Titanium Cross Section Evaluation

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S.Y. Oh[*,**], T. Kawano[*], S. Kahler[*], D. Dashdorj[†], and S. Cowell[*]

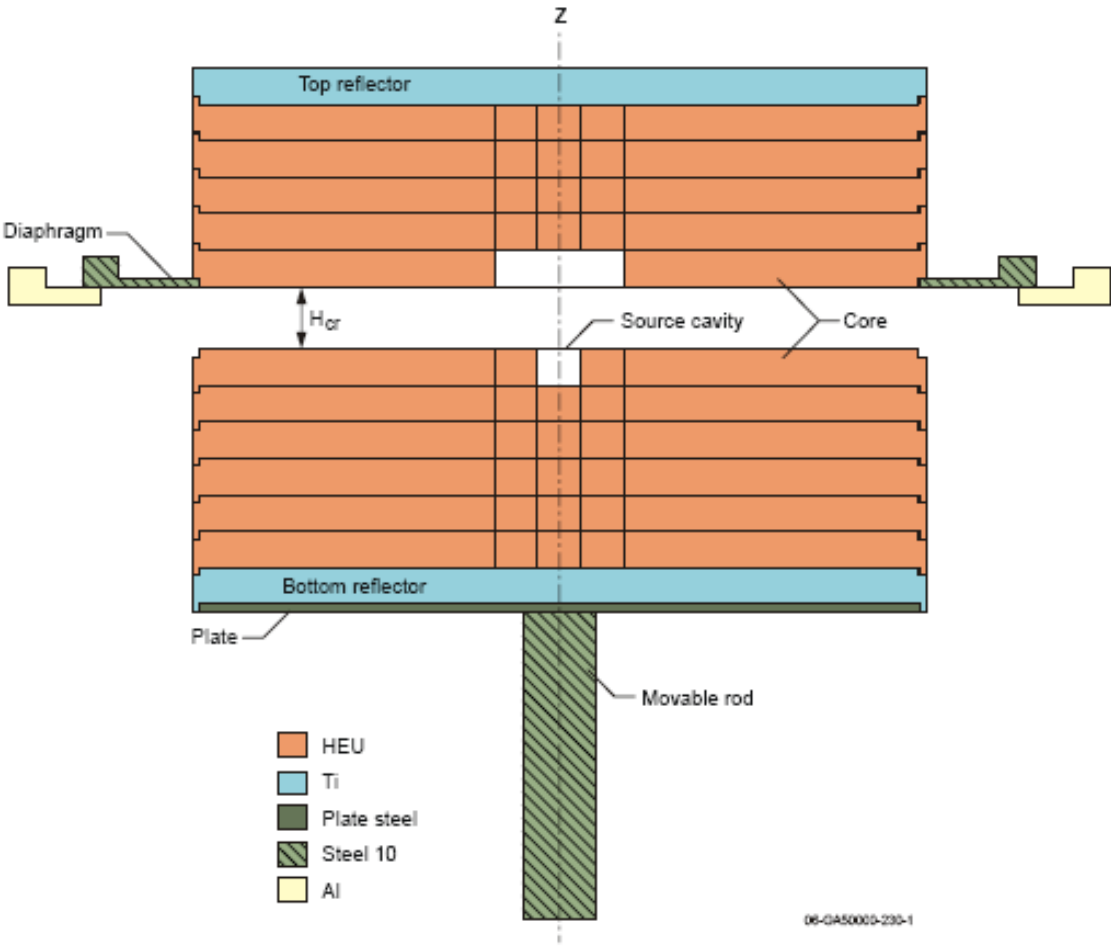
[*] Los Alamos National Laboratory, Los Alamos, NM 87545 USA
[**]Visiting staff from the Korea Atomic Energy Research Institute, Daejeon, Korea
[†] North Carolina State University, Raleigh, NC 27695 USA

1. Why do we re-evaluate Ti data?

- Importance of Ti
  - Structural material
  - Requests from the Criticality Safety Program, …
- Any problem in ENDF/B-VII.0 Ti data?
  - Discrepancies in Criticality Benchmarks
  - Discrepancies in Shielding Benchmarks
- Any new data?
  - New compilation of resonance & thermal data (Mughabghab 2006)
  - Some experimental works by Dashdorj et al.(2005), Voinov et al.(2003), …
  - Reference Input Parameter Library (RIPL-2, 2003)

