A systematic TDDFT data for nuclear fission analysis - Tin isotopes

Takashi Nishikawa[1,2]*, Yoritaka Iwata*[2]*, and Satoshi Chiba*[2]
[1]Nuclear Engineering Ltd, Osaka 550-0001, Japan
[2]Tokyo Institute of Technology, Tokyo 152-8550, Japan

Abstract
Dissipation of nuclear many-body systems is studied by means of TDDFT+ Langevin model. Much attention is paid to the energy dependence of the friction coefficient, identifying the thermodynamic property of nuclear medium for given nucleon numbers, neutron-richness, and energies. In this article, following the preceding work showing a systematics on $Z = 92$ to 100 nuclei, macroscopic friction coefficients for $Z = 50$ nuclei are derived from a microscopic framework. The comparison between $Z = 92$ and $Z = 50$ cases clarifies the similarity and the difference of fissions between heavy and medium mass nuclei. It is not only the completion of a systematic theoretical database, but also pinning down the dissipative features of the r-process nuclei. In addition, the knowledge about the obtained fission probability and fission fragment yields is expected to be useful for both nuclear synthesis and nuclear engineering.

1 Introduction

Nuclear friction arises from the dissipation effect. Indeed, the microscopic dissipation in quantum dynamics leads to the macroscopic friction effect to be found in the collective dynamics. Needless to say, the dissipation is a concept to be associated with the time-reversal symmetry breaking. That is, the sufficient understanding of nuclear dissipation is expected to be useful for clarifying not only the breaking mechanism of time reversal symmetry, but also the origin of friction-like effect in the sub-atomic collective dynamics.

In this article, following the preceding work [1] showing the systematics on $Z = 92$ region (Uranium, Plutonium isotopes and so on), the dissipation in many-nucleon systems is studied by the collective friction effects. A systematics of friction coefficients for Tin isotopes (in the following, we call "Sn isotopes") is presented. As distinct from $Z = 92$ region, the investigation on $Z = 50$ region clarifies that the energy dependence itself is complicated.

2 Proposed method

The analysis of quasi-fission events is made based on the TDDFT+Langevin model being introduced in [1] after our preparatory works on nuclear fission [2–5], where the terminology "TDDFT" stands for the time-dependent density functional theory. The TDDFT+Langevin model, at the present stage, consists of three steps:

(i) calculate collision dynamics by the TDDFT to obtain the microscopic wave function,
(ii) using the wave function, the averaged friction coefficient is calculated,
(iii) using the friction coefficient, the fission fragment yields are calculated by the Langevin model,

where Sky3D [6] is employed for the TDDFT calculations, and fission dynamics is stochastically calculated by by 4D Langevin code [8].

By hybridizing the TDDFT and the Langevin calculations, the total amount of dissipation during the reaction is calculated as the averaged friction coefficient in macroscopic dynamics. The averaged friction coefficient means that the friction (function of energy and time) is averaged for time. This treatment

is practically reasonable in terms of providing a coefficient to the Langevin calculations and obtaining dissipation effect comparable to experiments, because only the time-averaged value can be measured in experiments. The outline of the above three steps is explained in the following (for details, see Ref. [1]).

(i) TDDFT calculation

For the TDDFT calculations, we employ three different effective nuclear interactions: SV-bas [9], SLy4 [10], and SkM* [11]. We carried out the TDDFT calculations of symmetric quasi-fission processes

$$ {}^{A}Z + {}^{A}Z \;\rightarrow\; {}^{2A}2Z \;\rightarrow\; {}^{A}Z + {}^{A}Z \,, \tag{1} $$

where A and Z are a mass number and a proton number respectively. In particular, Z is fixed to $Z = 50$ in this research, and several excitation energies for each choice of A are examined. Here the energy E is taken as the initial energy of the collision, and E/A is from 3 MeV to 10 MeV. The value of A is 100, 104, 108, $\cdots$ 132. Consequently, the TDDFT wave function including all the information about microscopic collision dynamics is obtained. The distance $R(t)$ between the center-of-mass of two colliding nuclei is extracted from the TDDFT wave function. For the details of $R(t)$, see Ref. [12]. It is remarkable that the collective distance $R(t)$ is affected by the microscopic quantum effect such as the shell effect.

