Calculation of fission fragment mass distributions for actinide nuclei with Langevin approach

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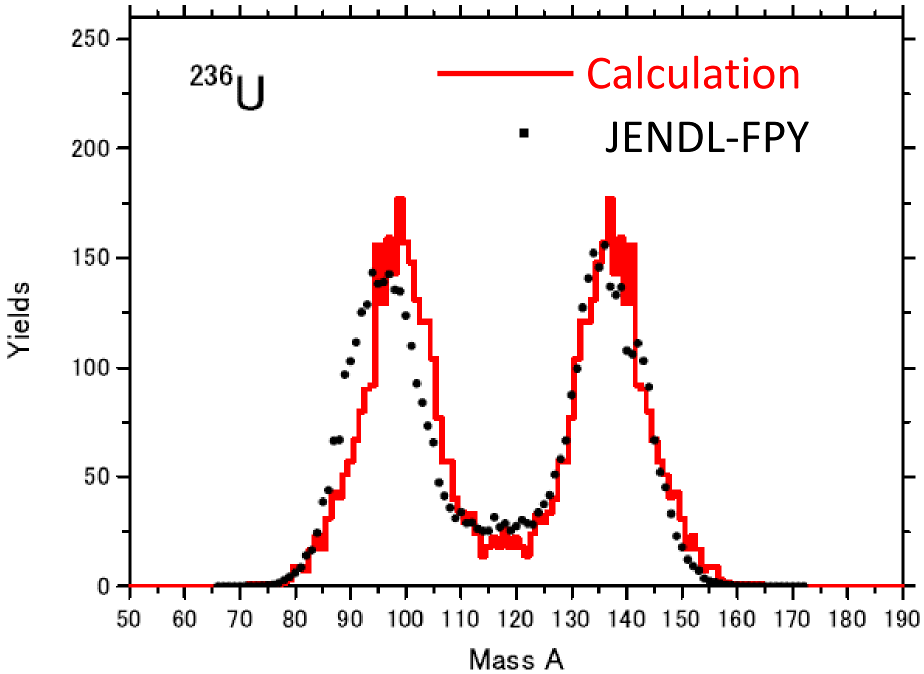
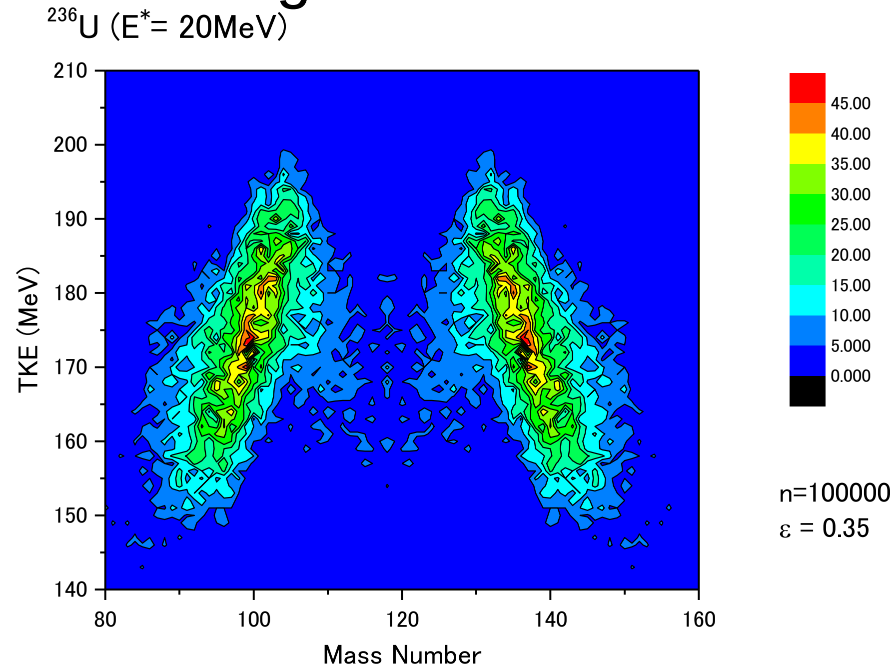
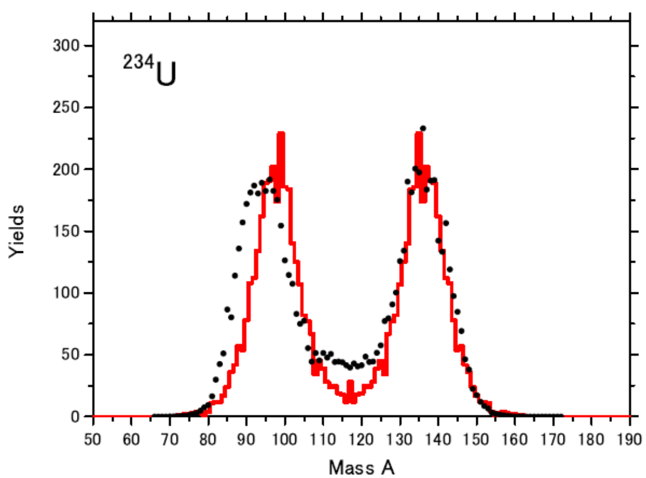
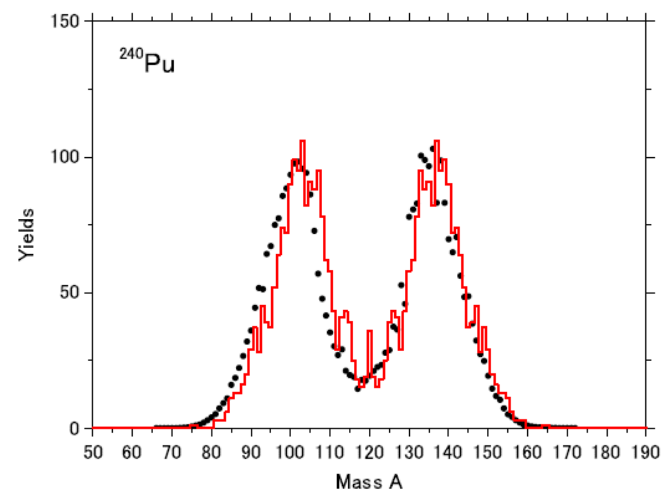
Present study includes the results of "Comprehensive study of delayed-neutron yields for accurate evaluation of kinetics of high-burn up reactors" entrusted to Tokyo Institute of Technology by the Ministry of Education, Culture, Sports, Science and Technology of Japan (MEXT).