1.1 Criticality Experiments Involving Ti

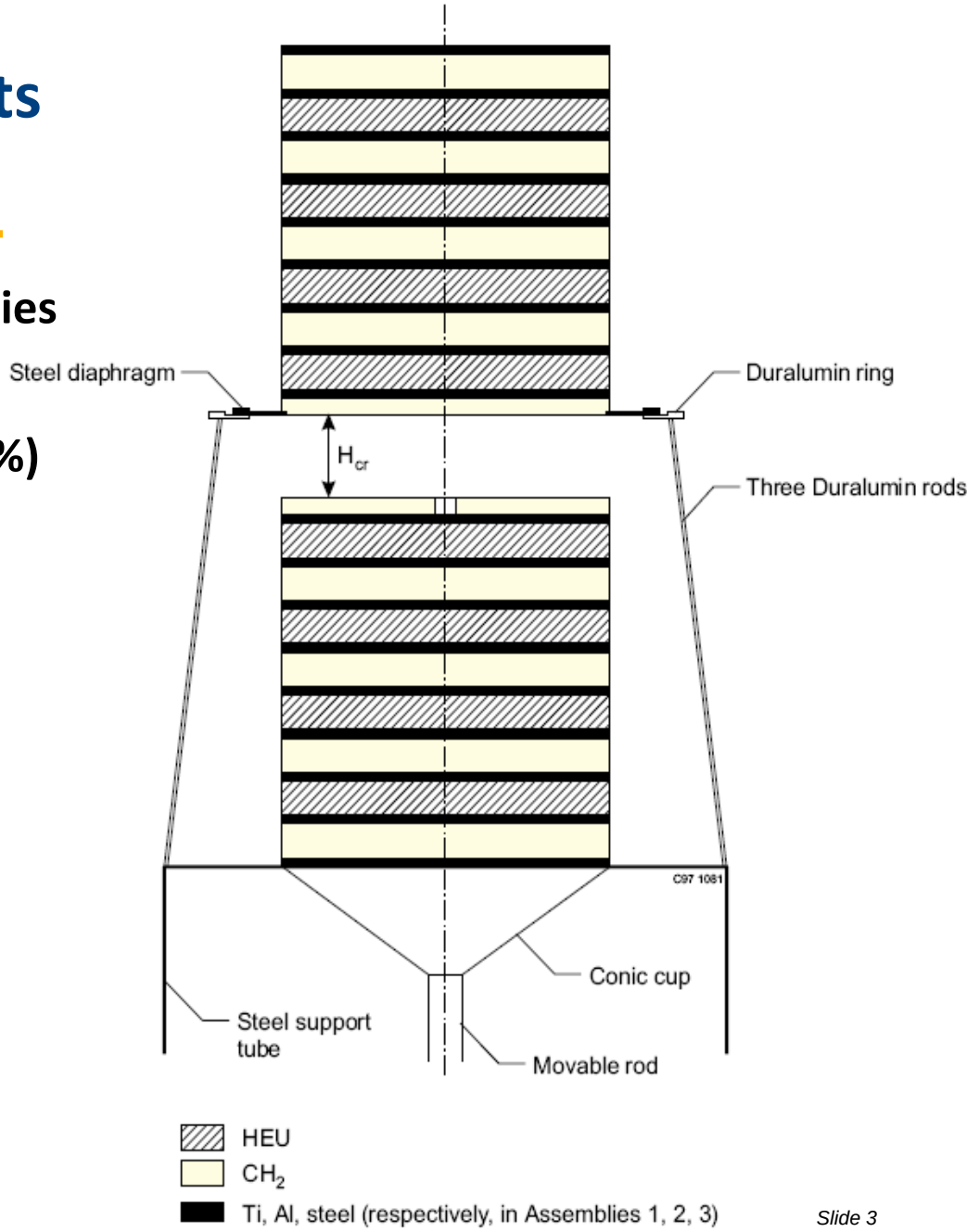
- **HEU-Metal-Fast (HMF) 079 Series (varying with Ti thickness)**



