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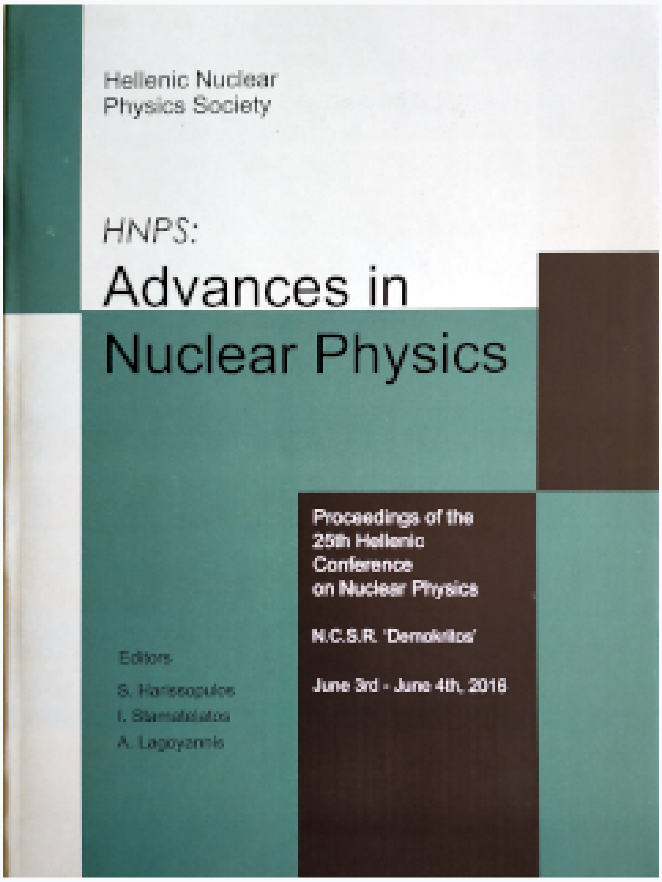

Systematic study of proton-induced spallation reactions with the Constrained Molecular Dynamics (CoMD) model

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Systematic study of proton-induced spallation reactions with the Constrained Molecular Dynamics (CoMD) model

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Abstract

Proton – induced spallation reactions on ^{238}U, ^{208}Pb, ^{181}Ta and ^{197}Au targets at high energies were studied and investigated using the microscopic Contrained Molecular Dynamics (CoMD) model. Total fission cross sections, the ratio fission cross section to residue cross section, mean kinetic energy of fission fragments, mass yield curves and the number of nucleons emitted, before and after scission, as well as the total nucleon multiplicity were calculated using the CoMD model and compared with experimental data from the literature. Some of our calculations showed satisfactory agreement with available experimental data.The calculations of cross sections and the ratio fission cross section to residue cross section as a function of the proton energy gave us the opportunity to estimate observables for unmeasured nuclides.

Keywords constrained modelular dynamics, spallation, spallation neutrons, ATW, ADS

INTRODUCTION

Spallation reactions induced by high-energy protons are of importance for fundamental research and technical applications in nuclear physics, as for instance, medical physics applications and nuclear-reactor technologies. The most important applications of these reactions are the spallation neutron sources, energy production techniques based on accelerator driven systems (ADS), transmutation of radioactive waste and radiation shield design for accelerators and cosmic devices. All these applications require the total fission cross section to be known with high accuracy in a wide proton energy range.

Since the accelerator driven system is considered as an option for the incineration of radioactive waste, many efforts have been made in providing experimental data on interactions in the energy range (100 – 1000 MeV) protons and neutrons with targets that are used in the ADS. Because of the variety of target nuclei and the wide range of energy of the beam particles, theoretical models and nuclear-reaction codes are needed.

Since the available experimental data on spallation reactions are rather poor and fragmentary, an experimental and theoretical work started at GSI Darmstadt [1]. In particular they measured the production of individual nuclides from charged-particle induced spallation reactions, using the inverse kinematics technique with the high resolution magnetic spectrometer FRS. Also improved codes [2] have been developed. However, there are still uncertainties concerning measured total fission cross sections and other observables.