Mass and TKE distributions of fission fragments $E^* = 20$ MeV





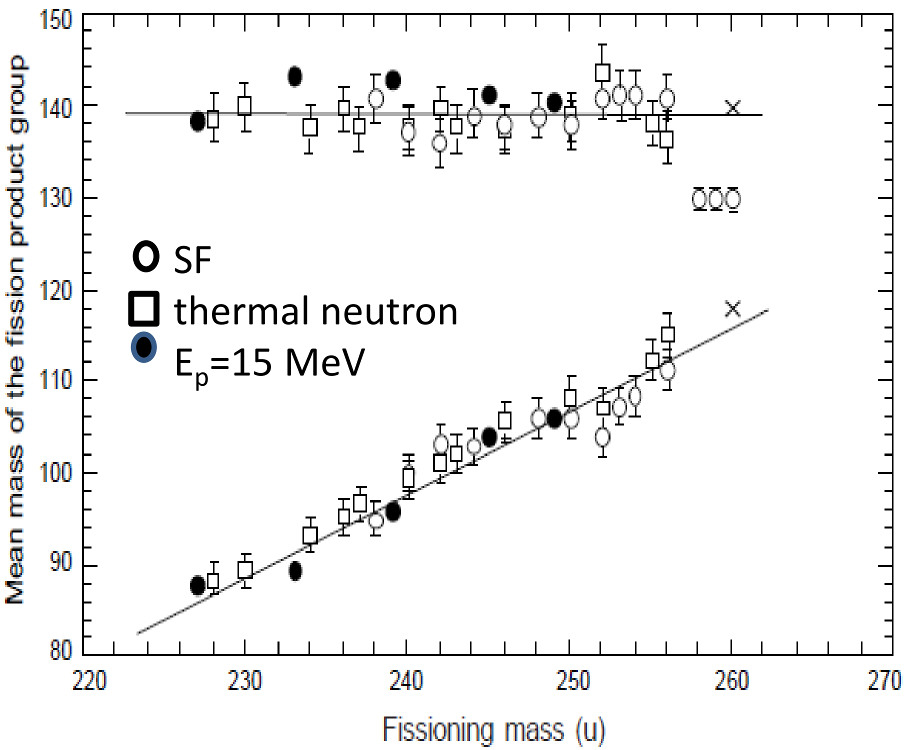




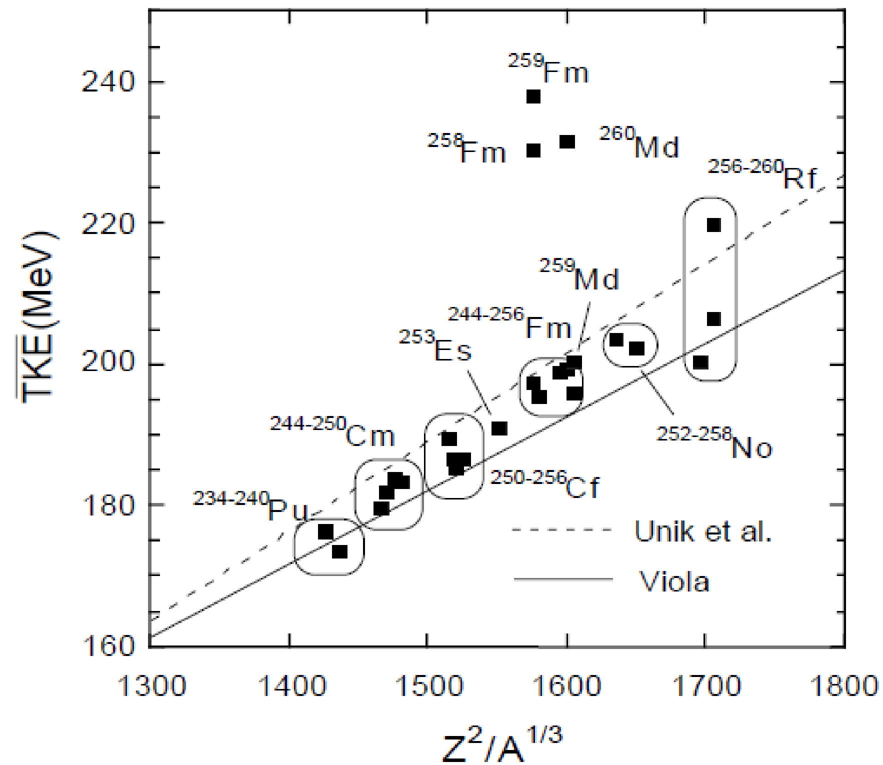
Y. Aritomo and SC, Phys. Rev. C 88, 044614-1-7.

Background

Mean mass of heavy and light fission fragments

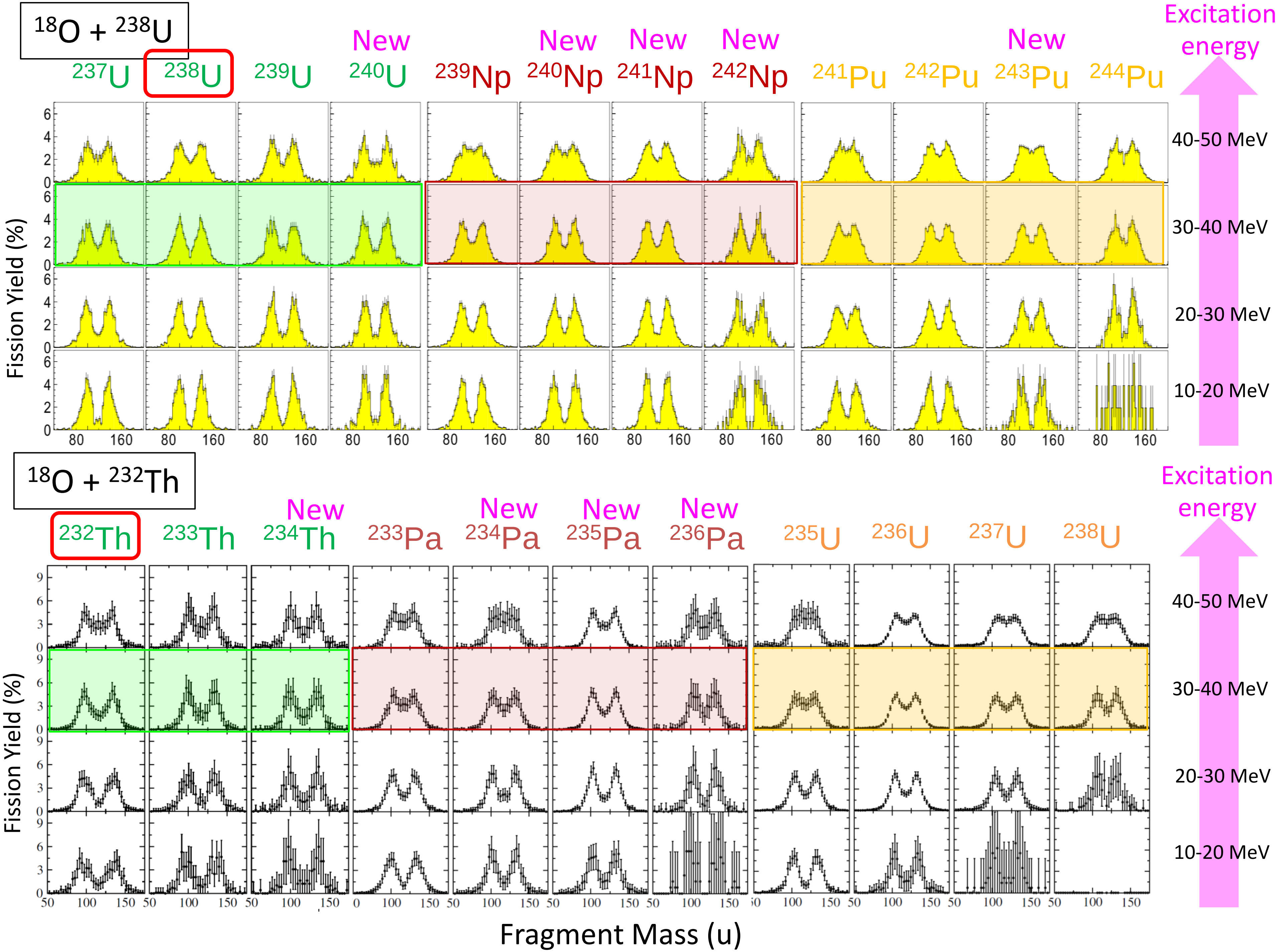


<TKE> as a function of Ec of fissioning system



T. Ohtsuki, Y. Nagame, H. Nakahara

How can we understand these well-established trends?


