

Effect of effective interaction potentials used in quantum molecular dynamics on nucleon-induced reactions

D. N. Kadrev^{1,2} and Y. Watanabe¹

¹*Department of Advanced Energy Engineering Science, Kyushu University, Kasuga, Fukuoka 816-8580, Japan*

²*Institute for Nuclear Research and Nuclear Energy, Bulgarian Academy of Sciences, Sofia 1784, Bulgaria*

A quantum molecular dynamics (QMD) model is applied to investigate the light-ion production in nucleon-induced reactions. The JQMD code is employed and the generalized evaporation model (GEM) is used to account for statistical decay processes after the QMD stage. In order to improve the ground state properties of the created nucleus other important effective interaction potentials, such as Pauli, momentum-dependent and Yukawa are added to the JQMD. The effect of the newly added effective interactions on the total reaction cross sections and differential cross sections of light-ion production in nucleon-induced reactions is also investigated.

1 Introduction

Various applications involving fast neutrons with energies over several tens of MeV have recently been developed, e.g., dosimetry at commercial aircraft altitudes, radiation therapy of cancer, soft-error estimation in microelectronic devices, accelerator-driven transmutation of nuclear waste, etc. Elementary interaction of a neutron with matter occurs via only a nuclear reaction because it has no charge. As a result, the kinetic energy is transferred into matter by light ions (p, d, t, ³He and ⁴He) and recoils produced by the nuclear reaction. As the incident neutron energy increases, it is known that emission of light ions with relatively high energy in the forward direction through direct and preequilibrium processes becomes important. Thus, it is necessary to enhance our understanding of these mechanisms and to establish a reliable model predicting accurately the energy and angular distributions of produced light ions from both viewpoints of fundamental nuclear physics and the above-mentioned applications.

To meet the needs, we have chosen the quantum molecular dynamics (QMD) model [1, 2] as one of the models describing the preequilibrium light-ion production in nucleon-induced reactions, and examined the applicability of the JAERI QMD (JQMD) code [2]. It has been found that the JQMD calculation can reproduce preequilibrium nucleon emission fairly well [2, 3], while it underestimates remarkably preequilibrium emission of light clusters (d, t, ³He and ⁴He) [4, 5]. More recent work [5] has suggested that implementation of a phenomenological surface coalescence model into the QMD leads to a reasonable description of preequilibrium light-cluster production in neutron-induced reactions. For further refinement, it is important to investigate how the model parameters used in the QMD calculations have an impact on the nucleon-induced light-cluster production.

It is well known that the usage of realistic initial ground state configuration in the QMD model is essential for the high predictable ability of the studied reactions. It has been found that the JQMD model can reproduce satisfactorily ground state properties of nuclei, e.g. the binding energy, root-mean-square radii, density and momentum distributions. The results show

overestimation of the root-mean-square radii in comparison with the experimental data, underestimation of the density in the center of the nucleus and its increase in the surface region and cannot reproduce experimentally observed high-momentum component of the total momentum distribution. One of the reasons for this is expected to be the simple effective interaction used in the JQMD model. It includes an attractive 2-body and repulsive 3-body simple Skyrme interactions, Coulomb and symmetry terms. The total wave function is a direct product of single-particle wave functions and is not antisymmetric. The fermionic properties of nucleons are taken into account only by checking the Pauli principle in the ground state and by the Pauli blocking effect in the collision process. It has been demonstrated [6] that it is possible to devise a Pauli potential so that the fermionic nature of the nucleons in a semiclassical manner could be reproduced, and this potential could yield an effect similar to that of the antisymmetrization of the total wave function.

In order to improve the ground state properties we modify the JQMD model by introducing the Pauli potential and also other important interactions such as momentum-dependent and Yukawa. The effects of these interactions on the total reaction cross sections and differential cross sections of light-ion production in nucleon-induced reactions are investigated.

2 The QMD model

The JQMD model is described in details in Ref. [2]. In this section we give only some basic equations and ingredients which are changed or added to the JQMD.

