Theoretical Study of decay heat and delayed neutron emission

- 4 year project of estimating decay heat and delayed neutron emission for U, Pu and minor actinides -

Hiroyuki Koura
Advance Science Research Center
Japan Atomic Energy Agency

Collaborate with:
S. Chiba (Tokyo Inst. Tech., TIT), T. Yoshida (TIT) and T. Tachibana (Waseda Univ.)
Understanding global properties of nuclei

Nuclear mass region

- (Extremely) Superheavy: Decay modes, Structure of superheavy double magic nuclei $^{298}_{114}$ and its neighboring, and beyond
- Proton-rich: $N=126$ neutron-deficient nuclei (Unknown peninsula): enhancement of existence due to the closed shell
- Neutron-rich: Change of closed shell, Fission in the superheavy, r-process nucleosynthesis

Medium-heavy n-rich region:
Astrophysics: r-process
Atomic Energy: Fission product from actinides

Chart of the Nuclides (KTUY mass+ decay model)

Prediction of decay modes of nuclei
(How far does the area of superheavy elements extend? - Decay modes of heavy and superheavy nuclei -
Purpose: High-precision prediction of operating characteristic properties of highly-burn-up nuclear reactor and innovative nuclear reactor where minor actinides accumulate from the following way:

1. Measurement of Fission Yield (FY) data via Surrogate reaction
2. Construction of method for obtaining delayed neutron rate and decay heat with gross theory of beta decay
3. Construction of theoretical method for obtaining Independent FY with Dynamical model (Two-center shell model + Langevin eq.)
4. Nuclear Data (including verification on reactor system)
Procedure

1. Surrogate reaction exp.

2. Gross theory of β decay
   - Strength function
   - β-ray spectra
   - γ-ray spectra
   - delayed neutron Yield, $\chi_d$
   - anti-neutrino spectra

3. Multi-dimensional dynamics of Fission (Langevin) model

4. Library, Summation Calculation
   - Analysis of decay heat data
   - $\beta_{eff}$ Analysis of Reactor Physics data
   - Neutrino production

courtesy of S. Chiba
\[ T_{1/2} = \frac{\ln 2}{\lambda} \]

\[ \lambda = \lambda_F + \lambda_{GT} + \lambda_1^{(0)} + \lambda_1^{(1)} + \lambda_1^{(2)} \]

(up to 1st forbidden)

\[ \lambda_F = \frac{m_e^5 c^4}{2\pi^3 \hbar^7} |g_V|^2 \int_{-Q}^{0} |M_F(E)|^2 f(-E) dE \]

\[ \lambda_{GT} = \frac{m_e^5 c^4}{2\pi^3 \hbar^7} |g_A|^2 3 \int_{-Q}^{0} |M_{GT}(E)|^2 f(-E) dE \]

\[ \lambda_1^{(2)} = \frac{m_e^5 c^4}{2\pi^3 \hbar^7} \left( \frac{m_e c}{\hbar} \right)^2 |g_A|^2 \int_{-Q}^{0} \sum_{ij} |M_{ij}(E)|^2 f_1(-E) dE \]

\[ \lambda_1^{(1)} = \frac{m_e^5 c^4}{2\pi^3 \hbar^7} \left( \frac{m_e c}{\hbar} \right)^2 \left[ |g_V|^2 \int_{-Q}^{0} |M_r(E)|^2 f_{1V}^{(1)}(-E) dE + |g_A|^2 \int_{-Q}^{0} |M_{\sigma \cdot r}(E)|^2 f_{1A}^{(1)}(-E) dE \right] \]

\[ \lambda_1^{(0)} = \frac{m_e^5 c^4}{2\pi^3 \hbar^7} \left( \frac{m_e c}{\hbar} \right)^2 |g_A|^2 \int_{-Q}^{0} |M_{\sigma \cdot r}(E)|^2 f_{1A}^{(0)}(-E) dE \]
Gross theory of beta decay

$$M_\Omega(E)^2 = \int_{\epsilon_{\text{min}}}^{\epsilon_{\text{max}}} D(E, \epsilon) W(E, \epsilon) \frac{dn_1}{d\epsilon} \, d\epsilon$$

$D(E, \epsilon)$: one particle strength function

half-life, energy distribution, delayed neutron probability
β-decay strength function

Neutron-rich side

Schematic view of β⁻ decay for light nuclei

Light nuclei : G-T dominance

Schematic view of β⁻ decay for heavy nuclei

Heavy nuclei : Competition between GT and 1st forbidden

No consideration with Pauli Principle $\leftrightarrow W(E, \epsilon) = 0$
Half-life measurement in the n-rich nuclei at RIBF: Gross theory vs QRPA

S. Nishimura, et al. PRL106(2011)

Nuclide Identification
Left from Black line: nuclei with known half-lives
Filled green: part of the r-process path (WP Approx.)

FIG. 3 (color online). Neutron number dependence of β-decay half-lives for (top) even-Z (a) Kr, (b) Sr, (c) Zr, and (d) Mo, and (bottom) odd-Z (e) Rb, (f) Y, (g) Nb, and (h) Tc. Filled circles and open triangles represent results from the present work and previous studies, respectively. The respective solid and dotted lines are predictions from the FRDM + QRPA models, while the dashed lines are from the KTUY + GT2.