18O + 238U
New
237U 238U 239U 240U
New New New
239Np 240Np 241Np 242Np
New
241Pu 242Pu 243Pu 244Pu
Excitation energy
40-50 MeV
30-40 MeV
20-30 MeV
10-20 MeV
Fission Yield (%)
18O + 232Th
New
232Th 233Th 234Th
New New New
233Pa 234Pa 235Pa 236Pa
235U 236U 237U 238U
Excitation energy
40-50 MeV
30-40 MeV
20-30 MeV
10-20 MeV
Fission Yield (%)
Fragment Mass (u)

Multi-dimensional Langevin Equation for nuclear fission

$$\frac{dq_i}{dt} = \left(m^{-1}\right)_{ij} p_j$$

$$\frac{dp_i}{dt} = -\frac{\partial V}{\partial q_i} - \frac{1}{2}\frac{\partial}{\partial q_i}\left(m^{-1}\right)_{jk} p_j p_k - \gamma_{ij}\left(m^{-1}\right)_{jk} p_k$$

Friction dissipation

Newton equation

q_i: deformation coordinate (nuclear shape)

two-center parametrization (z, δ, α) (Maruhn and Greiner, Z. Phys. 251(1972) 431)

p_i: momentum conjugate to q_i

m_{ij} : Hydrodynamical mass (inertia mass)

γ_{ij}: Wall and Window (one-body) dissipation (friction)

Needs for microscopic treatment of transport coefficients

$$\langle R_i(t)\rangle = 0,\ \langle R_i(t_1)R_j(t_2)\rangle = 2\delta_{ij}\delta(t_1 - t_2) : \text{white noise (Markovian process)}$$

$$\sum_k g_{ik} g_{jk} = T\gamma_{ij}$$

Einstein relation

Fluctuation-dissipation theorem

$$E_{\text{int}} = E^* - \frac{1}{2}\left(m^{-1}\right)_{ij} p_i p_j - V(q) = aT^2$$

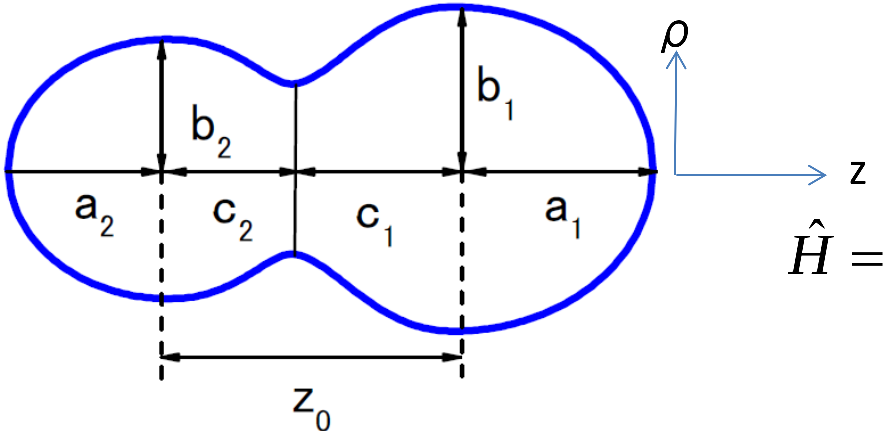
E_{int} : intrinsic energy, E^* : excitation energy

Neutron emission competition is taken into account

Shape parametrization and potential V : 2-center shell model

Shape parametrization

J. Maruhn and W. Greiner, Z. Phys, 1972



$$\hat{H} = -\frac{\hbar^2}{2m_0}\nabla^2 + V(\mathbf{r}) + V_{\mathrm{LS}}(\mathbf{r},\mathbf{p},\mathbf{s}) + V_{\mathrm{L}^2}(\mathbf{r},\mathbf{p}).$$

$$V(\rho,z) = \frac{1}{2}m_0 \begin{cases} \omega_{z1}^2 z'^2 + \omega_{\rho 1}^2 \rho^2, \quad z < z_1 \\ \omega_{z1}^2 z'^2\left(1 + c_1 z' + d_1 z'^2\right) + \omega_{\rho 1}^2\left(1 + g_1 z'^2\right)\rho^2, \\ \quad z_1 < z < 0 \\ \omega_{z2}^2 z'^2\left(1 + c_2 z' + d_2 z'^2\right) + \omega_{\rho 2}^2\left(1 + g_2 z'^2\right)\rho^2, \\ \quad 0 < z < z_2 \\ \omega_{z2}^2 z'^2 + \omega_{\rho 2}^2 \rho^2, \quad z > z_2, \end{cases}$$

$$z' = \begin{cases} z - z_1 & z < 0 \\ z - z_2 & z > 0 \end{cases}$$

$$z = \frac{z_0}{BR}$$ Normalized inter-fragment distance

$$B = \frac{3+\delta}{3-2\delta}$$

R : Radium of compound nucleus

$$\delta = \frac{3(a-b)}{2a+b}$$ Deformation of each fragment

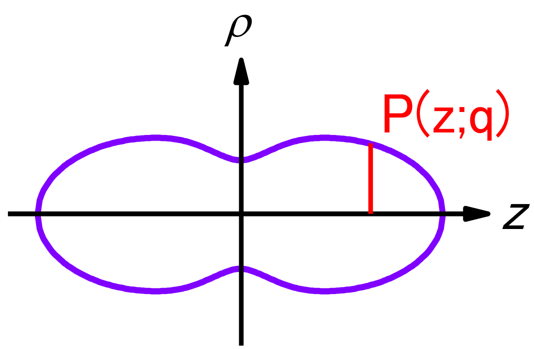
$$\alpha = \frac{A_1 - A_2}{A_{CN}}$$ Mass asymmetry

Transport coefficients (inertia mass)

Inertia Mass (Hydrodynamical mass)

Total kinetic energy of system

$$T = \frac{1}{2}\rho_m \int v^2 d^3 r = \frac{1}{2}\sum m_{ij}(q)\dot{q}_i \dot{q}_j$$



Werner-Wheeler approximation

$\nabla \cdot \vec{v} = 0$	Incompressible fluid
$\vec{v} = \dot{\rho}\vec{e}_\rho + \dot{z}\vec{e}_z$	Axially symmetric shape

$$\dot{z} = \sum A_i(z;q)\dot{q}_i$$

$$\dot{\rho} = \frac{\rho}{P}\sum B_i(z;q)\dot{q}_i$$

$$P = P(z;q)$$

For an incompressible fluid the total (convective) time derivative of any fluid volume must vanish

$$m_{ij} = \pi\rho_m \int_{z_{\min}}^{z_{\max}} P^2 \left(A_i A_j + \frac{1}{8} P^2 A_i' A_j' \right) dz$$

$$A_i(z;q) = \frac{1}{P^2(z;q)} \frac{\partial}{\partial q_i} \int_z^{z_{\max}} P^2(z';q)dz'$$

$$A_i(z;q) = -\frac{1}{P^2(z;q)} \frac{\partial}{\partial q_i} \int_{z_{\min}}^{z} P^2(z';q)dz'$$

$$B_i(z;q) = -\frac{1}{2} P \frac{\partial A_i}{\partial z}$$

K.T.R. Davies, A.J. Sierk, R. Nix, PRC 13 (1976) 2385

Transport coefficients (friction tensor)

