EPJ Web of Conferences **146**, 04025 (2017) DOI: 10.1051/epjconf/201714604025
ND2016

Effects of microscopic transport coefficients on fission observables calculated by Langevin equation and its systematics

Mark Usang[1,2,a], Fedir Ivanyuk[1,3], Chikako Ishizuka[1], and Satoshi Chiba[1]

[1] Tokyo Institute of Technology, Tokyo, Japan
[2] Malaysian Nuclear Agency, Bangi, Malaysia
[3] Institute for Nuclear Research, Kiev, Ukraine

Abstract. The Langevin dynamical description of fission observables is inspired by the random evolution of shape parameters across the potential surface. In these work, we shall use mass and friction tensors inspired from Linear Response Theory (microscopic transport coefficients) and obtain the fission observables associated with these calculations. We compare these microscopic results with calculations using hydrodynamical mass tensor and wall-window friction tensor (macroscopic transport coefficients). We are able to calculate the fission product yield, Coulomb kinetic energy and prescission kinetic energy from the Langevin calculation. This allows us to observe the systematic of average light and heavy mass fission product yield calculated using both microscopic and macroscopic calculations. We also compare the results of microscopic and macroscopic calculation total kinetic energy (TKE) with Viola's TKE systematics. In the case of ^{236,239}U compound nucleus, we do the microscopic calculation for several excitation energy up to 30 MeV and afterwards compare it to the TKE of experimental data and corresponding macroscopic TKE. Reasonable agreement of microscopic TKE to experiment is obtained which shows decreasing TKE with increasing excitation energy. Macroscopic TKE however, is independent of excitation energy and thus contrary to experimental data.

1. Introduction

Linear response theory [1–4] allowed us to obtain microscopic mass and friction tensor for a nucleus under perturbation such as in nuclear fission from the response function of these perturbations. The assumption is that the changes of nuclear shapes are due to the evolution of the shape as it travels randomly on a potential surface. Our potential is based on the two centre shell model [5] and the evolution is governed by Langevin equation.

Calculation of the Langevin equation for fission is done by solving the first order differential equations for collective coordinates, $q_\mu = (z_o/R_0, \delta, \alpha)$ and momentum conjugate of the collective coordinates, p_μ,

$$\frac{dq_\mu}{dt} = \left(m^{-1}\right)_{\mu\nu} p_\nu$$

$$\frac{dp_\mu}{dt} = -\frac{\partial V}{\partial q_\mu} - \frac{1}{2}\frac{\partial}{\partial q_\mu}\left(m^{-1}\right)_{\nu\sigma} p_\nu p_\sigma - \gamma_{\mu\nu}\left(m^{-1}\right)_{\nu\sigma} p_\sigma + g_{\mu\nu} R_\nu(t)\,. \quad (1)$$

The collective coordinates; z_0 is the elongation of the nucleus, R_0 the radius of spherical compound nucleus, δ is the deformation of fragments, and α is the mass asymmetry. We assume both the left deformation, δ_1 and right deformation, δ_2 is similar by setting $\delta = \delta_1 = \delta_2$. We also kept the neck parameter constant at $\epsilon = 0.35$. The trajectory is governed by the random force, $g_{\mu\nu}R_\nu(t)$. The random force is a product of white noise, $R_\nu(t)$ and temperature dependent strength factor, $g_{\mu\nu}$. The coefficient $g_{\mu\nu}$ is related to friction tensor and temperature via the Einstein relation

$$\sum_\sigma g_{\mu\sigma} g_{\sigma\nu} = T\gamma_{\mu\nu}\,. \quad (2)$$

We call this temperature the *local temperature* to differentiate it with the *transport temperature*, T_{tr} which is used in the calculation of microscopic mass, $m_{\mu\nu}$ and friction tensor, $\gamma_{\mu\nu}$. The microscopic mass and friction tensor calculation used in the current calculation are given and described by Ivanyuk [6] incorporates BCS approximations into the mean field Hamiltonian obtained in the current calculation using linear response theory at specific T_{tr}. As for the *local temperature*, T, it is determined according to the internal energy , E_{int} available to it. E_{int} is related to the excitation energy, E_x and level density parameter, a using the relationship,

$$E_{int} = E_x - \frac{1}{2}\left(m^{-1}\right)_{\mu\nu} p_\mu p_\nu - V(q, E_{int}) = aT^2\,. \quad (3)$$

Before any Langevin calculation is done, we calculate microscopic mass [7] and friction tensor [8] at several T_{tr} using linear response theory. The fission product yield for each T_{tr} in the case of ^{236}U is shown in Fig. 1. We afterwards interpolate the mass and friction tensor across

