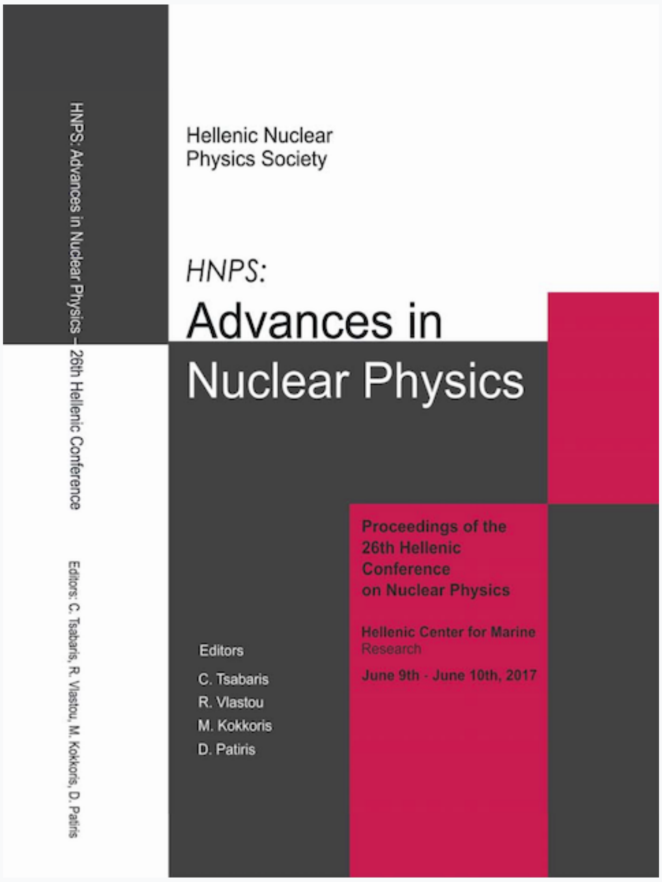
HNPS Advances in Nuclear Physics

Vol 25 (2017)

HNPS2017



Microscopic description of neutron-induced fission with the Constrained Molecular Dynamics (CoMD) Model: Recent progress

S. Papadimitriou, G. A. Souliotis, M. Veselsky, A. Bonasera

doi: [10.12681/hnps.1968](https://doi.org/10.12681/hnps.1968)

Microscopic description of neutron-induced fission with the Constrained Molecular Dynamics (CoMD) Model: Recent Progress

S. Papadimitriou[1,*], G.A. Souliotis[1] , M. Veselsky[2] and A. Bonasera[3,4]

[1] *Laboratory of Physical Chemistry, Department of Chemistry, National and Kapodistrian University of Athens, Athens 15771, Greece*
[2] *Institute of Physics, Slovak Academy of Sciences, Bratislava 84511, Slovakia*
[3] *Cyclotron Institute, Texas A & M University, College Station, Texas, USA*
[4] *Laboratori Nazionali del Sud, INFN, Catania, Italy*

Abstract The microscopic description of the mechanism of nuclear fission still remains a topic of intense nuclear research. Understanding of nuclear fission, apart from the theoretical many-body point of view, is of practical importance for energy pro-duction, as well as for the transmutation of nuclear waste. Furthermore, nuclear fission is essentially the process that sets the upper limit to the periodic table of the elements and plays a vital role in the production of heavy elements via the astrophysical rapid neutron-capture process (r-process).In the present work, we ini-tiated a systematic study of neutron-induced fission reactions using the code CoMD (Constrained Molecular Dynamics) of A. Bonasera and M. Papa[3] [4] [5]. In this paper, we present preliminary results of neutron-induced fission on 235U at neutron energies 10, 20, 50, 70 and 100 MeV. Calculated mass and energy distributions will be shown and compared with the recent experimental data of W. Loveland group[1] [2].It appears that the microscopic code CoMD is able to describe the complicated many-body dynamics of the n-induced fission process. Proper adjustment of the parameters of the effective interaction and possible improvements of the code will be implemented to achieve a satisfactory description of the experiment data.

INTRODUCTION

The study of the mechanism of nuclear fission, that is, the transformation of a single heavy nucleus into two receding fragments, has been a long journey of fruitful research and debate and, still today, is far from being complete. Motivated by the present state of affairs regarding fission research, in this work we initiated a study of neutron induced fission based on on the semi-classical microscopic N-body constrained molecular dynamics (CoMD) model of A.Bonasera and M.Papa [6]. In CoMD code the nucleons are considered as gaussian wavepackets which interact with a phenomenological effective interac-tion.The code implements an effective interaction with a nuclear-matter com-pressibility of K=200 (soft EOS) with several forms of the density-dependence of the nucleon symmetry potential. In addition, CoMD imposes a constraint in the phase space occupation for each nucleon restoring the Pauli principle at each time step of the collision). Proper choice of the surface parameter of the effective interaction has been made to describe fission. In addition,in order

* Corresponding author, email: soulioti@chem.uoa.gr

to introduce the fermionic nature of the system the code implies the Pauli principle through a proper constraint in the phase space.