Friction (One body friction)

Rayleigh dissipation function

$$F = \frac{1}{2}\frac{dE}{dt} = \frac{1}{2}\sum \gamma_{ij}(q)\dot{q}_i\dot{q}_j$$

↔

Incompressible fluid
constant two-body viscosity coefficient

$$F = \frac{1}{2}\mu\int \Phi(r)d^3r = \frac{1}{2}\sum \eta_{ij}(q)\dot{q}_i\dot{q}_j$$

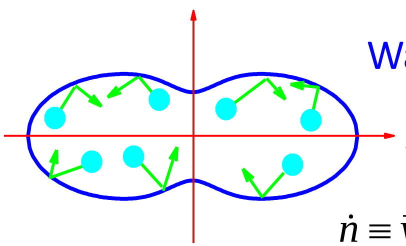
Loss of energy to particles inside the mean filed at the rate

$$\frac{dE}{dt} = \rho_S \bar{v}\int \dot{n}^2 dS$$

$\rho_S = \rho_S(q,z)$ mass density of nucleus

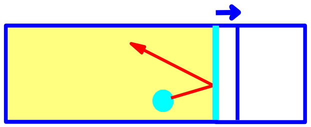
$\bar{v}$ average nucleon speed

$\dot{n}$ relative normal velocity of the wall



Wall formula

$$\dot{n} \equiv \vec{v}\cdot\hat{n} = \frac{\partial \rho_S}{\partial t}\left[1+\left(\frac{\partial \rho_S}{\partial z}\right)^2\right]^{-\frac{1}{2}}$$



$$= \sum_i \dot{q}_i \rho_S \frac{\partial \rho_S}{\partial q_i}\left[\rho_S^2 + \left(\rho_S \frac{\partial \rho_S}{\partial z}\right)^2\right]^{-\frac{1}{2}}$$

$$\gamma_{ij} = \frac{\pi\rho\bar{v}}{2}\int_{z_{\min}}^{z_{\max}} dz \frac{\partial \rho_S^2}{\partial q_i}\frac{\partial \rho_S^2}{\partial q_j}\left[\rho_S^2 + \frac{1}{4}\left(\frac{\partial \rho_S^2}{\partial z}\right)^2\right]^{-\frac{1}{2}}$$

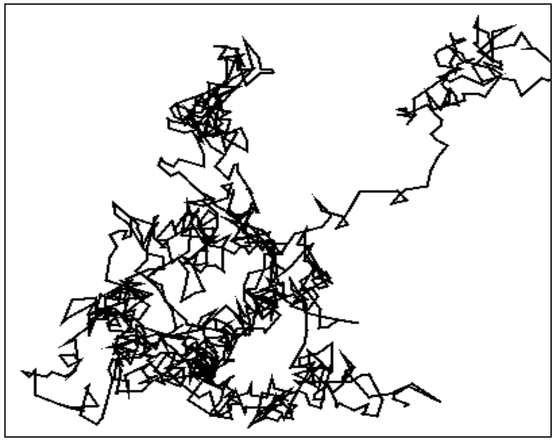
One body friction (Wall formula)