FIG. 4 (color online). Mass number dependence of the ratio of theoretical $T_{1/2}$ values from (a) FRDM + QRPA [16], (b) KTUY + GT2 [17,18], and (c) FRDM + GT2, to the experimental values deduced in the present work. (d) The difference between $Q_β$ values predicted by the FRDM and KTUY mass formulas.

Absolute Comparison of $T_{1/2}$

Pink : FRDM+QRPA
Dashed blue : KTUY+GT2

Ratio of theoretical $T_{1/2}$ to exp.

FRDM+QRPA: rather large discrepancy due to QRPA
KTUY+GT2: rather good reproduction
Decay Heat and Delayed neutron emission

**Decay heat:**
Fission products (FP) decays $\beta$-decay and $\gamma$ decay. These sum of each heats is decay heat.

$$f(t) = \sum_i \lambda_i \cdot \bar{E}_i \cdot N_i(t)$$

$$= \sum_i \lambda_i \cdot (\bar{E}_\beta + \bar{E}_\gamma) \cdot N_i(t)$$

$$\bar{E}_\gamma = \sum_j E_j^i I_j^\gamma / \text{number}$$

$$\bar{E}_\beta = \sum_j E_j^i I_j^\beta / \text{number}$$

$N_i(t)$: Production Yield at time $t$

**Delayed neutron rate:**
From fission theory and exp.

** Theory:**
$$\lambda_n = \sum_{\beta} \int_{0}^{\bar{E}_\gamma} \frac{\Gamma_n}{\Gamma_n + \Gamma_\gamma} \lambda_0(E) dE,$$

$$\lambda_n\text{exp} = \ln2 P_n\text{exp}/t_{1/2}.$$  

**Exp.:**
$$P_n: \text{Delayed neutron probability}$$

**Delayed neutron yield:**
$$\bar{v}_d = \sum_i P_{ni} Y_i$$

**Time-dependency of delayed neutron emission:**
$$n_d(t) = \sum_i P_{ni} \lambda_i Y_i(t)$$

(6-Group Approx.:)  
$$n_d(t) = \bar{v}_d \sum_{i=1}^{6} \alpha_i \lambda_i \exp(-\lambda_i t)$$

Both phenomena accompany $\beta$ decay.
Application of Gross theory of $\beta$-decay to atomic energy

1. Delayed neutron summation calculation


T. Tachibana, M. Yamada et al. (NDST 1988) 885

(First apply of Gross theory for summation cal.)

Goal: High precise reproduction for U, Pu, and reliable prediction for minor actinides (also energy dependency)

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Pandemonium Problem (Decay Heat)

2. Decay heat

\[ f(t) = \sum_i \lambda_i \cdot E_i^i \cdot N_i(t) \]

\[ = \sum_i \lambda_i \cdot (E_\beta^i + E_\gamma^i) \cdot N_i(t) \]

\( \lambda_i \): Decay constant of nuclide \( i \)
\( E_i^x \): Average energy /one decay
\( x = \beta, \gamma, \text{total} \)
\( N_i(t) \): Production Yield at time \( t \)

Real (correct) \( E_\beta, E_\gamma \)

Actual measurements of \( E_\beta, E_\gamma \)
(\( E_\beta \): overestimated, \( E_\gamma \): underestimated)

‘Virtual’ nuclide with such a incomplete decay scheme is referred to as ‘Pandemonium.’

‘ENDF’ in Fig. : Theory is applied for only unmeasured nuclides
‘App. Gross Theory’ in Fig. : Gross Theory is applied for not only unmeasured nuclides but also measured nuclides

- Lack of energy levels effects results of summation calc. in decay heat : Importance of nuclear structure

J. Katakura
TAGS: Total Absorption Gamma-ray Spectrometer

R.C. Greenwood, Idaho National Engineering and Environmental Laboratory

Taken from NDN 99, p14, T. Yoshida
time evolution of γ-ray heat

Enhancement of Solid red to blue due to TAGS data

Overestimation due to TAGS data (change for the worse)

T. Yoshida
Improvement of Gross theory for half-life, neutron emission and decay heat (in progress)

- Spin-parity of g.s. odd-odd
  - (odd-odd nuclei (J, J is large in most case) → even-even nuclei (0+))

- Spin-parity dependency of low-energy excited states

- Consideration of sum rules of one-particle strength function in high-energy part
  - (Analysis of $^{90}$Zr(p,n): broad distribution of strength function at 50MeV)
  - ...

Database

- β decay half-life, delayed neutron prob., spin-parity: extracted
- Decay heat: extracted
- TAGS data: extracted

ENSDF (May 2012 version)

Lowell (U-235, etc (3 nucl.)), Oak Ridge (3 nucl.), Yayoi (Univ. Tokyo) (3 nucl.), collab. with T. Yoshida (TIT)
Conclusion

• From this late fiscal year, we start a project for 3.5 year, related to delayed neutron and decay heat based on nuclear theory and experiment.

• We will develop a comprehensive code to calculate beta-decay, delayed neutron emission and decay heat, etc.

• Through this work, we will apply to understanding nuclear structure and decay, and will also apply to nuclear astrophysics as the r-process nucleosynthesis.