RESULTS AND DISCUSSION

In this work, we implement a special treatment of the surface parameter of the effective interaction in order to describe fission. The study of the preliminary stage of the process until the scission point was performed with a configuration of the ground state which has surface parameter C_S=-2, so the values of the radius and of the binding energy were close to the experimental ones. However, with this configuration the system does not undergo fission, only evaporation. In order to study the fission process, we performed calculations with surface parameter C_S=0. The problem with this choice is that the value of binding energy deviates from the experimental value. So, we introduced a time depen-dent surface parameter, in order to start with the correct configuration of the ground state and also drive the system into fission. For time t=0 fm/c the initial value of the surface parameter is $C_{S,O}$=-2 and for time=300 fm/c the final value of the surface parameter is $C_{S,F}$ =0. The value of the Cs parameter in every time step during these 300 fm/c is given by the linear function:

$$C_S(T) = C_{S,O} + C_{S,F} - C_{S,O}/T_F - T_F \qquad (1)$$

It is important to mention that in every step of the process we ensure the energy conservation of the system, by converting the change of potential energy into kinetic energy.

For a given reaction, a total approximately 2000 events were collected. For each event the impact parameter was chosen in the range b=0–7.5 fm, following a triangular distribution. Each event was followed up to 15000 fm/c and the phase space coordinates were registered every 100 fm/c. At each time step, fragments were recognized and their properties were reported.

In this presentation, we discuss preliminary results of fission for the reaction n+^{235}U at low and intermediate energies. In Fig. 1, we present the energy per nucleon as a function of the radius. In Fig. 1a) profile of the potential energy of the nucleons is shown, where protons are above neutrons because of the Coulomb interaction. In Fig. 1b) we show the distribution of the ki-netic energy where neutrons seem to be above protons. This happens because the nucleus ^{235}U has more neutrons than protons that occupy the same vol-ume,rendering the density of neutrons larger than that of the protons. In Fig. 1c) we present the total energy of the nucleus which has a local minimum at 2 fm and a total minimum at 7 fm. Fig. 1d) is pictured the variation of Coulomb interaction and in Fig. 1e) evolution of the surface term. The surface term has a maximum at about 4fm, whereas for distance values greater than 4fm the term behaves repulsively. Finally, in Fig. 1f) we show the number of neutrons, protons and nucleons versus radius. The maximum number of nucleons is found at a distance of 6 fm.