[a] e-mail: usang.m.aa@m.titech.ac.jp; mark_dennis@nm.gov.my

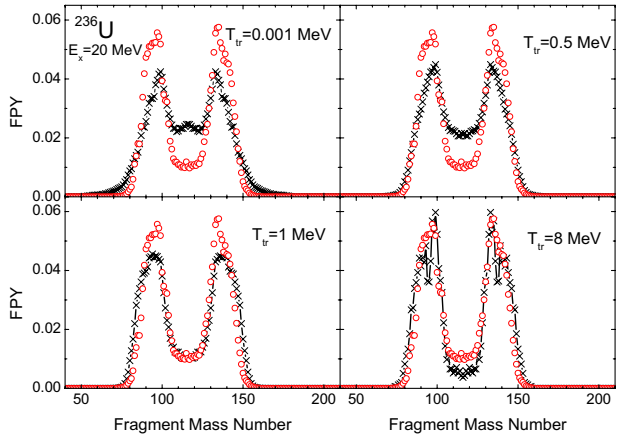

Figure 1. Langevin calculation for compound nucleus ^{236}U using microscopic transport coefficients at specific microscopic temperature, T_{tr} (black cross) in comparison to 14 MeV incident neutron from JENDL-4.0 fission product yield (red circle).

several T_{tr} to obtain mass and friction tensor at T_{tr} equal to the *local temperature*, T. We perform our calculation at $E_x = 20$ MeV and compare them with JENDL 14 MeV incident neutron data except in Sect. 3.1 where the calculation is done for a range of excitation energy. Previously [9], we have shown for ^{236}U detailed analysis of the fission observables calculated using Langevin equation with microscopic transport coefficients.

2. Mass yield systematics

In Fig. 2, excellent agreement can be seen of the yield using microscopic transport coefficients in comparison to macroscopic transport coefficients and JENDL fission product yield. The discrepancy at the peak and valley of the yield can be easily removed or at least reduced by adjusting shell corrections. In the current microscopic calculation, full shell and pair correction ($\Phi(E_{int})_{sh,pair} = 1$) are used but we could optionally use Randrup & Möller [10] shell and pair correction formula,

$$\Phi(E_{int})_{sh,pair} = \frac{1 + e^{E_1/E_0}}{e^{E_{int}/E_0} + e^{E_1/E_0}}. \qquad (4)$$

The formula above can be reduced to Ignatyuk shell correction [11] by setting $e^{E_1/E_0} = 0$. The parameter $E_0 = 15$ MeV is interpreted as the shell damping energy, and E_1 is the energy shift, as explained in Ref. [10]. As a note, the macroscopic calculation is done using $E_1 = 30$ MeV for both shell and pairing.

The average mass of the light fragments, $\langle A_L \rangle$ and average mass of the heavy fragments, $\langle A_H \rangle$ in Fig. 3 shows that for many actinides, our calculation follows the systematic of 14 MeV incident neutron JENDL-4.0 fission product light and heavy mass yield averages with very little deviation, with either microscopic or macroscopic calculation. The current calculation shows that our results are consistent with the bimodal fission argued by Ohtsuki [12].

This mass distribution of light and heavy mass averages is first demonstrated by Flynn [13] but the mass distribution used by Flynn is determined from fission product yield due to thermal neutron, reactor neutron and spontaneous fission. Hence Flynn's mass distribution will