(ii) Friction coefficient

By substituting $R(t)$ into the macroscopic equation of motion describing nuclear dynamics,

$$ \mu\ddot{R}(t) + \frac{dV(R(t),E)}{dR} + \gamma(R(t),E)\dot{R}(t) = 0 \,, \tag{2} $$

the master equation for the collective motion for a given energy E is obtained, where the reduced mass μ is a constant, and the potential V can disappear by adjusting the initial time t_i and final time t_f to satisfy $V(R(t_i),E) = V(R(t_f),E)$. Note that $V(R(t),E)$ includes both the nuclear and the Coulomb interactions. Though the determination scheme is not exactly the same, the combination of the TDDFT and Eq. (2) has already been studied in Refs. [13, 14]. Consequently, for an input $R(t)$, the friction coefficient γ for the collective dynamics is obtained as an output, where the dissipation effect included in the TDDFT is known as the quantum one-body dissipation. The averaged friction coefficient $\overline{\gamma}(E) = \int_{t_i}^{t_f} \gamma(R(t),E)\{\dot{R}(t)\}^2 dt / \int_{t_i}^{t_f} \{\dot{R}(t)\}^2 dt$ is obtained by

$$ \overline{\gamma}(E) = \frac{\{\frac{1}{2}\mu\dot{R}^2(t_i) + V(t_i)\} - \{\frac{1}{2}\mu\dot{R}^2(t_f) + V(t_f)\}}{\int_{t_i}^{t_f}\{\dot{R}(t)\}^2 dt} \,, \tag{3} $$

where $\overline{\gamma}(E)$ is averaged for time t. t_i and t_f are usually taken as the initial and the final time of reaction. Again, this treatment is practically reasonable in terms of introducing a coefficient to the Langevin calculations and obtaining comparable theoretical results to experiments. Note that $\overline{\gamma}(E)$ values at extraordinary energies, which are too low or too high to be treated by the TDDFT, are also obtained using the extrapolation method being explained in Ref. [1].

(iii) Langevin calculation

Fission dynamics is obtained by the Langevin model equations:

$$ \begin{aligned} \frac{dq_\mu}{dt} &= m_{ij}^{-1} p_j, \\ \frac{dq_\mu}{dt} &= -\frac{dV}{dq_\mu} - \frac{1}{2}\frac{d}{dq_\mu} m_{ij}^{-1} q_i q_j - \gamma_{ij} m_{ij}^{-1} p_j - g_{ij} R_j, \end{aligned} \tag{4} $$

where a part of γ_{ij}, more precisely γ_{11}, is replaced with $\overline{\gamma}(E)$, and the values obtained by the Wall-and-Window formula [7] are employed for the other components. Indices i, j $(1 \le i, j \le 4)$ mean collective