In the present work we used the CoMD model, which is described in the references [11-15].With this model we were able to reproduce (p,f) cross sections, mass yield curves, fission to residue cross sections, and neutron multiplicities for the targets ^{238}U, ^{208}Pb, ^{181}Ta at 200, 500 ,1000 MeV and ^{197}Au at 800 MeV. We chose these targets because they are important especially for accelerator-driven systems (ADS). For example tantalum alloys and lead–bismuth eutectic are optimum materials for the construction of spallation neutron sources. In our work, we compared our CoMD calculations with experimental data taken from refs. [3-10].

COMD RESULTS AND COMPARISONS TO EXPERIMENTAL DATA

The present work was based on the use of the microscopic CoMD model in order to simulate the p-induced spallation reactions at intermediate and high enegies on heavy targets (^{238}U, ^{208}Pb, ^{181}Ta and ^{197}Au) . Below we present the mass yield curve of the reaction p(500 MeV) + ^{208}Pb, the ratio fission cross section to residue cross section for the targets ^{238}U, ^{208}Pb, ^{181}Ta and ^{197}Au and finally the neutron multiplicity for the reaction p(500 MeV) + ^{208}Pb at 200, 500 and 1000 MeV. We compare the CoMD calculations with available experimental data as it is shown on the corresponding figures.

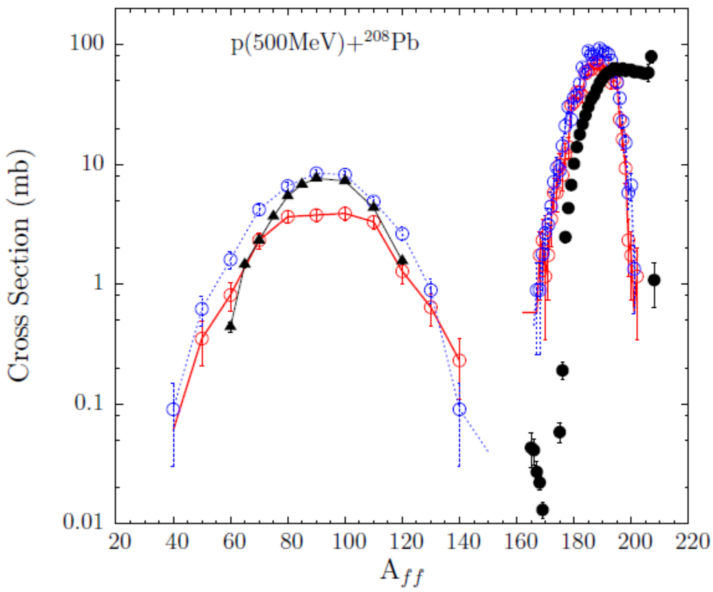

Fig. 1. Mass yield curve of fission fragments and heavy residues from the reaction p (500 MeV) + ^{208}Pb, calculated with the CoMD code. Experimental data: black triangles [3], black circles [4], red points: CoMD calculations with the “standard” symmetry potential, blue points: CoMD calculations with the “soft” symmetry potential.

In Fig. 1, we show the mass number of the fragments as a function of the proton energy for the reaction p (500 MeV) + ^{208}Pb, calculated with the microscopic CoMD code. The CoMD calculations are compared with the experimental data of Rodriguez-Sanchez et al. [3] and Audouin et al. [4]. The red points represent the standard symmetry potential and the blue points the soft potential. Similarly, in this figure we distinguish two regions of fragments. One region has the fission fragments with the smaller mass numbers and the other region has the heavy residues with larger mass numbers, close to the target. We can observe that in the region with the fission fragments, the CoMD calculations are in overall agreement with the experimental data [3], which are indicated with black points. It seems that the cross sections for the fragments produced with the standard potential are lower than the cross sections produced with the soft symmetry potential. In the region with the heavy residues, the CoMD calculations are in agreement with data [4], although at heavier mass numbers there is a discrepancy with the data. We see also that the two symmetry potentials are in mutual agreement.