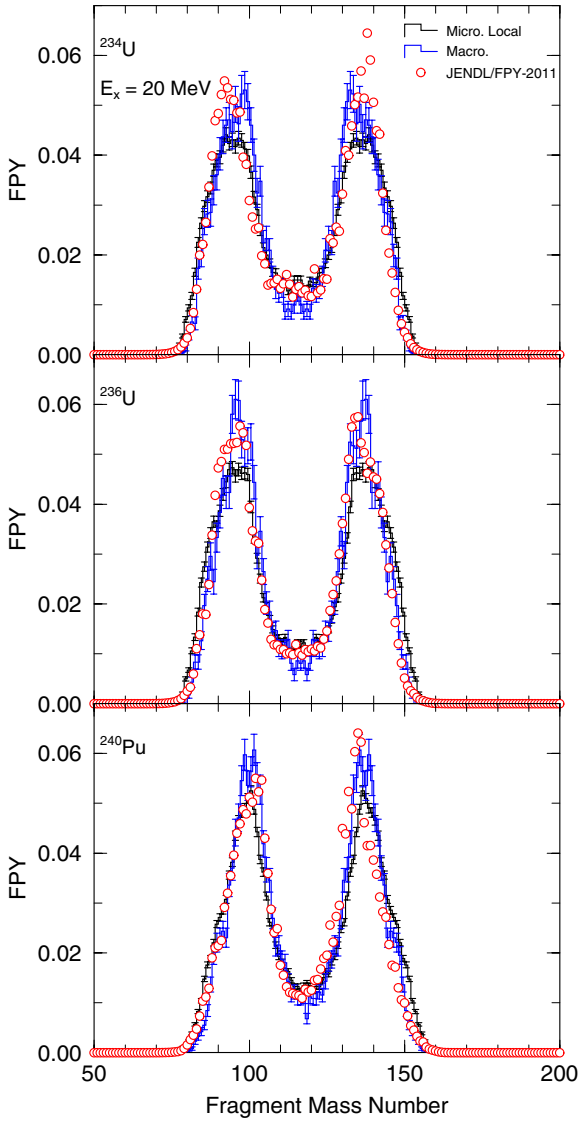

Figure 2. Langevin calculation for compound nucleus ^{234}U, ^{236}U and ^{240}Pu using both microscopic and macroscopic transport coefficients fission fragment mass yield results.

have a slightly heavier mass averages at $\langle A_H \rangle \approx 140$, in contrast to the 14 MeV incident neutron evaluated results used in Fig. 3 that has $\langle A_H \rangle \approx 135$. Flynn's $\langle A_L \rangle$ distribution against compound mass is also slightly steeper.

3. Total kinetic energy systematics

We define in our calculation the total kinetic energy (TKE) at scission as the sum of prescission kinetic energy E_{pre} and Coulomb energy E_{Coul} of the fission fragments.

$$TKE = E_{Coul} + E_{pre}\,. \qquad (5)$$

We calculate E_{Coul} by assuming that the point charge of the fission fragments is proportional to its mass and is separated by a distance equal to the distance between the length of these fragments at scission. E_{pre} on the other hand, is the kinetic energy of our trajectory for the elongation, Z_{z_0} at scission. This allows us to observe the TKE of our calculation and compare them with experiments, evaluated data and available systematics. We are however aware that our definition of TKE is different from Eq. (7) in the paper by Straede [15].

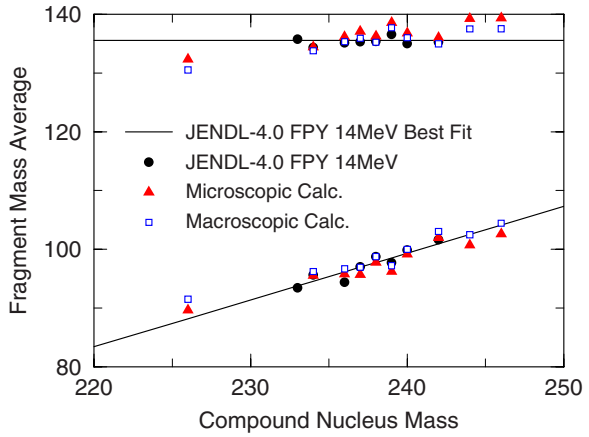

Figure 3. Light and heavy mass average systematics for macroscopic and microscopic calculation in comparison to JENDL's 14 MeV incident neutron fission fragment light and heavy mass average.

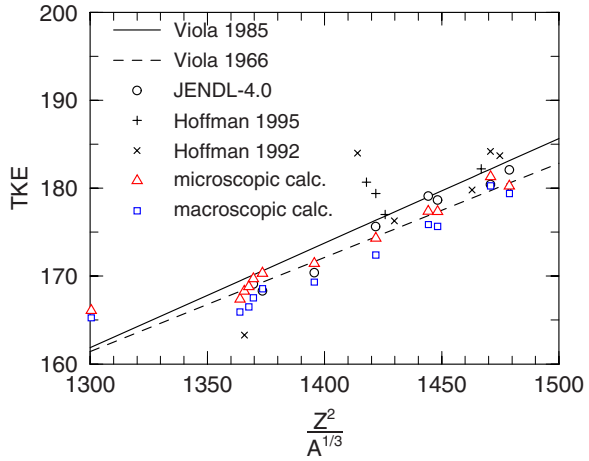

Figure 4. TKE systematics in comparison to the systematic by Viola [14].