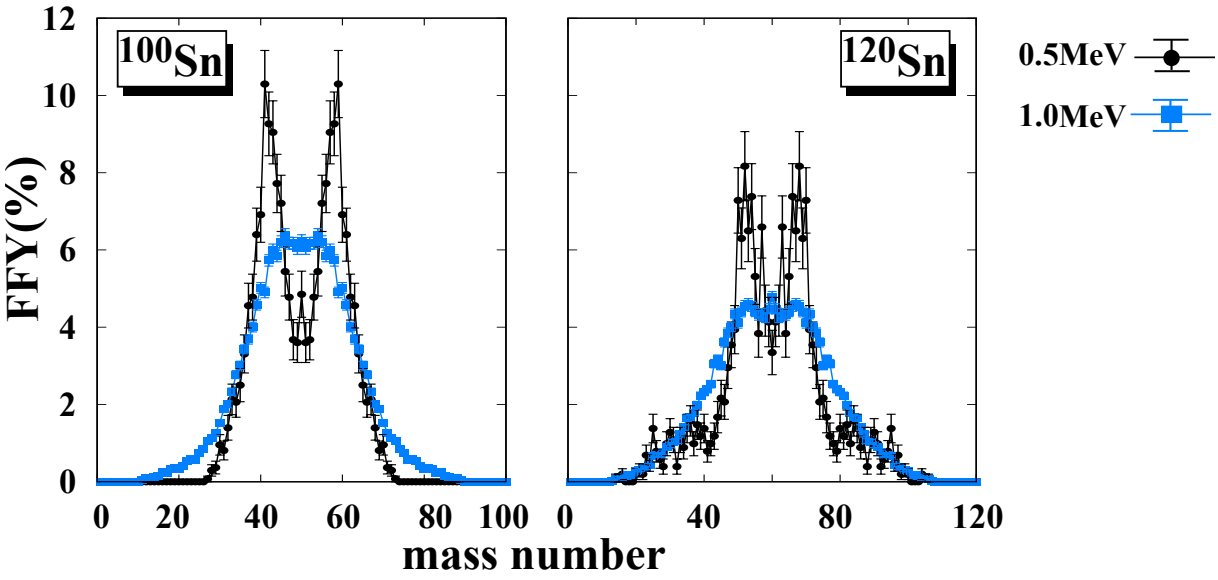

Fig. 1: (Color online) Fission fragment yield (FFY) calculated by the TDDFT+Langevin model (SV-bas). The FFYs at 0.5 MeV and 1 MeV per nucleon are shown for ^{100}Sn and ^{120}Sn. The corresponding fission probability is 0.006 % for 0.5 MeV, and 2.61 % for 1.0 MeV in case of ^{100}Sn, and 0.004 % for 0.5 MeV, and 2.67 % for 1.0 MeV in case of ^{120}Sn.

Table 1: The friction coefficient $\overline{\gamma}(E)$ of unit $\hbar$ is calculated for Sn isotopes (Z=50) using three effective nuclear interactions (SV-bas, SLy4, and SkM*). The energy is $E = 20$ MeV ($E/A \sim$0.17 MeV) being calculated by the extrapolation method. In the column "Average", the averaged values for those three interactions are shown.

N	SV-bas	SLy4	SkM*	Average
54	52.0	41.0	50.9	48.0
58	52.6	44.8	43.9	47.1
62	55.1	47.3	45.2	49.2
66	57.7	49.9	52.1	53.2
70	60.7	52.0	53.8	55.5
74	63.7	53.9	57.4	58.3
78	67.6	57.6	57.4	60.9
82	61.1	54.3	56.0	57.1

coordinate. Detailed explanation is shown in Ref [8]. Although the stochastic aspect of the dynamics is introduced in the Langevin model, its dynamics accounts only for the nucleus degrees of freedom. The Langevin calculations enable us to incorporate the stochastic aspect of reaction dynamics resulting in both fission and fusion dynamics.

As a result, the refined friction coefficients for $^{2A}2Z$ are obtained in an energy dependent manner, and they are employed in the Langevin calculation. The coefficient is refined in terms of including the microscopic quantum effect obtained by a less phenomenological and time-dependent theoretical framework.

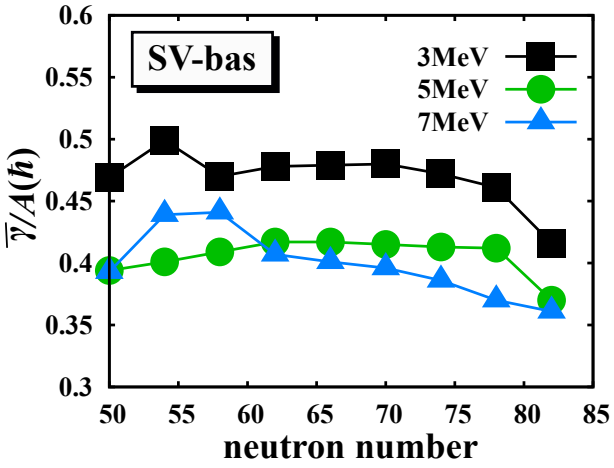

Fig. 2: (Color online) Energy and mass dependence of friction coefficient $\overline{\gamma}$ per nucleon, where A denotes the mass number. The amplitude of $\overline{\gamma}$ stands for the amount of dissipated energy at a given excitation energy.

3 Result

Figure 1 shows the fission fragment yield (FFY) for ^{100}Sn and ^{120}Sn. The transitions from symmetric fission to asymmetric fission are well described. In this case, the mass number is too small for low-energy fission events including spontaneous fission to take place, while collision-fissions such as fusion-fission and quasi-fission appear by giving a sufficient high energy. In this case, we found no corresponding experimental fission data to compare, so that the calculation is carried out as the prediction for future research in the context of figuring out the role of collision-fission events in nuclear synthesis, as well as for the completion of the theoretical $\overline{\gamma}$ database. By comparing low and high energy cases, the energy dependence is remarkable in which asymmetric fissions are favored for lower energies and symmetric fissions are favored for higher energies. The shell effect is seen in the mass yield $A = N + Z = 40$ or 48. $A = 40$ nuclei are more produced in the fission of ^{100}Sn, while $A = 48$ nuclei are mainly obtained in the fission of ^{120}Sn. For the higher energies, fission probabilities are calculated to be around 3% for both ^{100}Sn and ^{120}Sn. Fission events with quite small fission probability are calculated based on the microscopic TDDFT dynamics. The present prediction is worth believing by accounting for the agreement between the TDDFT+Langevin result and the experimental FFY in Uranium and Plutonium isotopes [1].

