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Development of dynamical model for simulation of nuclear spallation

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The aim of this article is development of Ultra Relativistic Quantum Molecular Dynamic model for calculations of nuclear spallation and multifragmentation. The results of this dynamical approach is analyzed in comparison with the model of statistical (multi)fragmentation, namely, the cascade model including evaporation and multifragmentation, developed in the framework of percolation model.

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1. Introduction

As a challenging tasks for theoretical models nuclear spallation and/or multifragmentation are the subjects of intensive theoretical and experimental investigations. There are two theoretical approaches describing multifragmentation: statistical and dynamical. In statistical multifragmentation models an excited remnant achieves thermal equilibrium state and then expands, eventually reaching the freeze–out volume. At this point it fragments into neutrons, light charged particles and IMFs. In dynamical models IMFs are formed at the fast stage of nuclear collision via dynamical forces between nucleons during the evolution of the total system of interacting projectile and target. In this case the whole system and its parts (projectile and target remnants) never pass through states of thermal equilibrium. Well known models of statistical description of disintegration of the excited nuclei include evaporation and multifragmentation [1]. At the same time the Quantum Molecular Dynamic (QMD) model was successful for calculations of isotopes generation at collision energies less than 0.3 AGeV [2, 3]. For higher energies a new version of QMD, Ultra Relativistic Quantum Molecular Dynamic, UrQMD, model has been developed. However, there is a serious deficiency in UrQMD: it does not take into account formation the residual nucleus and its fragmentation. In this paper we propose UrQMD modification, adding nuclear spallation and multifragmentation. Parameters of the modification are adjusted by comparison with the Modified Cascade Model, including evaporation, fission and multifragmentation. The modified UrQMD is compared with the experimental data on spallation of the iron nucleus irradiated by protons.

2. Modified Cascade Model

The intranuclear cascade model is one of the basic tools for analyzing spallation and multifragmentation processes in nuclear collisions. In the traditional cascade model of hadron-nucleus and nucleus-nucleus interactions, particle production is treated in two stages. In the first fast stage, intranuclear cascade occurs inside the target and (or) the projectile nuclei and some nucleons from the target and projectile nuclei are knocked out, together with mesons. In the second stage, residual nuclei (generally, in an excited state) divide into two remnants in the fission channel or evaporate protons, neutrons and/or light nuclei, including helium isotopes. However, experimental data indicate that, at intermediate energies, a third competing process, multifragmentation, comes into play, in which excited remnants break up into intermediate mass fragments (IMF). In statistical multifragmentation models, an excited remnant achieves thermal equilibrium state and then expands, eventually reaching the freeze–out volume. At this point it fragments into neutrons, light charged partiles and IMFs. In paper [4] the process of nuclear multifragmentation has been implemented into cascade-evaporation model in the framework of percolation theory, together with evaporation and fission channels of the disintegration of excited remnants.

3. UrQMD modification

The UrQMD model [5, 6] is a microscopic model based on a phase space description of nuclear reactions. It describes the phenomenology of hadronic interactions at low and intermediate energies ($\sqrt{s} < 5$ GeV) in terms of interactions between known hadrons and their resonances. At higher

energies, $\sqrt{s} > 7$ GeV , the excitation of color strings and their subsequent fragmentation into hadrons are taking into account. The model is based on the covariant propagation of all hadrons considered on the (quasi-)particle level on classical trajectories in combination with stochastic binary scattering, color string formation and resonance decay. It represents a Monte Carlo solution of a large set of coupled partial integro-differential equations for the time evolution of the various phase space densities of particle species $i = N, \Delta, \Lambda$, etc. The main ingredients of the model are the cross sections of binary reactions, the two-body potentials and decay widths of resonances. The equations of motion of the many-body system is calculated by means of a generalized variational principle. The Hamiltonian H of the system

$$H = \sum_i T_i + \frac{1}{2}\sum_{ij} V_{ij} \tag{3.1}$$

contains a kinetic term T_i and mutual interactions V_{ij}. The time evolution equations are solved numerically. The equations have the same structure as the classical Hamilton equations. The interaction is based on a non-relativistic density-dependent Skyrme-type equation of state with additional Yukawa- and Coulomb potentials. The Skyrme potential consists of a sum of two- and a three-body interaction terms. The two-body term, which has a linear density-dependence models the long range attractive component of the nucleon-nucleon interaction, whereas the three-body term with its quadratic density-dependence is responsible for the short range repulsive part of the interaction.

A projectile or target nucleus is modeled according to the Fermi-gas ansatz. The wave-function of the nucleus is defined as the product wave-function of the single nucleon Gaussians. In configuration space the centroids of the Gaussians are randomly distributed within a sphere with radius $R(A)$,

$$R(A) = r_0(\frac{1}{2}[A + (A^{\frac{1}{3}} - 1)^3])^{\frac{1}{3}}, \tag{3.2}$$

where r_0 is a parameter.

Impact parameter of a collision is sampled according to the quadratic measure ($dW \sim bdb$). At given impact parameter centers of projectile and target are placed along the collision axis in such a manner that a distance between surfaces of the projectile and the target is equal to 3 fm. Momenta of nucleons are transformed in the system where the projectile and target have equal velocities directed in different directions of the axis. After that the time propagation starts. During the calculation each particle is checked at the beginning of each time step whether it will collide within that time step. A collision between two hadrons will occur if $d < \sqrt{\sigma_{tot}/\pi}$, where d and σ_{tot} are the impact parameter of the hadrons and the total cross-section of the two hadrons, respectively. After each binary collision or decay the outgoing particles are checked for further collisions within the respective time step.