Terrell [16] argues that if charge divides in the same ratio as the mass ratio, $\langle A_L \rangle / \langle A_H \rangle$, the kinetic energy should be proportional to $Z^2/r_0 A^{1/3}$. He showed through a linear square fit that the TKE is proportional to $0.121 Z^2 A^{-1/3}$. This is further demonstrated by Viola [14] by the linear equation given in 1966

$$TKE = 0.1071 \frac{Z^2}{A^{1/3}} + 22.2 \text{ MeV}, \quad (6)$$

and in 1985,

$$TKE = 0.1189 \frac{Z^2}{A^{1/3}} + 7.3 \text{ MeV}, \quad (7)$$

In Fig. 4 we show that our calculations are within this systematic established by Viola and are very close to the TKE of several actinides given by JENDL.

3.1. Excitation energy dependence

Currently we are able to show that the TKE of ^{239,236}U compound nucleus at various excitation energy are roughly consistent with experimental results at various incident energy by assuming that the excitation energy of the compound nucleus for the actinides in experimental is

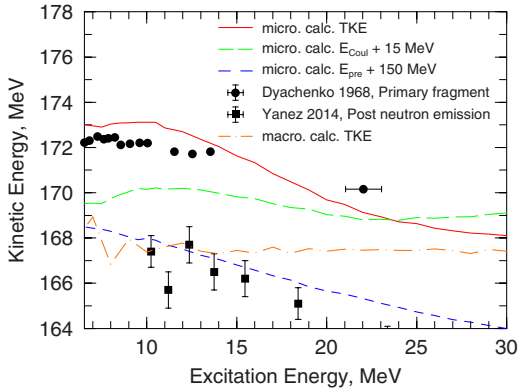

Figure 5. TKE dependence on excitation energy, E_x for ^{236}U. Comparisons are made with data by Dyachenko et al. [17] (EXFOR asc. 40235) and Yanez et al. [18] (EXFOR asc. 14394) for U-235 induced by neutrons assuming $E_x = E_n + B_n(A_{U236})$.

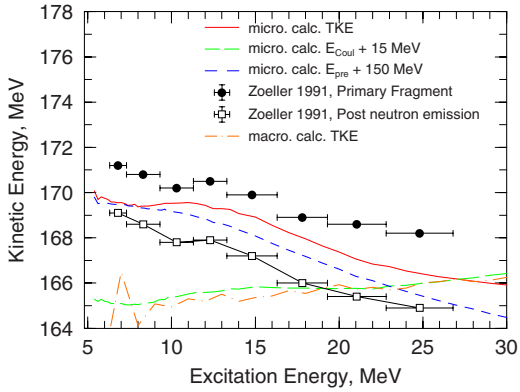

Figure 6. TKE dependence on excitation energy, E_x for ^{239}U. Comparisons are made with data by Zoeller [19] (EXFOR asc. 22799) for U-238 induced by neutrons assuming $E_x = E_n + B_n(A_{U239})$.

approximately equal to the sum of the incident energy and neutron binding energy of the compound nucleus, $B_n(A_c)$ as in the following manner

$$E_x = E_n + B_n(A_c)\,. \quad (8)$$

This is demonstrated for ^{236}U compound nucleus in Fig. 5 and on Fig. 6 in the case of ^{239}U compound nucleus.

Influence and contributions from E_{pre} and E_{Coul} for each calculation to the TKE at each excitation energy can also be seen from the figures. E_{pre} in general, tends to decay with increasing excitation energy while E_{Coul} seems to fluctuate around a fixed constants. This indicates that the decay of TKE at increasing excitation energy is generally due to E_{pre} component.

Our calculated TKE for ^{236}U slightly overestimates experimental data at low excitation energy but overestimate it at high excitation energy. For ^{239}U, our calculation underestimates the TKE. These deviations however, are very small as was illustrated in Fig. 5 and Fig. 6. We are also unable to show the onset of pair breaking at 1.5 MeV $\leqslant E_n \leqslant$ 2.0 MeV as indicated by Straede and his co-workers [15] at the moment but these could be due to insufficient scission events in our calculations to get a reliable enough statistics.

4. Conclusion

Observables of fission such as mass yield and TKE from the calculation of Langevin equation using microscopic transport coefficient at $E_x = 20\,\mathrm{MeV}$ gives a good approximation of the fission yield in comparison to evaluated data of JENDL-4.0 fission product yield 14 MeV incident neutron. This is demonstrated by the fitness of the microscopic calculation yields alongside evaluated data and the proximity of its heavy and light fragment mass averages to corresponding JENDL's mass fragment averages. The TKE's of these calculations also seem to adhere very well to the systematics of Viola's and JENDL's TKE.

