/3}$$

and where the parameters γ_1 , γ_2 and γ can be taken as $\gamma_1 = 0.072$, $\gamma_2 = 0.257$ and $\gamma = 0.052$ MeV⁻¹.

Figure 1. Comparisons of the MSDM simulations with the Fermi-gas level density (dot lines) and Ignatyuk formula (solid lines)

The formation cross-sections of the mass and charge distribution; the fission and spallation products of the residuals are shown at the $p + {}^{208}Pb$ reaction with proton energy of 1 GeV. The squares and dots denote the experimental data by T. Enqvist of GSI [8].



Calculation results

Figure 1 shows the calculation results by using the MSDM code with the Fermi-gas level density (dot lines) and Ignatyuk formula (solid lines) for the formation cross-section of the mass and charge distributions at fission (Zn – Figure 1) and spallation (Tm – Figure 1) products. The dots represent experimental data [8] of a proton-induced reaction on ²⁰⁸Pb with energy of 1 GeV. The simulations of MSDM with Fermi-gas level density were: 50% larger than the experimental data at the fission peak, lower at the spallation part and two times larger at the regions of $50 \le Z \le 70$ and $120 \le A \le 160$. The same conditions were seen in the isotopic production cross-sections of the fission (Zn) and spallation (Tm) products. It is clear that simulations by MSDM with Ignatyuk formula level density were in good agreement with experimental data, more so than by MSDM code with Fermi-gas level density.

Figure 2 gives the formation cross-section of residue charge and mass distribution for ²⁰⁸Pb with proton energy of 1 GeV. Good agreement was achieved for both charge and mass spectra for MSDM simulations with experimental data [6,8]. Two components can be found in Fig. 2: a fragmentation peak (collecting the heavy residuals left after evaporation of remnant products close to targets, Z~80 and A~200) and a broad fission peak (centred around Z~40 and A~100, half the target mass number). The

MSDM calculations showed a left peak around A~4 since the MSDM simulations included light particles (such as p, d, t, ³He, ⁴He emission), which were not present in the measured data. Calculations performed using the INCL4+KHSv3p model, the LAHET code (v2.7) and YIELDX (Silberberg's semi-empirical method) are shown together with the present work in Figure 2. Fission fragments of the residual products simulated by LAHET are much lower than the experimental data in fission distribution and are in good agreement with the fragmentation peak. YIELDX results show large deviation from experimental data.

Figure 2. Residual charge (left) and mass (right) production cross-sections for ²⁰⁸Pb with incident proton energy of 1 GeV

The squares represent experimental data by Yu. E Titarenko at ITEP [6], the dash line denotes the GSI experimental data [8]. The predictions of the INCL4+KHSv3p model [25] for charge distribution are given by the dot/dash line, the simulations of the LAHET and YIELDX codes are shown by the open circles and dot lines, respectively. The vertical step lines show the simulations of the MSDM code with the Ignatyuk formula.



Summary

In the present work, the Ignatyuk formula of the level density was adopted to replace the Fermi-gas level density in the MSDM code in order to take into account the shell effects on level densities and their decrease with increasing excitation energy. With this change, the calculation results of MSDM (for the formation cross-section of charge and mass distribution of proton-induced spallation reactions on ²⁰⁸Pb with an energy of 1 GeV) were in good agreement with the experimental data.

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