The QMD model is a semi-classical simulation model in which each nucleon state is represented by a Gaussian wave function of width L

$$\phi_i(\mathbf{r}) = \frac{1}{(2\pi L)^{3/4}} \exp \left[-\frac{(\mathbf{r} - \mathbf{R}_i)^2}{4L} + \frac{i}{\hbar} \mathbf{r} \cdot \mathbf{P}_i \right], \quad (1)$$

where R_i and P_i are the centers of position and momentum of the i -th nucleon, respectively. The total wave function is assumed to be a direct product of these wave functions.

The one-body distribution function is obtained by the Wigner transform of the wave function,

$$f(\mathbf{r}, \mathbf{p}) = \sum_i f_i(\mathbf{r}, \mathbf{p}), \quad f_i(\mathbf{r}, \mathbf{p}) = 8 \exp \left[-\frac{(\mathbf{r} - \mathbf{R}_i)^2}{2L} - \frac{2L(\mathbf{p} - \mathbf{P}_i)^2}{\hbar^2} \right]. \quad (2)$$

The equation of motion of nucleons is given by the Newtonian equations

$$\dot{\mathbf{R}}_i = \frac{\partial H}{\partial \mathbf{P}_i}, \quad \dot{\mathbf{P}}_i = -\frac{\partial H}{\partial \mathbf{R}_i}, \quad (3)$$

and the stochastic two-body collision term.

The Hamiltonian H in the present work consists of the kinetic energy and the energy of two-body effective interactions

$$H = T + V_{\text{local}} + V_{\text{Pauli}} + V_{\text{MD}} + V_{\text{Yukawa}}, \quad (4)$$

where $T = \sum_i \sqrt{m_i^2 + \mathbf{P}_i^2}$ is the kinetic energy including the mass term. V_{local} , V_{Pauli} , V_{MD} and V_{Yukawa} are the local potential, the Pauli potential, the momentum-dependent (MD) potential and the Yukawa potential parts, respectively.

For the local potential part we adopt the effective interaction used in the JQMD model. It contains the Skyrme type, the Coulomb and the symmetry terms,

$$V_{\text{local}} = \frac{A}{2\rho_0} \sum_i \langle \rho_i \rangle + \frac{B}{\rho_0^\tau (1+\tau)} \sum_i \langle \rho_i \rangle^\tau + \frac{e^2}{2} \sum_{i,j(\neq i)} \frac{c_i c_j}{|\mathbf{R}_i - \mathbf{R}_j|} \text{erf} \left(|\mathbf{R}_i - \mathbf{R}_j| / \sqrt{4L} \right) + \frac{C_s}{2\rho_0} \sum_{i,j(\neq i)} (1 - 2|c_i - c_j|) \rho_{ij}, \quad (5)$$

where erf denotes the error function, c_i is 1 for protons and 0 for neutrons and $\langle \rho_i \rangle$ is an overlap of density with other nucleons defined as

$$\langle \rho_i \rangle \equiv \sum_{j \neq i} \rho_{ij} \equiv \sum_{j \neq i} \int d\mathbf{r} \rho_i(\mathbf{r}) \rho_j(\mathbf{r}) = \sum_{j \neq i} (4\pi L)^{-3/2} \exp \left[-(\mathbf{R}_i - \mathbf{R}_j)^2 / 4L \right], \quad (6)$$

with

$$\rho_i(\mathbf{r}) \equiv \int \frac{d\mathbf{p}}{(2\pi\hbar)^3} f_i(\mathbf{r}, \mathbf{p}) = (2\pi L)^{-3/2} \exp \left[-(\mathbf{r} - \mathbf{R}_i)^2 / 2L \right]. \quad (7)$$

In addition to the JQMD effective interaction we include also Pauli potential, momentum-dependent term and Yukawa potential.