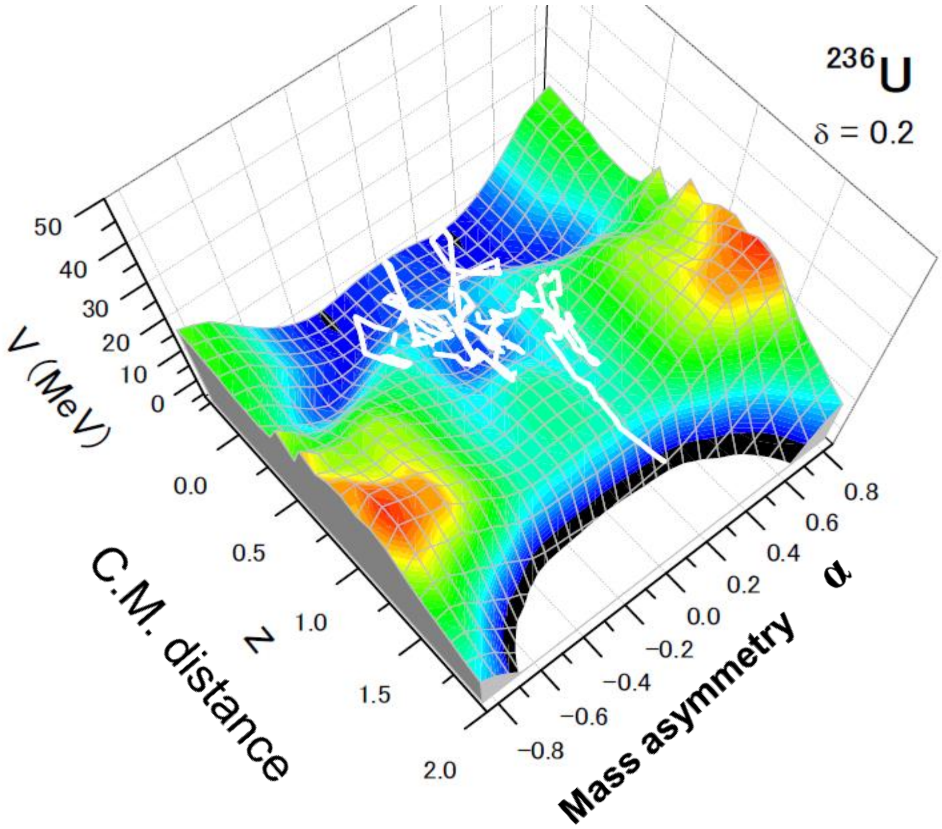
A.J. Sierk, R. Nix, PRC 21 (1980) 982

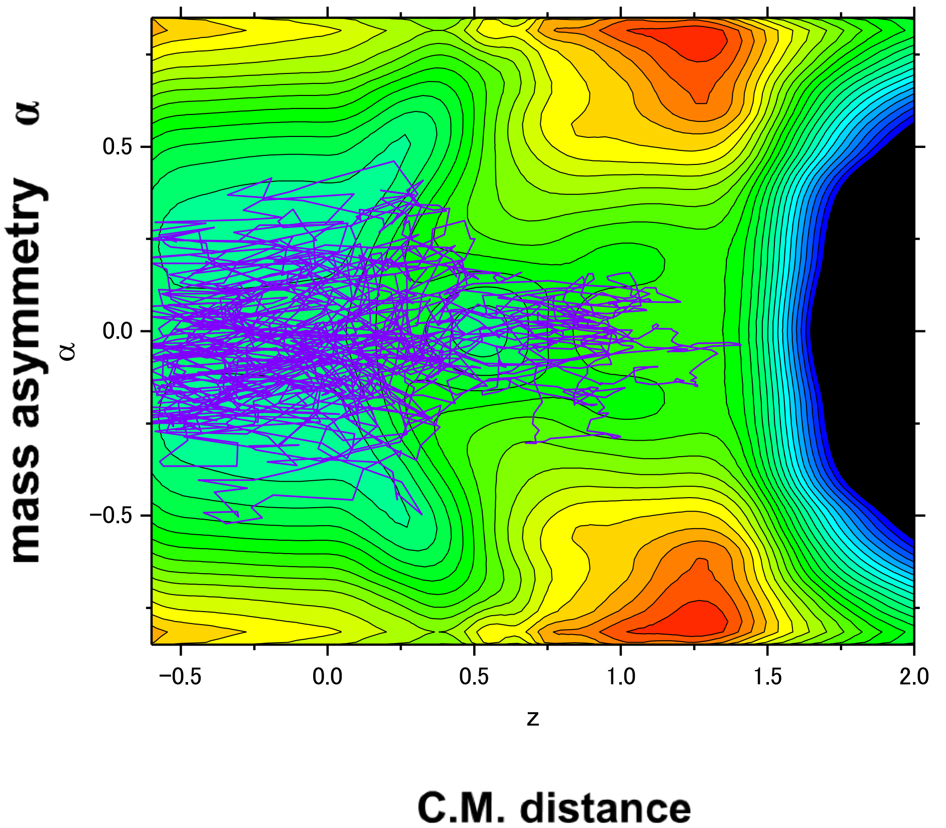
Potenaial V and fission process of ^{236}U by Langevin equation (E*=20 MeV)

The Langevin trajectories do not necessarily follow the multi-dimensional potential minima