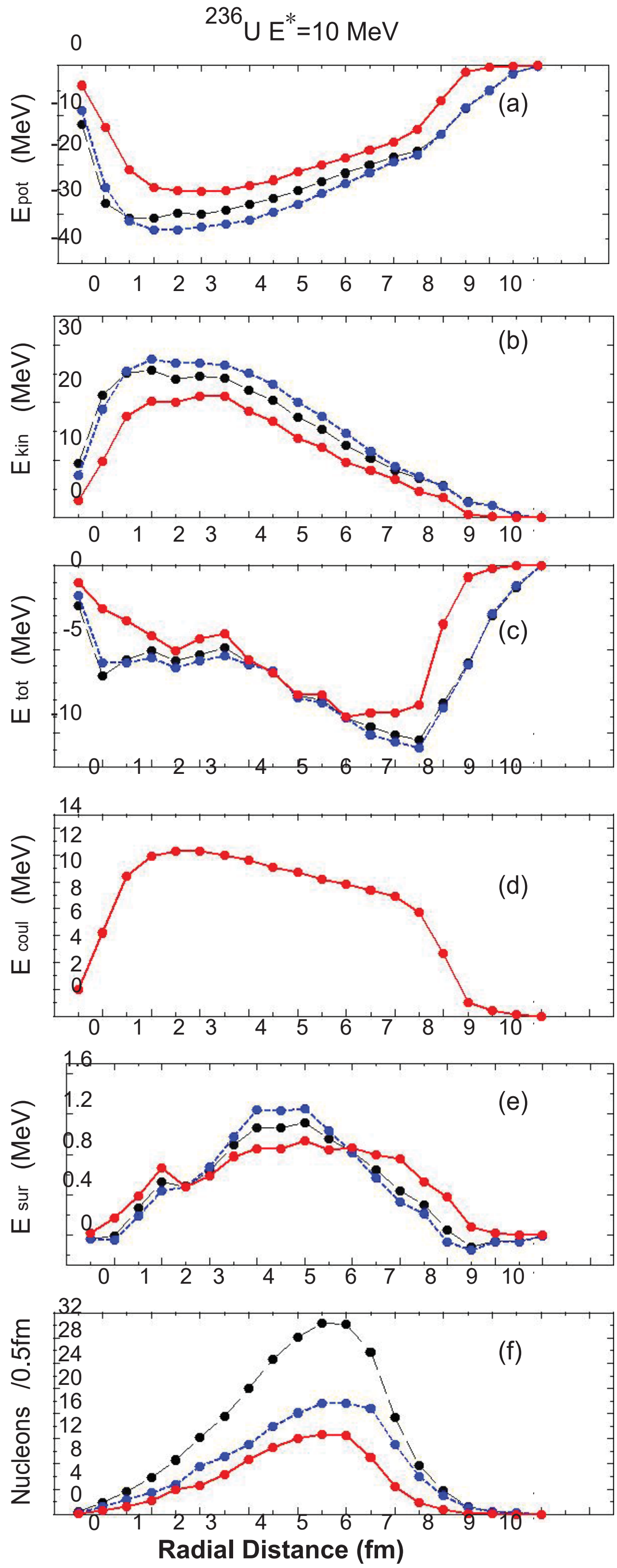


Fig. 1. (Color online) Calculated energy terms per nucleon versus radial distance. Red line: protons. Blue line: neutrons. Black line: nucleons. a) Potential energy per nucleon. b) Kinetic energy. c) Total energy. d) Energy Coulomb. e) Surface energy. f) Nucleons/0.5 fm.

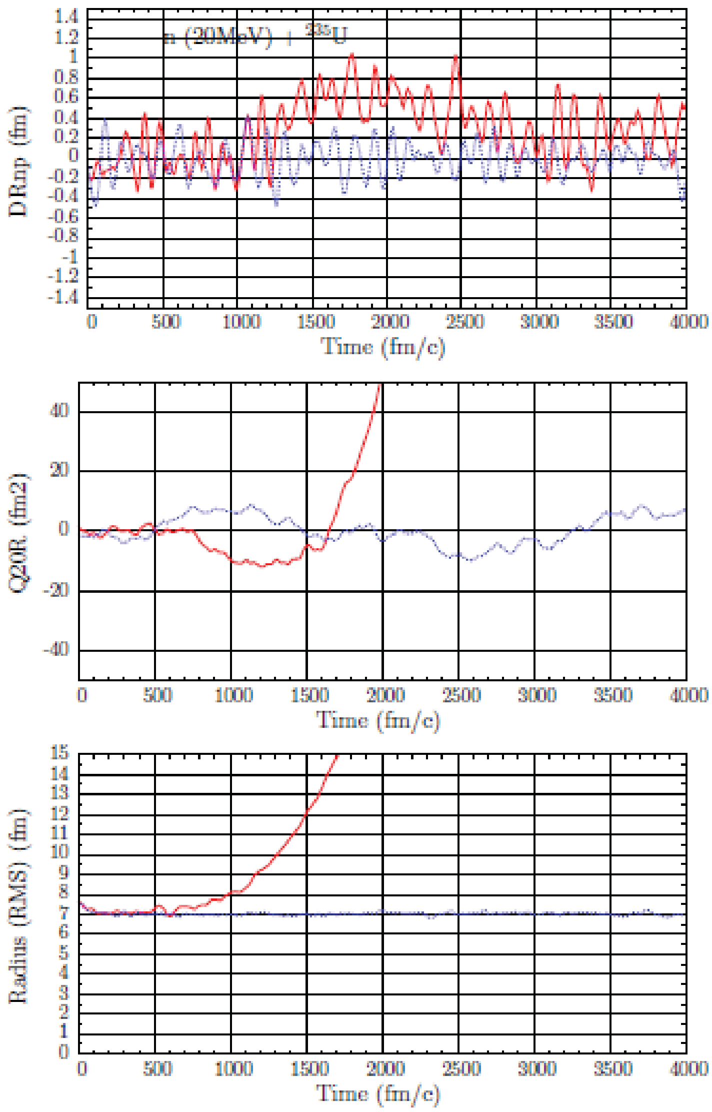


Fig. 2. (Color online) CoMD calculations on important macroscopic quantities of the nucleus versus time for the reaction n(20MeV)+^{235}U. Red continuous line: Cal-culation with Cs=0. Blue dotted line: Calculation with C_S=-2. a)Relative distance between the centres of mass of protons and neutrons (GDR). b)Time evolution of the quadrupole moment(GQR). c)Time evolution of the radius(GMR).