The Pauli potential [6, 7] is introduced for the sake of simulating fermionic properties of nucleons in a semiclassical way. This phenomenological potential prohibits nucleons of the same spin σ and isospin τ from coming close to each other in the phase space. Here we employ the Gaussian form of the Pauli potential

$$V_{\text{Pauli}} = \frac{C_P}{2} \left(\frac{\hbar}{q_0 p_0} \right)^3 \sum_{i,j(\neq i)} \exp \left[-\frac{(\mathbf{R}_i - \mathbf{R}_j)^2}{2q_0^2} - \frac{(\mathbf{P}_i - \mathbf{P}_j)^2}{2p_0^2} \right] \delta_{\tau_i \tau_j} \delta_{\sigma_i \sigma_j}. \quad (8)$$

The momentum-dependent term [7] is introduced as a Fock term of the Yukawa-type interaction. It is divided into two ranges so as to fit the effective mass and the energy dependence of the real part of the optical potential, as

$$V_{\text{MD}} = \frac{C_{\text{ex}}^{(1)}}{2\rho_0} \sum_{i,j(\neq i)} \frac{1}{1 + [(\mathbf{P}_i - \mathbf{P}_j) / \mu_1]^2} \rho_{ij} + \frac{C_{\text{ex}}^{(2)}}{2\rho_0} \sum_{i,j(\neq i)} \frac{1}{1 + [(\mathbf{P}_i - \mathbf{P}_j) / \mu_2]^2} \rho_{ij}. \quad (9)$$

The Yukawa potential [6, 8] has the form

$$V_{\text{Yukawa}} = \frac{C_Y}{2} \sum_{i,j(\neq i)} \frac{\exp(L/\gamma_Y^2)}{2|\mathbf{R}_i - \mathbf{R}_j|} \left\{ \exp\left(-\frac{|\mathbf{R}_i - \mathbf{R}_j|}{\gamma_Y}\right) \left[1 - \text{erf} \left(\frac{2L/\gamma_Y - |\mathbf{R}_i - \mathbf{R}_j|}{\sqrt{4L}} \right) \right] - \exp\left(\frac{|\mathbf{R}_i - \mathbf{R}_j|}{\gamma_Y}\right) \left[1 - \text{erf} \left(\frac{2L/\gamma_Y + |\mathbf{R}_i - \mathbf{R}_j|}{\sqrt{4L}} \right) \right] \right\}. \quad (10)$$

Two sampling methods are employed in the JQMD model for creation of the ground state, random packing and frictional cooling. The random packing method accepts initial configurations which binding energy per nucleon lies within ± 0.5 MeV interval of the liquid-drop model value. The frictional cooling method cool or heat the system to adjust the binding energy to the liquid-drop model value. We also use the Metropolis sampling method [9], which give possibility to obtain a ground state at certain temperature, and so to examine the thermostatic properties of nuclei.

The QMD simulations of nucleon-induced reactions are performed up to certain time (100–150 fm/c in our case) and then at the end of dynamical stage we switch to statistical decay calculations. The generalized evaporation model (GEM) [10] is used to account for the decay processes.

3 Results and Discussion

The modified QMD model has been used to explore the effect of the different effective interactions on the ground state properties of nuclei, reaction cross sections and light-ion production in nucleon-induced reactions. Calculations have been done for several nuclei of interest, such as ^{12}C , ^{16}O , ^{27}Al , and ^{28}Si .

We use two parameter sets, which take into account different effective interactions. They are listed in Table 1 along with the JQMD one. The first of them (denoted as P&MD) in addition to the JQMD interaction includes Pauli and momentum-dependent potentials and is taken from Ref. [11], the other one (Yukawa) with Pauli and Yukawa potentials is from [12]. We use the

Table 1: Parameters of the model for the different interactions.

	JQMD	P&MD	Yukawa
A (MeV)	-219.4	-127.86	-163.0
B (MeV)	165.3	204.28	125.95
L (fm ²)	2.0	1.75	1.0
τ	1.33	1.33	1.67
C_P (MeV)		140	30
q_0 (fm)		1.644	5.81
p_0 (MeV)		120	400
$C_{\text{ex}}^{(1)}$ (MeV)		-258.54	
$C_{\text{ex}}^{(1)}$ (MeV)		-375.60	
μ_1 (MeV)		2.35	
μ_2 (MeV)		0.4	
C_Y (MeV fm)			-0.498
γ_Y			1.4

JQMD values for the saturation density $\rho_0 = 0.168 \text{ fm}^{-3}$ and the symmetry energy parameter $C_s = 25 \text{ MeV}$.