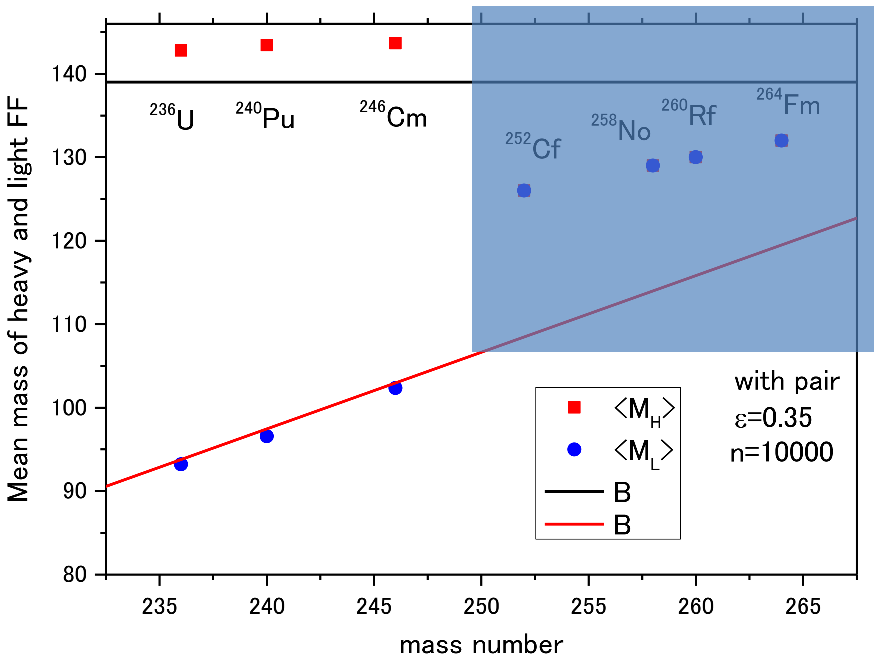
Trajectory on potential energy surface

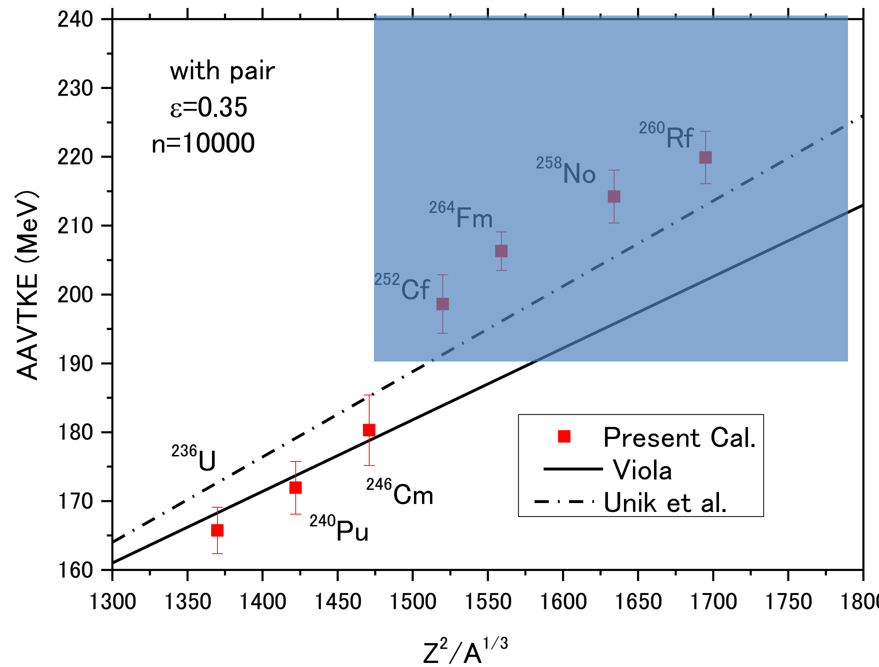


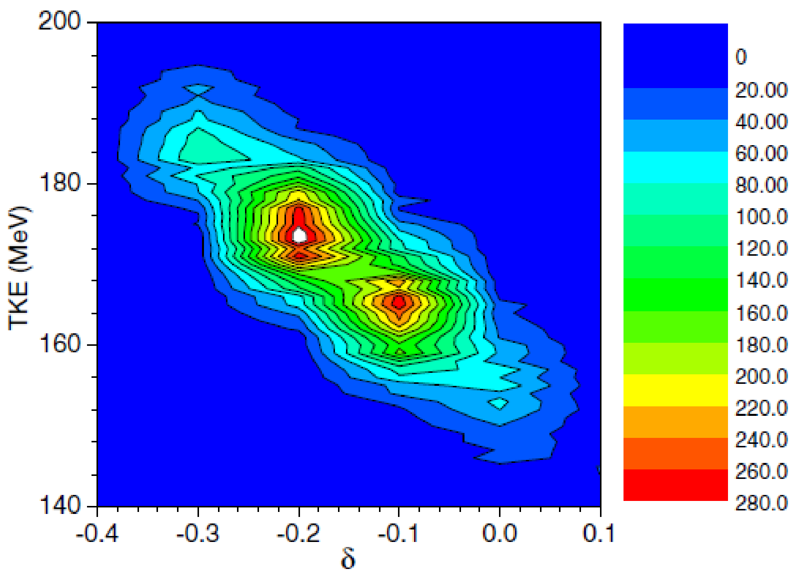




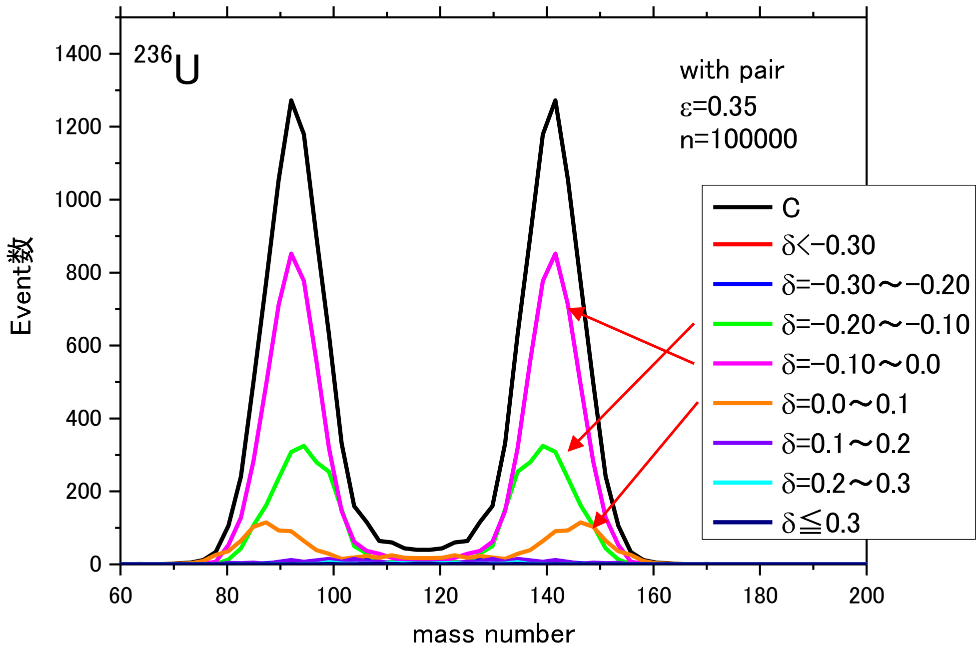
Mean mass of FF and <TKE> E*=20MeV

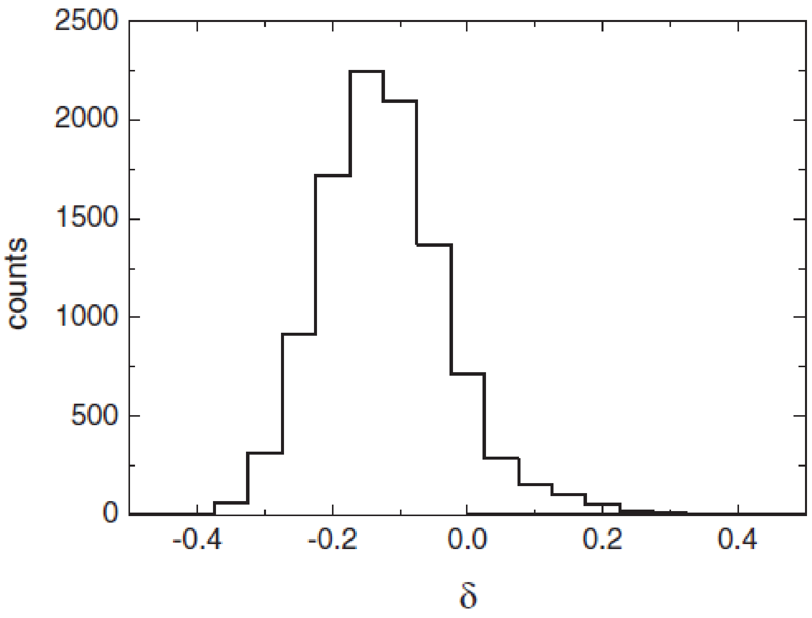




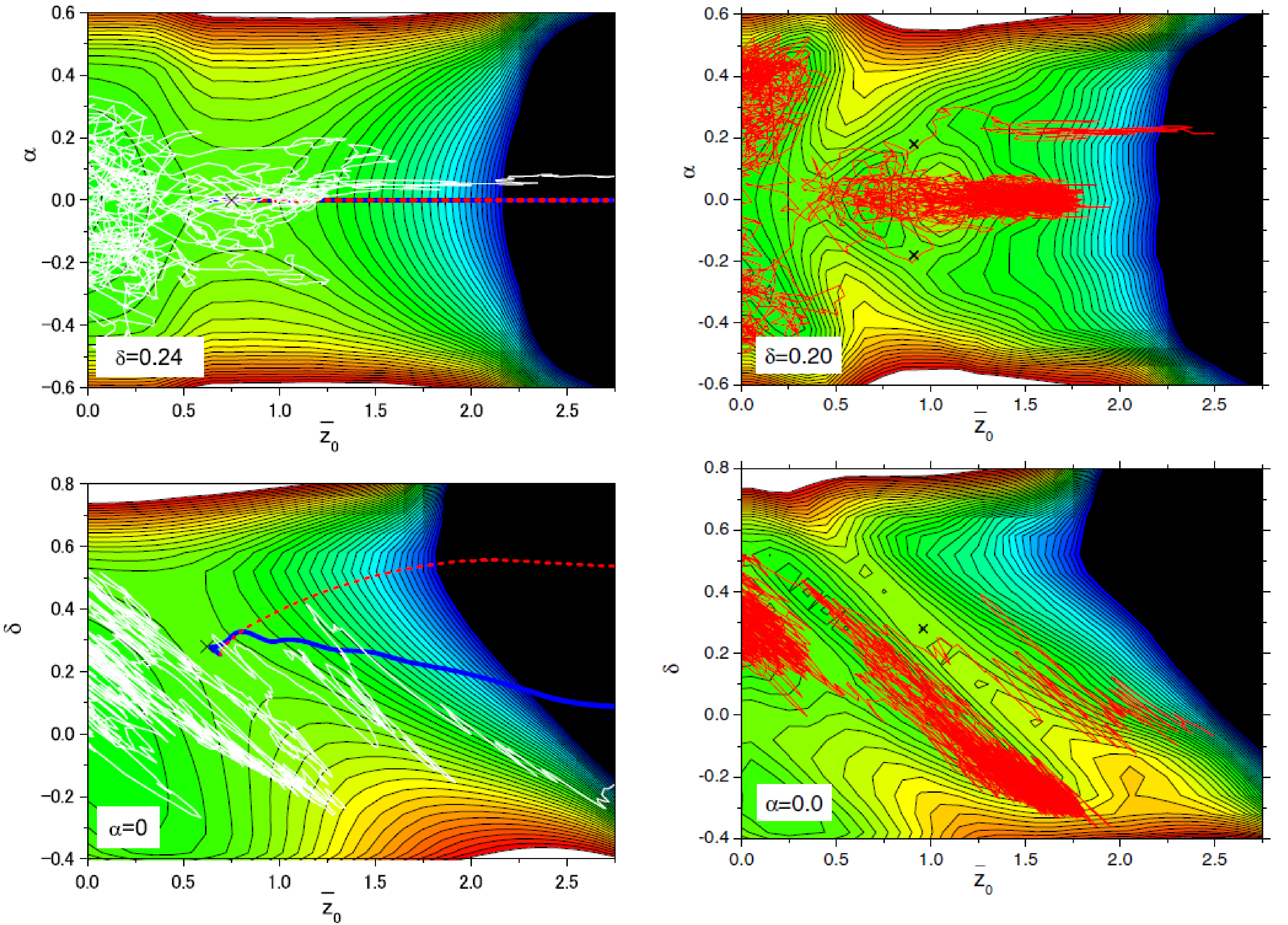


δ-dependence in asymmetric FFMD of ^{236}U