The coefficient $\overline{\gamma}$ at the energy closed to the Coulomb barrier is shown in Table 1. Fission at or around the barrier energy is useful to analyze the low-energy fission events such as quasi-fission, photo-fission, neutron-induced fission and so on.

Energy and mass dependence of $\overline{\gamma}$ can be found in Fig. 2. As a trend, the amplitude of $\overline{\gamma}$ becomes smaller for higher energies. Such a trend is reasonable, because the shorter duration time in higher energy collisions should lead to the smaller amount of dissipated energy in reaction processes. As a more weak dependence, the value of $\overline{\gamma}$ becomes smaller for more neutron-rich cases. However, Note that the neutron number dependence is not definitely monotonous. Although some local extremal values can be found in Fig. 2: e.g., maximum at $N = 54$ and $E/A = 3$ MeV, their origins are not easy to be identified, because many factors such as shell effect and/or pauli effect may contribute in certain complicated manners. The detail investigation on the energy and mass dependence of $\overline{\gamma}(E)$ is a future problem in which the different properties of effective nuclear interaction should be investigated more carefully. Consequently, for Sn isotopes, the energy dependence ($\sim$0.1 $\hbar$ difference in $\overline{\gamma}/A$) is more prominent than the neutron-richness or mass dependence ($\sim$0.05 $\hbar$ difference in $\overline{\gamma}/A$). With respect to the total amount of dissipated energy during the fission process, the most dissipative isotope can be different depending on the energy. In

Table 2: The friction coefficient $\overline{\gamma}(E)$ of unit $\hbar$ calculated for Sn isotopes (Z=50) using three effective nuclear interactions (SV-bas, SLy4, and SkM*). The energy is taken for 3 MeV, 5 MeV and 7 MeV per nucleon. In the column "Average", the averaged values for those three interactions are shown.

a) $E/A = 3$ MeV

N	SV-bas	SLy4	SkM*	Average
50	46.9	43.0	49.0	46.3
54	51.9	44.2	50.5	48.8
58	50.7	47.8	50.8	49.8
62	53.6	48.3	52.1	51.3
66	55.6	49.2	53.4	52.7
70	57.6	50.3	55.5	54.5
74	58.5	51.1	56.2	55.3
78	59.0	51.9	57.1	56.0
82	54.9	48.8	53.3	52.4

b) $E/A = 5$ MeV

N	SV-bas	SLy4	SkM*	Average
50	39.4	32.7	36.4	36.1
54	41.7	35.3	39.5	38.8
58	44.2	37.4	41.7	41.1
62	46.8	39.0	43.7	43.1
66	48.3	40.2	44.9	44.5
70	49.8	41.3	45.9	45.7
74	51.2	41.7	46.7	46.5
78	52.7	40.2	46.3	46.4
82	48.8	37.1	43.1	43.0

c) $E/A = 7$ MeV

N	SV-bas	SLy4	SkM*	Average
50	39.3	30.0	35.1	34.8
54	45.6	30.8	39.6	38.7
58	47.6	31.9	38.0	39.2
62	45.6	33.7	39.2	39.5
66	46.6	34.4	40.1	40.4
70	47.5	34.6	40.8	41.0
74	47.8	33.1	40.0	40.3
78	47.4	31.6	38.4	39.1
82	47.7	30.9	37.8	38.8

fact, ^{128}Sn ($N = 78$) is the most dissipative for low energies up to $E/A = 6.0$ MeV (SV-bas), while isotopes with smaller neutron numbers are rather dissipative for higher energies; ^{124}Sn ($N = 74$), ^{120}Sn ($N = 70$), and ^{116}Sn ($N = 66$) are the most dissipative nuclei for $E/A = 7.0, 8.0$ and 9.0 MeV, respectively. This fact implies that the neutron-richness contributes to the dissipation (leading to fission) rather prominently for higher energies. Accordingly, the energy and mass dependences of $\overline{\gamma}$ are shown. It will provide us a clue to discover the origin of quantum one-body dissipation.