The ground state in the JQMD and with the P&MD parameter set is generated by the frictional cooling method. In order to investigate the thermostatic properties of the ground state and to check the effect of the temperature on the reaction cross section, the ground state for the P&MD parameter set is created also using the Metropolis sampling method at temperature $T = 3 \text{ MeV}$. For the Yukawa parameter set we use random packing because of difficulties in the creation of stable ground state by means of the frictional cooling and adjustment of the binding energy.

In Fig. 1 we show the density $\rho(r)$ and momentum $n(p)$ distributions of the ground state of ^{12}C and ^{28}Si nuclei calculated with different parameter sets. The corresponding root-mean-square radii are listed in Table 2. The QMD simulations are performed up to 150 fm/c and the averaged quantities over 1000 events are plotted. The results are compared with the empirical density distribution of Negele [13] and with “experimental” total momentum distribution deduces by y -scaling analysis [14] of inclusive electron-scattering data. The results of both parameter sets show improvement of the ground state properties in comparison with the JQMD ones. We have higher density in the center of nucleus and not so wide surface shape, root-mean-square radii are smaller and closer to the experimental ones, and the momentum distributions develop a high-momentum component. The inclusion of the Pauli and momentum-dependent potentials shows, for the ^{12}C case, fair agreement of the density distribution and root-mean-

square radius with the empirical ones. Increasing of the temperature of the system leads to rearrangement of the nucleons from the center to the periphery. The momentum distribution of ^{12}C calculated with Yukawa parameter set is in better agreement with the experimental data.