Y. Aritomo, S.C and F.A. Ivanyuk, Phys.Rev.C 90, 054609-1-8(2014)



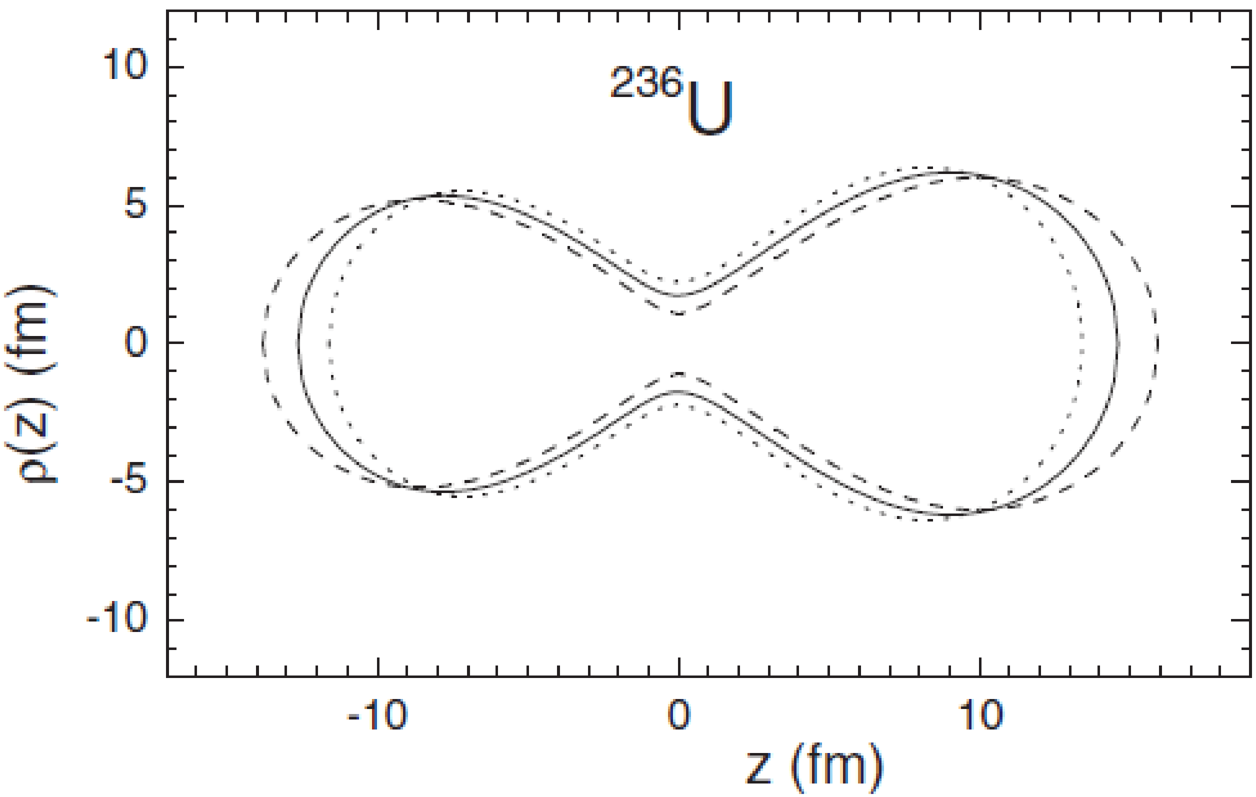
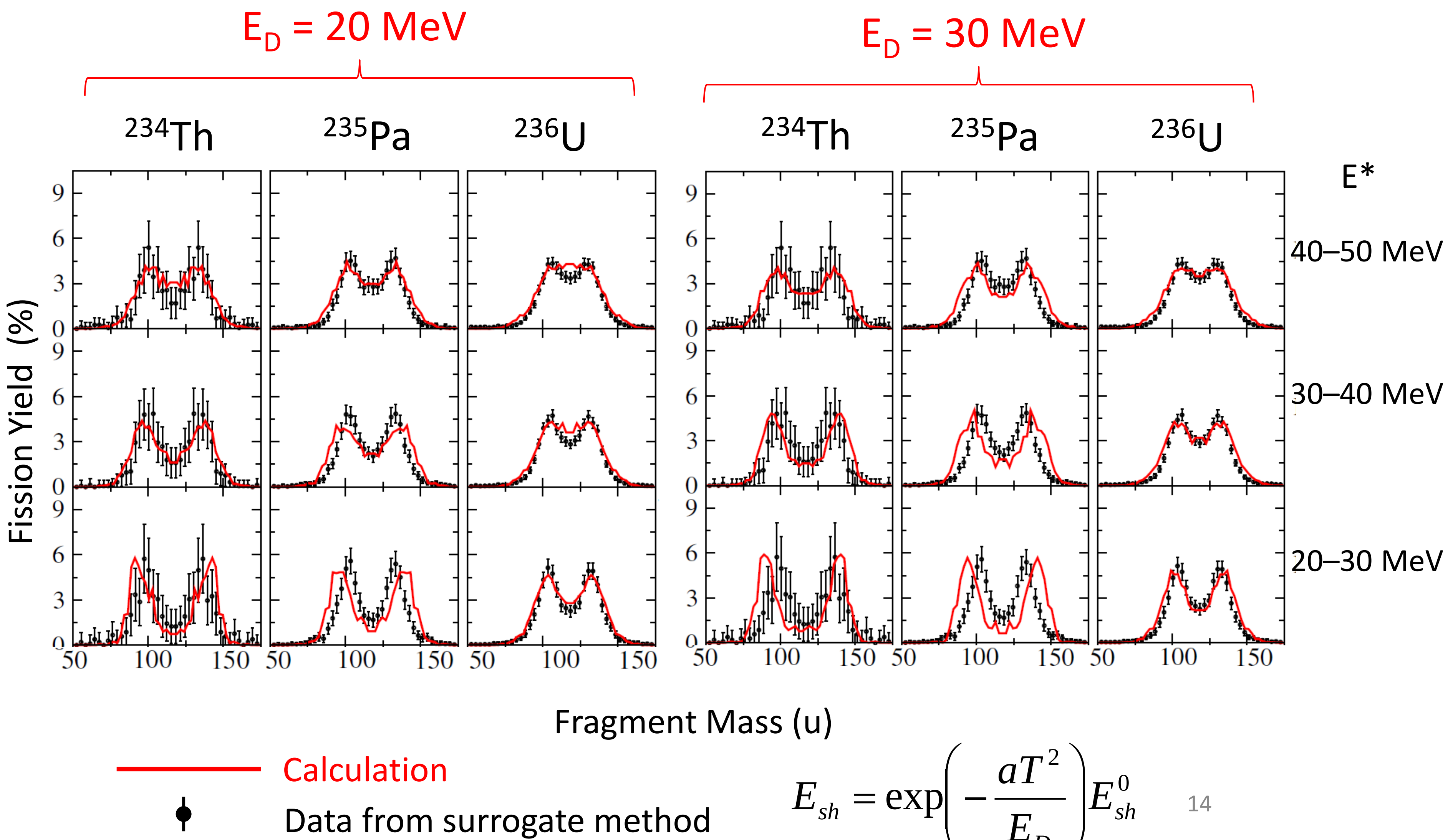


FIG. 5. Nuclear shapes around the scission point of ^{236}U. The dot, solid, and dashed line corresponds to the nuclear shape at $\{\bar{z}_0, \delta, \alpha\} = \{2.5, -0.2, 0.2\}$, $\{2.5, 0, 0.2\}$, and $\{2.5, 0.2, 0.2\}$.