4 Summary

The friction coefficients utilizable to the Langevin calculations have been obtained based on the TDDFT framework. In a more microscopic point of view, possible dissipation for a given excitation energy is systematically obtained for Sn isotopes. Since the low-energy heavy-ion reactions ($\sim E/A < 10$MeV) have known to be well described by the TDDFT(for a review, see [15]), the reliability of proposed method is expected to be sufficiently high.

The obtained coefficient has been used in the TDDFT+Langevin model calculation. It is the first time attempt to carry out the TDDFT+Langevin model calculations for medium-mass nuclei. Even based on the quantum and less-phenomenological input, it will open-up a new way to study the stability and the related stochastic dynamics of medium and heavy mass nuclei. The proposed method requires only a system of light-weight calculations, so that it is advantageous to make up a large-scale theoretical database.

In terms of the future utility in nuclear engineering, the obtained coefficients are summarized in Table 2. Table 2 shows the calculated coefficient $\overline{\gamma}$ for Sn isotopes ($Z = 50$). The $\overline{\gamma}$ values depend more prominently on the energy than on neutron-richness. The smaller $\overline{\gamma}$ is calculated for a heavier case ($N = 82$), where such a trend can be found for $Z = 92$ region. According to the preceding result [1], $\overline{\gamma}$ values distribute from 110 to 120 for the uranium isotopes ($N = 142$ to 150). It also tells us another aspect of the mass dependence; i.e., Z dependence. Table 2 provides a part of theoretical database of systematic friction coefficients.

Sn isotopes are regarded as the fission product of U and Pu isotopes. From this point of view, calculating the FFY of Sn is the product of the secondary fission. Asymmetric fission producing $A = 40$ or 48 nucleus occurs for low energy, while symmetric fission producing $A = 50 \sim 60$ occurs for high energy. Because the secondary fission can occur when the energy in the field of nuclear synthesis or nuclear reactor is sufficiently high, the FFYs of Sn isotopes constrain a possible scenario of nuclear synthesis, as well as a possible control of nuclear reactors.

Acknowledgement

Numerical computation was carried out at a workstation system at Tokyo Institute of Technology (AEGIS system). This work was supported by JSPS KAKENHI Grant No. 17K05440. One of the authors (Y. I.) is grateful to Prof. Dr. Hans Feldmeier for presenting an essential idea at the preparatory stage of this research.

References

[1] T. Nishikawa, Y. Iwata, and S. Chiba, in preparation.

[2] T. Nishikawa, Y. Iwata, and S. Chiba, to appear in JAEA-Conf (2018).

[3] Y. Iwata and S. Heinz, Exotic Nuclei, EXON-2012, World Scientific, 153 (2013).

[4] Y. Iwata and S. Heinz, CERN Proceedings 2012 - 002, 241 (2013).

[5] Y. Iwata, JAEA-Conf 2015-003, INDC(JPN)-201, 93 (2015).

[6] J. A. Maruhn, P.-G. Reinhard *et al.*, Comput. Phys. Commun. **185** 2195 (2014).

[7] T. Dossing and J. Randrup, Nucl. Phys. A **475** 557-568 (1987),

[8] M. D. Usang, F. A. Ivanyuk, C. Ishizuka, and S. Chiba, Phys. Rev. C **94** 044602 (2016).

[9] P. Klüpfel, P.-G. Reinhard, J. Bürvenich, and J. A. Maruhn, Phys. Rev. C **79** 034310 (2009).

[10] E. Chabanat, P. Bonche, P. Haensel, J. Meyer, and F. Schaeffer, Nucl. Phys. **A 635**, 231 (1998).

[11] J. Bartel, P. Quentin, M. Brack, C. Guet, and H.B. Hakansson, Nucl. Phys. **A 386**, 79 (1982).

[12] Y. Iwata, H. Feldmeier, and J. A. Maruhn, AIP Conf. Proc. 1377, 365 (2011).

[13] K. Washiyama and D. Lacroix, Phys. Rev. C **78** 024610 (2008).

[14] K. Washiyama, D. Lacroix, and S. Ayik, Phys. Rev. **C 79** 024609 (2009).
[15] C. Simenel, and A. S. Umar, Prog. Part. Nucl. Phys. **103**, Nov. 2018, 19 (2018).