Implementation of the fragments and residue production in UrQMD are performed by the following manner. On the first stage of the process of nuclear collision the time evolution of the spatial distributions of nucleons and mesons (pions, kaons, etc) are traced. Then, taking into account relative momenta of nucleons, and a mutual nucleon-nucleon potential in (3.1), the nucleon clusters are formed. On the next step the nuclear fragments are shaped from these clusters, and their kinetic energies, masses and binding energies are calculated. There is one important problem: how long

should the process of cluster/fragment formation be prolonged. Indeed the dynamical evolution of the cluster/fragment formation can continue infinite time. When the dynamical cluster/fragment formation should be stopped could be defined from comparison with yield of fragments (including excited ones) in MCAS. On the last stage of the interaction the decay of the excited fragments to smaller ones with the usage of the EVAPOR code of MCAS are calculated. At the moment the excitation energy of fragments are simulated from the spectra given by MCAS. Stages of fragments generation and decay of excited of them into smaller ones are compared with MCAS stages of (multi)fragmentation/spallation and evaporation correspondingly.

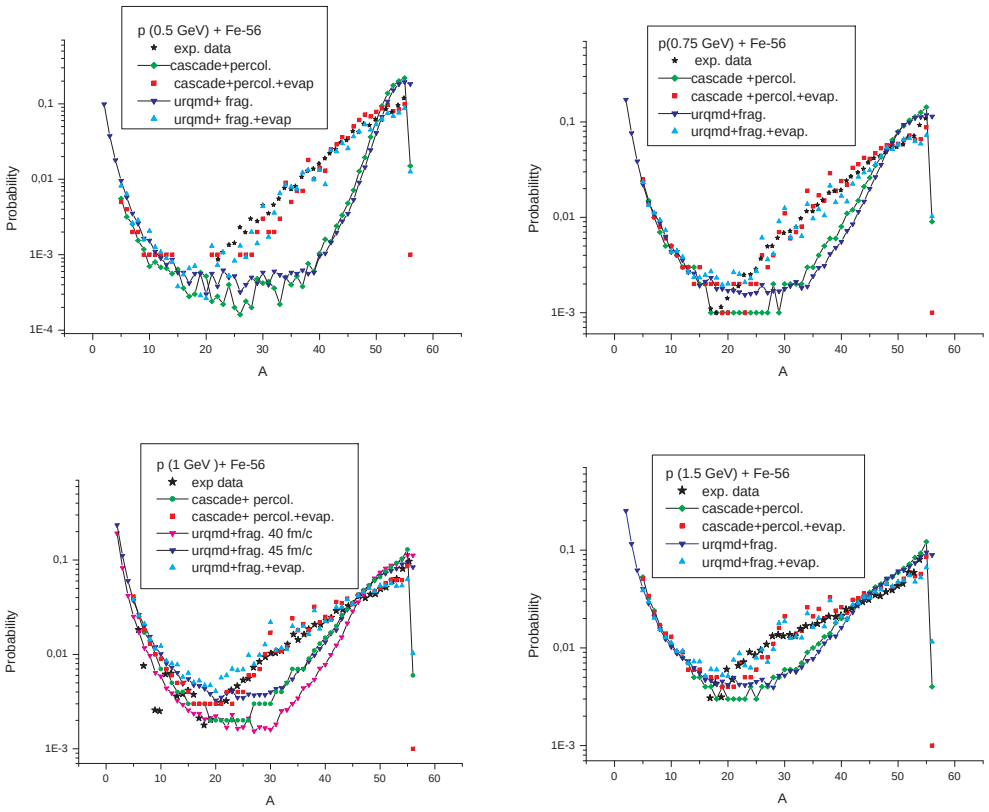

Figure 1: Mass distributions of fragments before evaporation (intermediate stage) and evaporated fragments (final stage) in $p + ^{56}Fe$ + p reaction. Experimental data are depicted by black stars.

4. Results

Adequacy of the modified UrQMD, the Dynamical Model, to describe fragments production is demonstrated by comparison of simulation at different stages of the evolution process with MCAS (Fig. 1). By this comparison we can stop the process of the fragments formation at a certain time. The mass distribution of fragments at the formation times 40 fm/c and 45 fm/c for the energy 1 GeV is given in Fig. 1. One can see that 45 fm/c more preferable for adequacy of UrQMD and MCAS

results. The final mass distributions of fragments, simulated by the modified UrQMD and MCAS, are compared with the experimental data from GSI Darmstadt.The mass distributions of light and intermediate-mass nuclides have been measured in the reaction $p+^{56}Fe$ at different energies [7]. The experiment has been performed in inverse kinematics irradiating a thin liquid-hydrogen target by iron beam. The points on plots of the Figure 1 depict the mass distributions calculated by the Dynamical model and MCAS at different stages of the fragment formation. UrQMD+fragment and CASCADE+percolation correspond to stages before evaporation. At the final, evaporation stage, the excited fragments can emit protons, neutrons, and light nuclei, deuterons, tritons, He-3, He-4. As one can see there is a satisfactory agreement between statistical and dynamical models and experimental data.

5. Conclusion

The Dynamical model of spallation/fragmentation of nuclei in hadron-nucleus and nucleus-nucleus reactions in the framework UrQMD has been developed. Isotopes production calculated by Modified Cascade and Dynamical Models quite agree with experimental data. Thus, UrQMD which is very popular and effective in simulation of particle production in intermediate and high energies can used for description of spallation/fragment formation, as well.

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