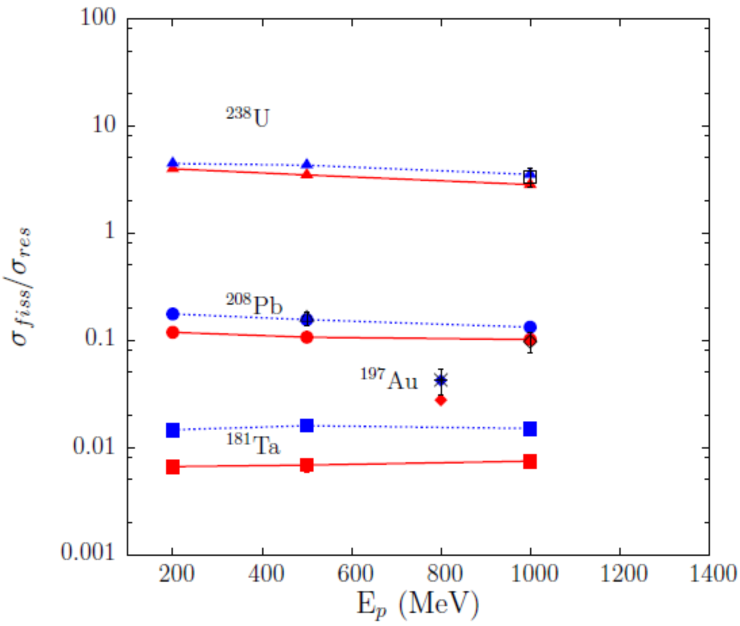

Fig. 2. Fission cross section to residue cross section ratio as a function of the proton energy at 200, 500 and 1000 MeV for the targets ^{238}U, ^{208}Pb and ^{181}Ta and ^{197}Au at 800 MeV calculated with the CoMD code.The calculations are compared with experimental data. Red points: CoMD calculations with the “standard” symmetry potential, blue points: CoMD calculations with the “soft” symmetry potential. Experimental data: open square [6], open triangle [5], rhombus [7], star [8, 9].

In Fig. 2, we present the ratio of fission cross section to residue cross section as a function of the proton energy for ^{238}U, ^{208}Pb and ^{181}Ta at 200, 500 and 1000 MeV and ^{197}Au at 800 MeV. We compare our calculations with the indicated experimental data. At first, we can observe that the ratio of ^{238}U is about 8, which confirms that it is a high fissile nucleus. This value means that it has much higher possibility to undergo fission than evaporation. We notice also that the CoMD calculations at 1000 MeV are in good agreement with the data of Bernas et al. [19]. The ratio of fission cross section to residue cross section for ^{208}Pb, calculated with the CoMD calculations, is about 10%. This demonstrates that lead target has a modest fissility. It appears that our calculations are in good agreement with the data of Fernandez et al. [5] at 500 MeV, especially the results with the soft symmetry potential. At 1000 MeV, the CoMD calculations with the standard potential are in good agreement with the data of Enqvist et al. [7]. Next, we presented the ratio of ^{197}Au at 800 Mev and this is about 6%. This shows that it has intermediate fissility in relation with tantalum and lead. We also compare our results with experimental data [8, 9]. The CoMD calculations with the soft symmetry potential are in very good agreement with the data. For ^{181}Ta, the ratio is only about 1%, as calculated from the CoMD, showing its low fissility. This low value confirms that ^{181}Ta is a low fissility target and shows its tendency to undergo mostly evaporation. In general, we can point out that the CoMD calculations with the soft potential are higher than the standard potential.