In Fig. 2, we present the evolution of three moment of the nucleus as a function of time for the reaction n(20MeV)+^{235}U. The continuous red line corresponds to the calculation with surface parameter Cs=0 and the dashed blue line to the calculation with surface parameter CS=-2. In Fig. 2a) we show the distance between the centres of mass for the Fermi gases of protons and neutrons on z-axis of the nucleus. The blue line with CS=-2 oscillates harmonically around the center of mass of the system, while the red line curve with CS=0 shows an abrupt increase. Similar pattern is observed in the time evolution of the radius of the nucleus, as we see in Fig. 2c). The distributions in Fig. 2b) and 2c) indicate that with CS=0, the system undergoes fission, while with CS=-2 the only way of de-excitation is the evaporation.

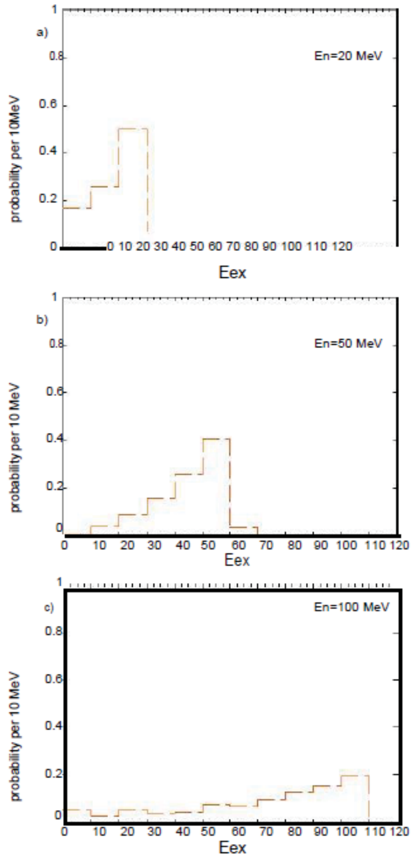


Fig. 3. (Color online) CoMD calculations on the distribution of the excitation energy of the compound nucleus at 3000 fm/c.a) probability of the excitation energy for the reaction n(20 MeV)+^{235}U. b) probability of the excitation energy for the reaction n(50 MeV)+^{235}U. c) probability of the excitation energy for the reaction n(100 MeV)+^{235}U.

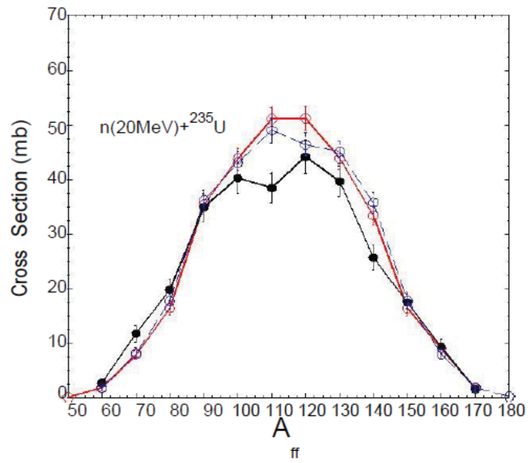


Fig. 4. (Color online) CoMD calculated yield curves for the fission reaction n(20MeV)+235 U. Open red points: CoMD calculations with standard symmetry potential and CS=0 . Open blue points: CoMD calculations with standard symmetry potential and CS=0. Full black points: CoMD calculations with standard symmetry potential and CS=2. Pink open triangles: experimental data of the Loveland group [1].

In Fig. 3, we display the distribution of the excitation energy of the nucleus at 3000 fm/c taken as a representative time before fission. We performed calculations with three different neutron energies: 20,50 and 100 MeV. In Fig. 3a) and 3b) which correspond to the calculations with 20 and 50 MeV, respectively, the most probable excitation energy is near the projectile energy. In the calculation at 100 MeV [Fig. 3c)] the excitation energy shows a broad distribution, due to particle emission of the compound nucleus before the scission point.

In Fig. 4, we show the calculated mass distributions for the reaction n(20 MeV)+235U. The distributions with open symbols connected with dotted (blue) and solid (red) lines have surface parameter CS=0 and show a quite symmetric fission [7]. The calculations shown by the full points connected with black line have time dependent surface parameter CS(T) and suggest a rather asymmetric fission as expected for this low-energy fission reaction [2].