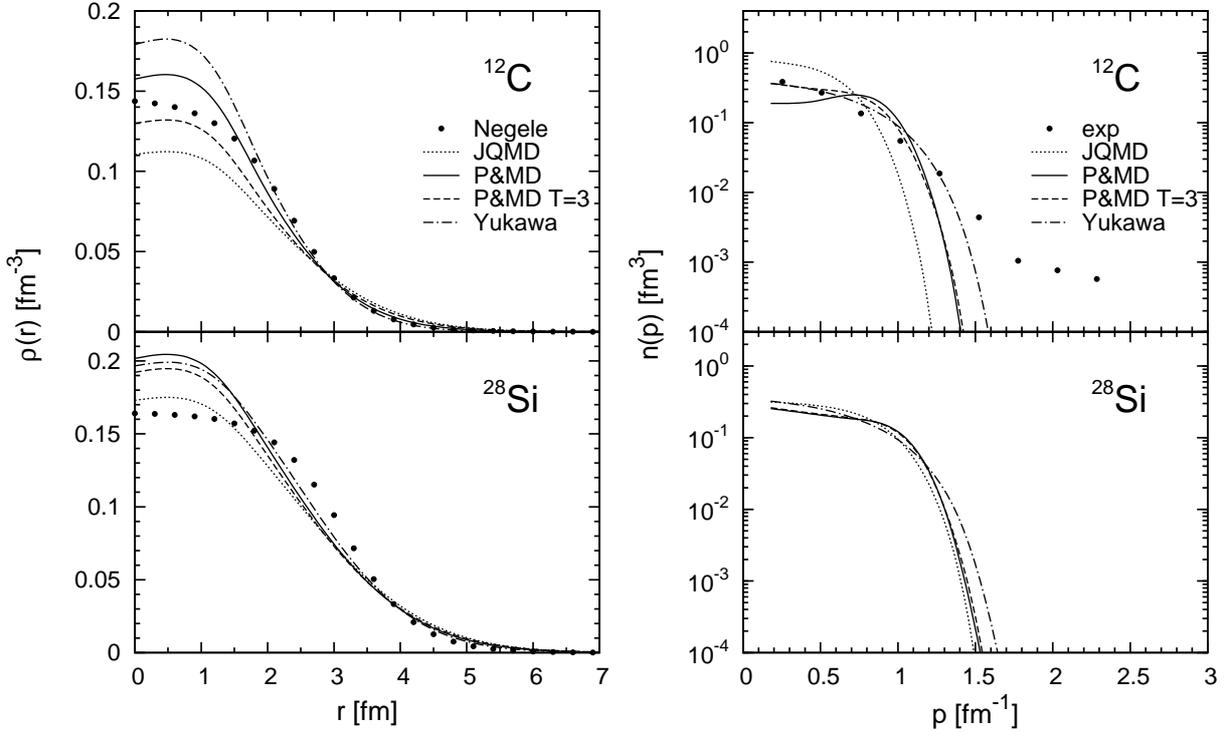


Figure 1: Density (left) and momentum (right) distributions of the ground state of ^{12}C and ^{28}Si obtained with different parameter sets.

Table 2: Root-mean-square radii (in fm) of ^{12}C and ^{28}Si obtained with different parameter sets.

Nucleus	JQMD	P&MD	P&MD $T = 3$ MeV	Yukawa	Negele
^{12}C	3.082	2.771	2.987	2.555	2.707
^{28}Si	3.488	3.413	3.447	3.265	3.165

A comparison between QMD calculations of the total reaction cross section for the proton-induced reaction on ^{12}C is shown in Fig. 2. The results are averaged quantities over time evolution up to 100 fm/c and over 10^4 events. The experimental data are taken from Ref. [15]. The JQMD model describes satisfactorily the reaction cross section, especially at high energies. The QMD calculations with the Pauli and momentum-dependent parameter set underestimate the experimental cross section for whole energy spectrum, but reproduce very well the energy dependence. We can improve the results by increasing the temperature of the ground state. The calculations with the Yukawa parameter set show good agreement with the experimental data. Similar results have been obtained for the ^{27}Al nucleus.

The results with the P&MD parameter set for angle-integrated energy spectra of light-ion production for ^{28}Si in neutron-induced reaction at incident energy 96 MeV are presented in Fig. 3. The QMD simulations are performed with 10^6 events and up to 100 fm/c. It can be seen that the JQMD results reproduce very well the proton production, but show large underestimation

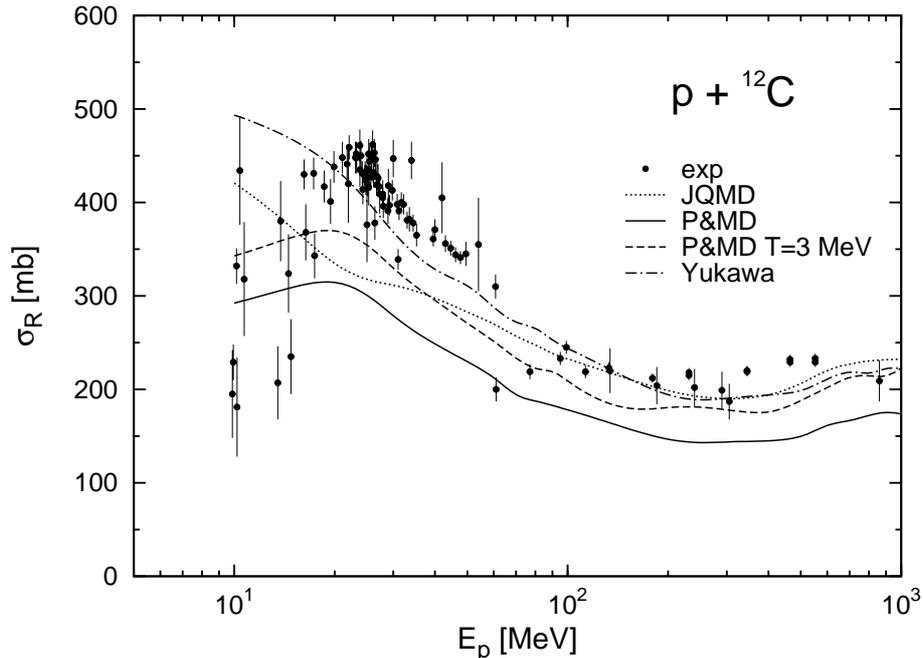


Figure 2: Total reaction cross section of ^{12}C for incident proton.

for other light clusters. The introduction of Pauli and momentum-dependent potentials with present parameters doesn't change significantly the description of light-ion emission. The proton cross sections are slightly reduced, while for the cross sections of other light clusters we have small enhancement. The results for the double-differential cross sections are similar. Thus, the present work indicates that the effective interaction potentials used in QMD calculations have little influence on preequilibrium light-cluster production in neutron-induced reactions. It should be noted that agreement with the experimental data is fairly improved by implementation of a phenomenological coalescence model into the QMD calculation as shown in our recent work [5].