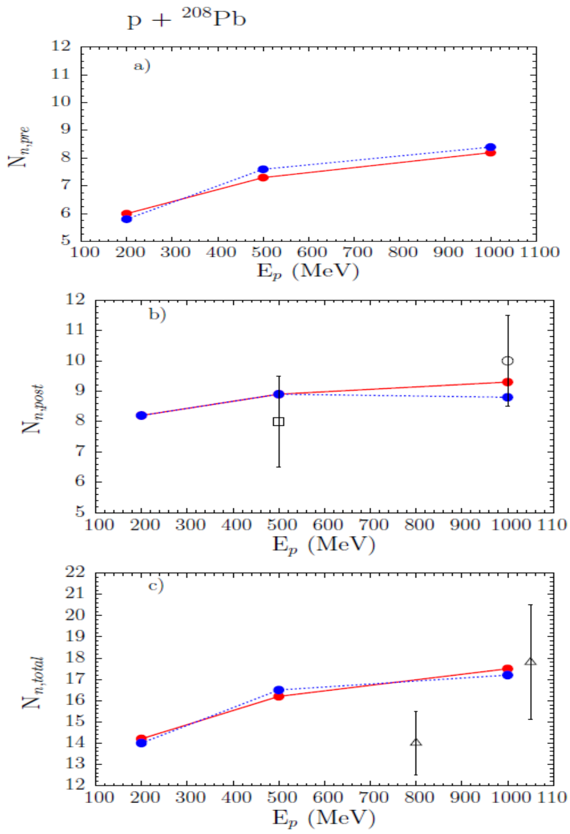

Fig. 3. a) neutron multiplicity before fission, b) neutron multiplicity after scission and c) total neutron multiplicity as a function of the proton energy for the reaction p + ^{208}Pb at 200, 500 and 1000 MeV. The calculations are obtained with the CoMD code and are compared with experimental data. Red points: CoMD calculations with the "standard" symmetry potential, blue points: CoMD calculations with the "soft" symmetry potential. Experimental data: open square [5], open circle [7], open triangle [10] (displaced at 1100 from 1200).

In Fig. 3, we show the neutron multiplicity before scission, after scission and the total neutron multiplicity as a function of the proton energy for the reaction p + ^{208}Pb at 200, 500 and 1000 MeV. The CoMD calculations are represented with red points for the standard symmetry potential and with blue points with the soft symmetry potential. In panel a), we can observe that as the proton energy increases, the number of neutrons that are emitted before scission increases. This happens because of the higher proton energy. In panel b), the number of neutrons that are emitted after scission increases as the proton energy increases, particularly in the calculations with the standard potential. We can point out that our CoMD calculations are higher than the data of Fernandez et al. [5] at 500 MeV, but within the error bar. At 1000 MeV our results are within the error bar of the data of Enqvist et al [7]. In panel c) we present the total neutron multiplicity, which increases as the proton energy increases. Our calculations are compared with the experimental data of Leray et al. [10] at 800 and 1200 MeV. At 800 MeV we have not yet performed calculations with the CoMD code. At 1000 MeV our calculations are in agreement with the data of ref. [10] at 1200 MeV (which for display purposes, has been displaced at 1100 MeV).

DISCUSSION AND CONCLUSIONS

From our calculations with the microscopic code CoMD, we see that the code is able to describe the full dynamic of the spallation process at high energies. We point out that we studied these targets because of the available experimental data in recent literature and because of their importance in the current applications of spallation.We observed that the fission of Pb (and also U, Ta, Au) target is symmetric due to the high excitation energy and because the shell effects at high energies are fully washed out. Also the ratio of fission over residue cross sections gave us the chance to make estimations for targets, such as ^{181}Ta, where there are no experimental data and validate the existent data. Concerning the neutron multiplicities of p + ^{208}Pb, we found that they were also well reproduced, in comparison to experimental data. In general the CoMD calculations agree with the available experimental data for a broad range of observables that we have studied so far. We plan to present in detail the results of the present study in a full paper [16].

We conclude that further theoretical and experimental work of p-induced spallation reactions is needed, and we propose the systematic study of the above observables and comparison with experimental data. Besides the microscopic code CoMD, the use of phenomenological models INC and SMM and the comparison between them is considered important. We would like also to propose measurements in inverse kinematics concerning the ^{181}Ta target.

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