In Fig. 5 we present the total kinetic energy of the fission fragments versus the kinetic energy of the neutron projectile. Our calculations with the CoMD model were performed with the soft and the standard symmetry potential and they were compared with the experimental data at the corresponding energies of Loveland and al. [1]. The calculation with time dependent surface parameter CS(t) describe better the experimental data at low energies, while the calculations with CS=0 describe better the experimental values for higher neutron energies.

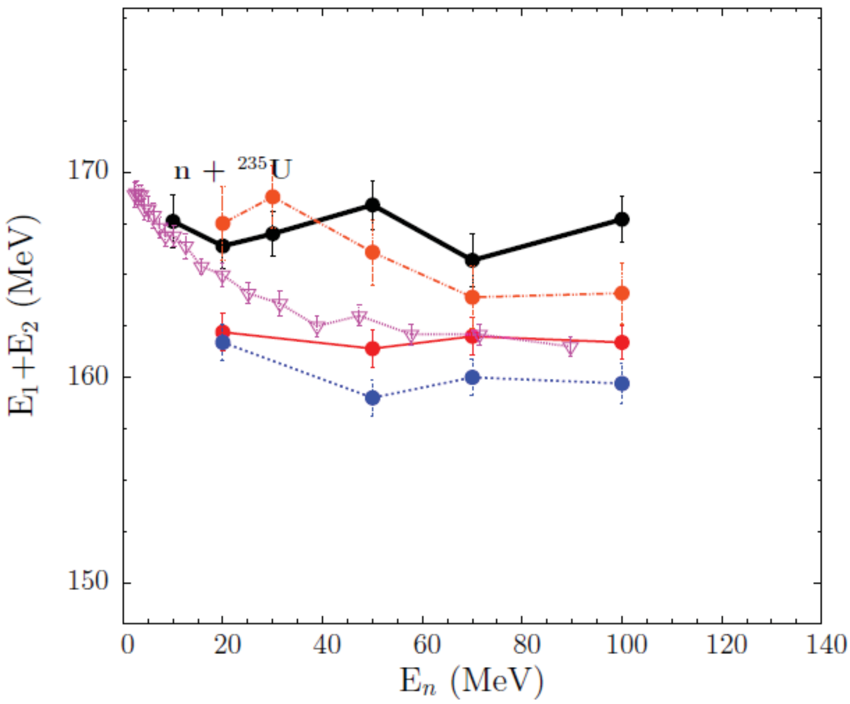


Fig. 5. (Color online) CoMD calculations on average total energy of fission fragments with respect to incident neutron energy. Red points connected with thin dotted lines: CoMD calculations with standard symmetry potential and Cs=0. Blue points connected with dotted line: CoMD calculations with soft symmetry potential and Cs=0. Black points: CoMD calculations with standard symmetry potential and Cs=-2. Pink open triangles: experimental data of the Loveland group [1].

CONCLUSIONS

In the present work we employed the semi-classical microscopic code CoMD to describe neutron induced fission, at several energies on ^{235}U. We intend to study systematically the neutron induced fission by calculating a number of representative observables such as: mass yield curves, cross sections, energy distributions, the fission time scale and the pre-fission and post-fission neutron and proton emission. We mention that the code does not include the effect of spin-orbit interaction in the mean filed, as a result of the absence of spin dependence in the effective nucleon-nucleon interaction. We intend to add such a dependence in order to improve our ability to examine low energy fission.

References

[1] R. Yanez, W. Loveland, J. Kind, J.S. Barett, Total kinetic energy release in the fast neutron induced fission of 235U arXiv:1605.09690v2 [nucl-ex] (2016)

[2] W. Loveland, J. King, Total kinetic energy release in the fast neutron induced fission of 232Th and 235U, arXiv:1702.01790v1 [nucl-ex] (2017).

[3] M. Papa, T. Maruyama, and A. Bonasera, Constrained Molecular dynamics approach to fermionic systems, Phys.Rev. C64, 024612 (2001).

[4] M.Papa, G.Guluilani, and A. Bonasera, Constrained Molecular Dynamics II: a N-body approach to fermionic systems, J. Comp. Phys. 208, 403 (2005).

[5] A. Bonasera, M. Bruno, C.O. Dorso and P.F. Mastinu, Critical phenomena in nuclear fragmentation, Riv. Nuovo Cimento 23,1 (2000).

[6] M. Papa, Many-body in semiclassical molecular dynamics and Skyrme interaction, Phys. Rev.C87,014001 (2013).

[7] N.Vonta, G.A. Souliotis, M. Veselsky, and A. Bonasera, Microscopic dynamical description of proton induced fission with the constrained molecular dynamics model, Phys. Rev.C 92, 024616 (2015).