4 Conclusions

The JQMD model is used to explore the preequilibrium light-cluster production in nucleon-induced reactions at intermediate energies. In order to improve ground state properties of nuclei, new effective interactions, for instance Pauli, momentum-dependent and Yukawa, are added to the nuclear Hamiltonian. Two parameter sets are used, the first one includes the Pauli and momentum-dependent potentials, the second one – the Pauli and Yukawa potentials.

The inclusion of the Pauli potential and momentum-dependent interaction leads to enhancement of the density distribution and the root-mean-square radii of nuclei. Calculations show underestimation of the proton-induced total reaction cross section but the energy dependence is reproduced rather well. Increasing of the temperature of the system leads to enhancement of the results.

The introduction of the Yukawa potential improves the nucleon momentum distribution, it develops a high-momentum component in accordance to the experimental data. The proton-induced total reaction cross section is reproduced rather well.

Newly added interactions with present parameter sets don't affect significantly the JQMD description of the light-cluster emission in nucleon-induced reactions.

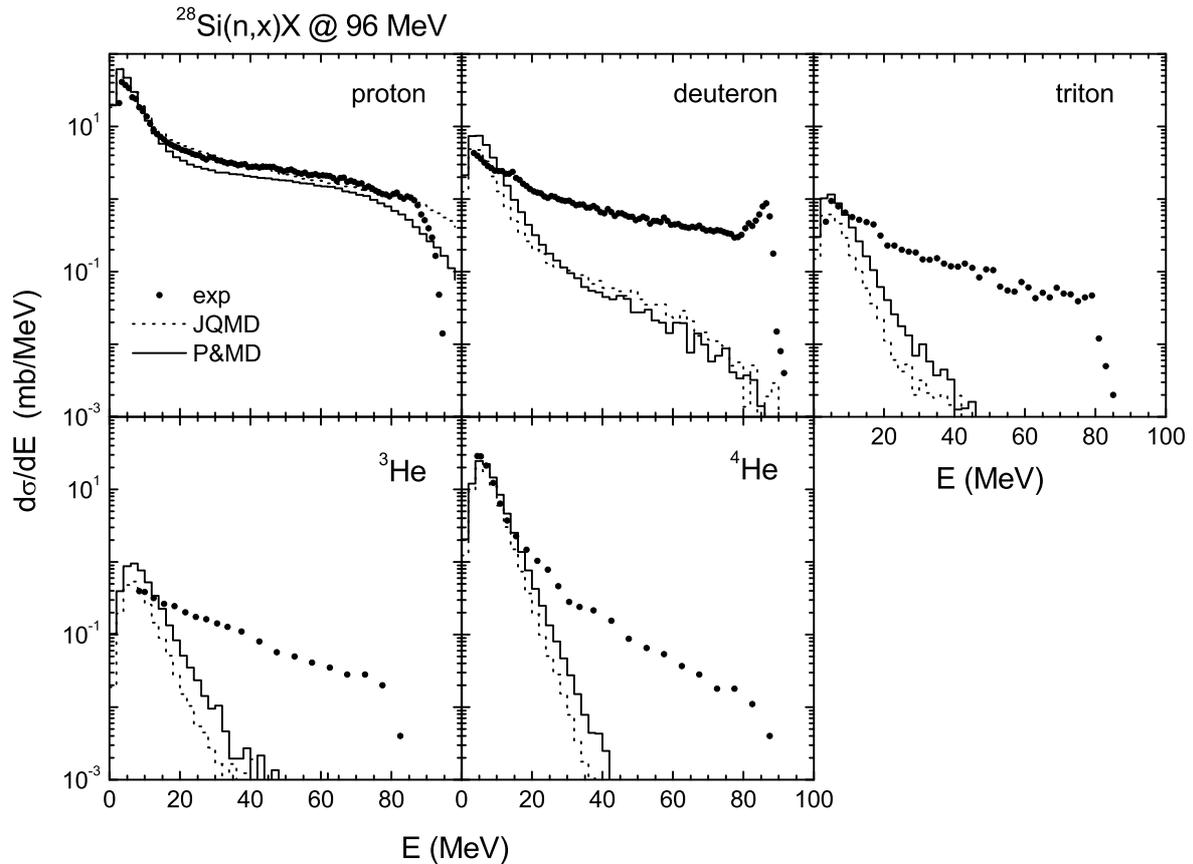


Figure 3: Angle-integrated energy spectra of light ions produced from neutron-induced reaction on ^{28}Si at 96 MeV. The experimental data are taken from [16].

Acknowledgments

The authors would like to thank Drs. K. Niita and S. Chiba for valuable comments on this work. D.N.K. is grateful to the Japan Society for the Promotion of Science (JSPS) for a postdoctoral fellowship. This work is partly supported by the Grants-in-Aid (No.17-05374) for Scientific Research from JSPS.

References