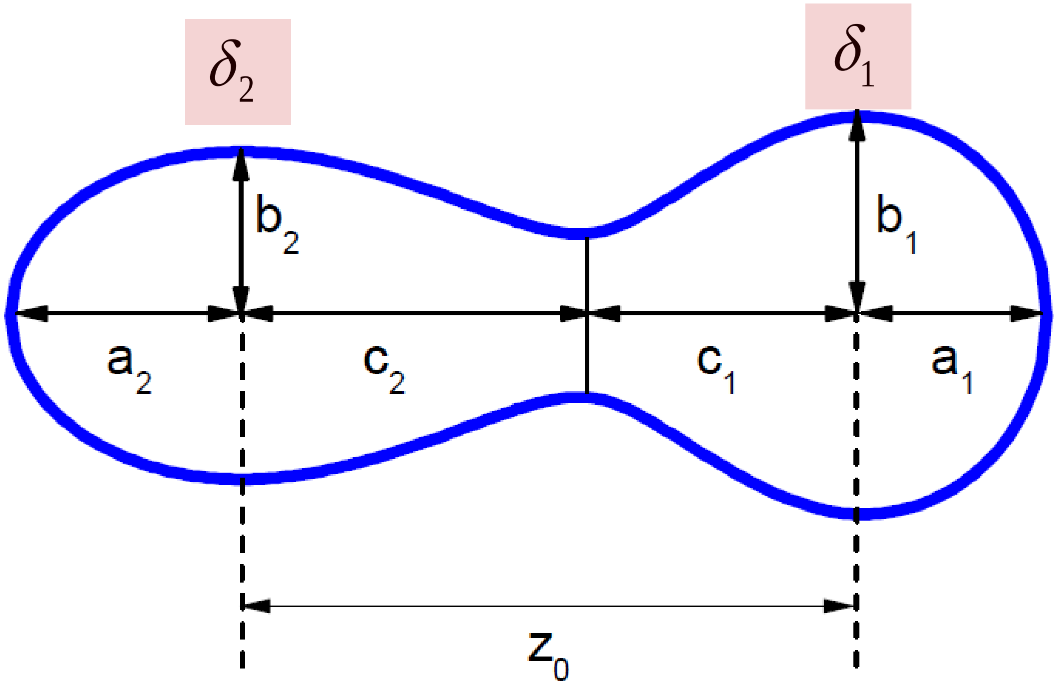
Comparison of measured (by surrogate method) and Langevin calculation



$$E_{sh} = \exp\left(-\frac{aT^2}{E_D}\right)E_{sh}^0$$

4-dimensional calculation

2 center shell model
(Maruhn and Greiner,
Z. Phys. 251(1972) 431)



$$q(z, \delta_1, \delta_2, \alpha)$$

$$z = \frac{z_0}{BR}$$

$$B = \sqrt{B_1 B_2}$$

$$B_1 = \frac{3+\delta_1}{3-2\delta_1}, \quad B_2 = \frac{3+\delta_2}{3-2\delta_2}$$

R Radius of compound nucleus

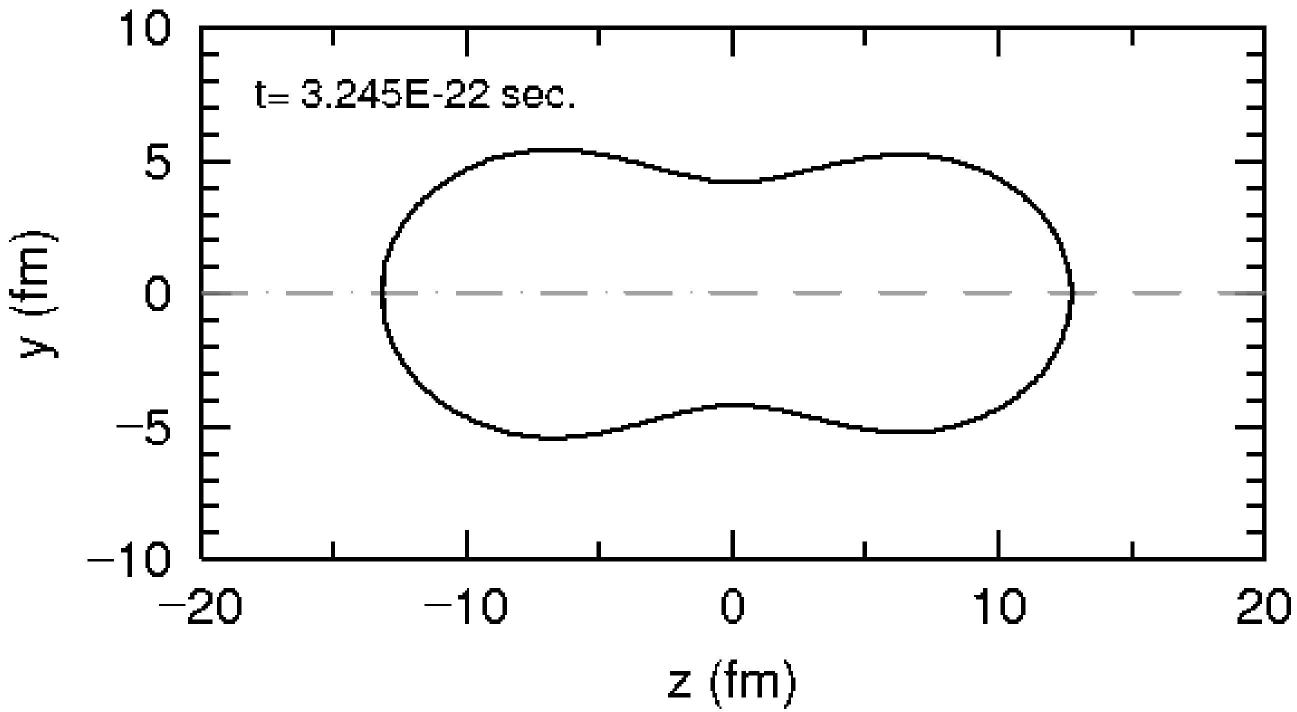
$$\delta 1 = \frac{3(a_1 - b_1)}{2a_1 + b_1}, \quad \delta 2 = \frac{3(a_2 - b_2)}{2a_2 + b_2}$$

$$\alpha = \frac{A_1 - A_2}{A_1 + A_2}$$

$$V(q, \ell, T) = V_{DM}(q) + \frac{\hbar^2 \ell(\ell+1)}{2I(q)} + V_{SH}(q, T)$$

Time evolution by 4-dimensional Langevin calculation

^{236}U E^{*}=20 MeV



Summary

- Results of Langevin calculations at Tokyo Tech were summarized

- 3D calc. : Good for FFMD and <TKE> in U to Cm region
- negative δ is important in this model
- trajectories in -45 deg. in δ-z plain : importance of non-diagonal terms in the transport coefficients
- 4-D calc. and microscopic transport coefficients : ongoing