Examination of the TKE's calculated at various excitation energy for ^{236,239}U shows that our results follow experimental results closely. Additionally, TKE trends for these two actinides to gradually decrease at higher excitation energy seems to be the contribution of E_{pre}. E_{pre} in our calculations experience a consistent decrease at increasingly higher excitation energy while E_{Coul} seems to be fluctuating around a constant value with no clear indication of increasing or decreasing at higher excitation energy.

There are many improvements that could be done to the present result such as adjusting the pair and shell correction for each nuclide for a better fit to fission product yield or improving the statistics of our calculations for example. In other words, we are fairly optimistic that our calculation of the Langevin equation using microscopic transport coefficients could be further improved as more physics are introduced into the calculation.

The current study includes the results of "*Comprehensive study of delayed-neutron yields for accurate evaluation of kinetics of high-burn up reactors*" entrusted to Tokyo Institute of Technology by the Ministry of Education, Culture, Sports, Science and Technology of Japan (MEXT). Our appreciations to Profs. T. Wada (Kansai University) for the fruitful and informative discussions. M.D. Usang and F.A. Ivanyuk would also like to express their gratitude to the Laboratory for Advanced Nuclear Energy, Institute of Innovative Research, Tokyo Institute of Technology, for the hospitality during the visits to Japan.

References

[1] S. Yamaji, H. Hofmann, R. Samhammer, Nucl. Phys. A **475**, 487 (1987)
[2] H. Hofmann, Phys. Rep. **284**(4), 137 (1997)
[3] F. Ivanyuk, H. Hofmann, Nucl. Phys. A **657**(1), 19 (1999), ISSN 0375-9474, http://www.sciencedirect.com/science/article/pii/S0375947499003243
[4] F. Ivanyuk, S. Chiba, Y. Aritomo, J. Nucl. Sci. Technol. **53**(6), 737 (2016)
[5] J. Maruhn, W. Greiner, Z. Phys. **251**(5), 431 (1972)
[6] F.A. Ivanyuk, *The shell effects in the collective transport coefficients*, in *Proc. of Int. Conf. on Nucl. Phys."Nuclear shells-50 years".-Singapore: World Scientific*, edited by Y. Oganessian, R. Kalpakchieva (2000), pp. 456–465
[7] K.T.R. Davies, A.J. Sierk, J.R. Nix, Phys. Rev. C **13**, 2385 (1976), http://link.aps.org/doi/10.1103/PhysRevC.13.2385
[8] A.J. Sierk, J.R. Nix, Phys. Rev. C **21**, 982 (1980), http://link.aps.org/doi/10.1103/PhysRevC.21.982
[9] M.D. Usang, F.A. Ivanyuk, C. Ishizuka, S. Chiba, Phys. Rev. C **94**, 044602 (2016), http://link.aps.org/doi/10.1103/PhysRevC.94.044602
[10] J. Randrup, P. Möller, Phys. Rev. C **88**(6), 064606 (2013)
[11] A. Ignatyuk, K. Istekov, G. Smirenkin, Sov. J. Nucl. Phys. (Engl. Transl.); (United States) **29**(4) (1979)
[12] T. Ohtsuki, Y. Nagame, H. Nakahara, *Bimodal nature of nuclear fission*, in *Heavy Elements and Related New Phenomena*, edited by W. Greiner, R.K. Gupta (World Scientific, 1999), pp. 507–535, ISBN: 9789814525305
[13] K.F. Flynn, E.P. Horwitz, C.A.A. Bloomquist, R.F. Barnes, R.K. Sjoblom, P.R. Fields, L.E. Glendenin, Phys. Rev. C **5**, 1725 (1972), http://link.aps.org/doi/10.1103/PhysRevC.5.1725
[14] V. Viola, K. Kwiatkowski, M. Walker, Phys. Rev. C **31**(4), 1550 (1985)
[15] C. Straede, C. Budtz-J rgensen, H.H. Knitter, Nuclear Physics A **462**(1), 85 (1987), ISSN 0375-9474, http://www.sciencedirect.com/science/article/pii/0375947487903812
[16] J. Terrell, Phys. Rev. **113**, 527 (1959), http://link.aps.org/doi/10.1103/PhysRev.113.527
[17] P.P. Dyachenko, B.D. Kuzminov, M.Z. Tarasko, Soviet Journal of Nuclear Physics **80**(2), 165 (1969)
[18] R. Yanez, L. Yao, J. King, W. Loveland, F. Tovesson, N. Fotiades, Phys. Rev. C **89**, 051604 (2014), http://link.aps.org/doi/10.1103/PhysRevC.89.051604
[19] C. Zöller, Ph.D. thesis, Technische Hochschule Darmstadt, Darmstadt, Germany (1991)