- [1] J. Aichelin, Phys. Rep. **202**, 233 (1991) and references therein.
- [2] K. Niita, S. Chiba, T. Maruyama, T. Maruyama, H. Takada, T. Fukahori, Y. Nakahara, and A. Iwamoto, Phys. Rev. C **52**, 2620 (1995).
- [3] S. Chiba, O. Iwamoto, T. Fukahori, K. Niita, T. Maruyama, T. Maruyama, and A. Iwamoto, Phys. Rev. C **54**, 285 (1996).
- [4] Y. Watanabe, in *Perspectives on Nuclear Data for the Next Decade*, Workshop Proceedings, Bruyères-le-Châtel, France, 26-28 September 2005, edited by E. Bauge (OECD Nuclear Energy Agency, Paris, 2006), p. 95.
- [5] Y. Watanabe and D. N. Kadrev, in *Proceedings of the Tenth International Symposium on Neutron Dosimetry*, Uppsala, Sweden, 2006, Radiat. Prot. Dosim. (to be published).

- [6] G. Peilert, J. Konopka, H. Stöcker, W. Greiner, M. Blann, and M. G. Mustafa, Phys. Rev. C **46**, 1457 (1992).
- [7] T. Maruyama, K. Niita, K. Oyamatsu, T. Maruyama, S. Chiba, and A. Iwamoto, Phys. Rev. C **57**, 655 (1998).
- [8] S. A. Bass *et al.*, Prog. Part. Nucl. Phys. **41**, 225 (1998).
- [9] N. Metropolis, A. W. Rosenbluth, M. N. Rosenbluth, A. H. Teller, and E. Teller, J. Chem. Phys. C **21**, 1087 (1953).
- [10] S. Furihata, Nucl. Instrum. Methods Phys. Res. B **171**, 251 (2000).
- [11] S. Chiba, K. Niita, T. Fukahori, T. Maruyama, T. Maruyama, and A. Iwamoto, in *Nucleon-nucleus optical model up to 200 MeV*, Proceedings of a Specialists Meeting, 13-15 November 1996, Bruyères-le-Châtel, France (OECD Nuclear Energy Agency, Paris, 1997), p. 49.
- [12] Khaled Abdel-Waged, Phys. Rev. C **74**, 034601 (2006).
- [13] J. W. Negele, Phys. Rev. C **1**, 1260 (1970).
- [14] C. Ciofi degli Atti, E. Pace, and G. Salmè, Phys. Rev. C **43**, 1155 (1991).
- [15] R. F. Carlson, At. Data Nucl. Data Tables **63**, 93 (1996).
- [16] U. Tippawan *et al.*, Phys. Rev. C **69**, 064609 (2004).