1.1 Criticality Experiments Involving Ti (cont.)

- **HEU-Metal-Fast (HMF) 034 Series**

  - HMF-034.1 Ti interleaved (thermal fission fraction ~ 10%)



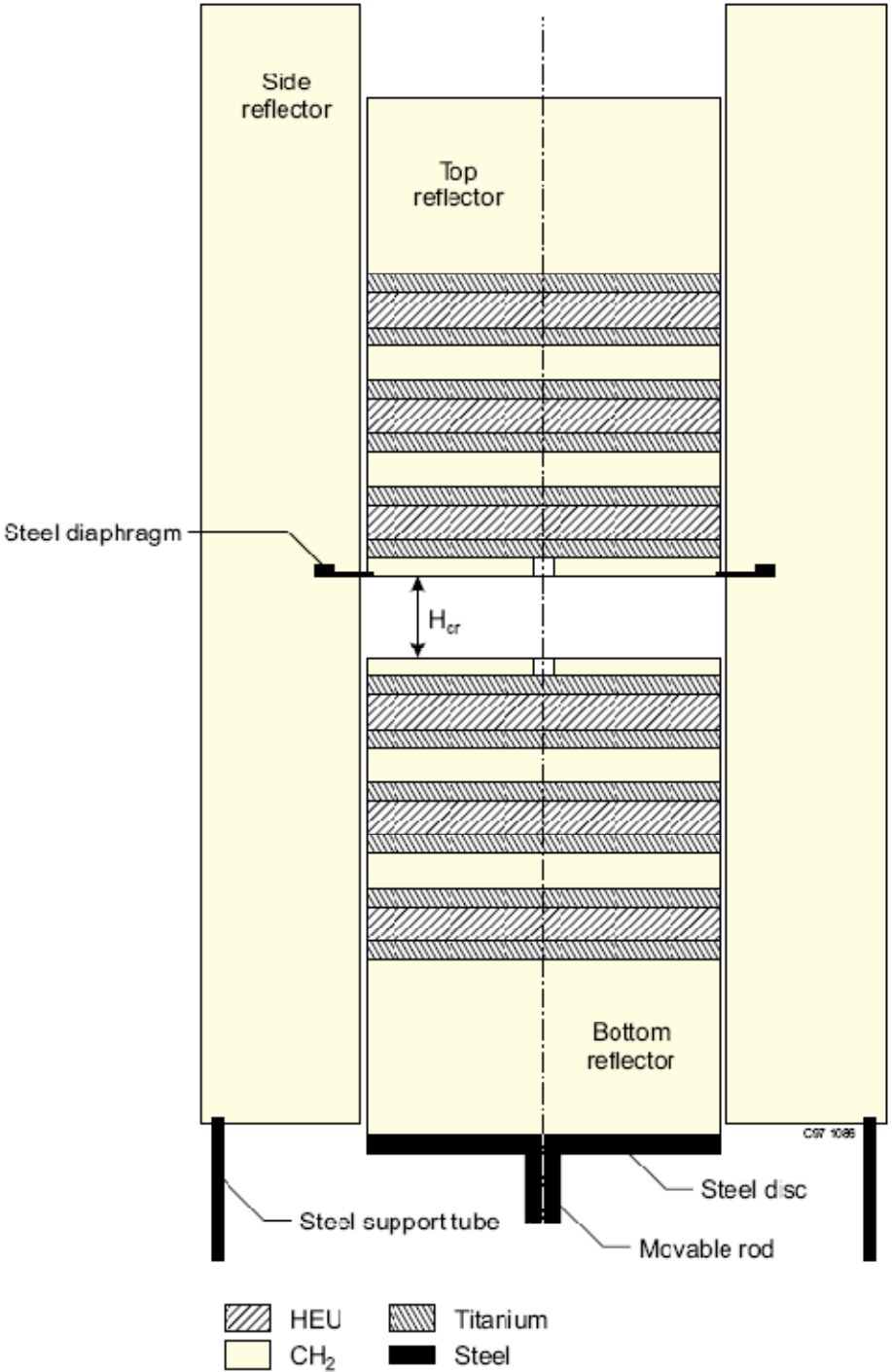
1.1 Criticality Experiments Involving Ti (cont.)

- **HEU-Metal-Mixed (HMM) 1 & 15**

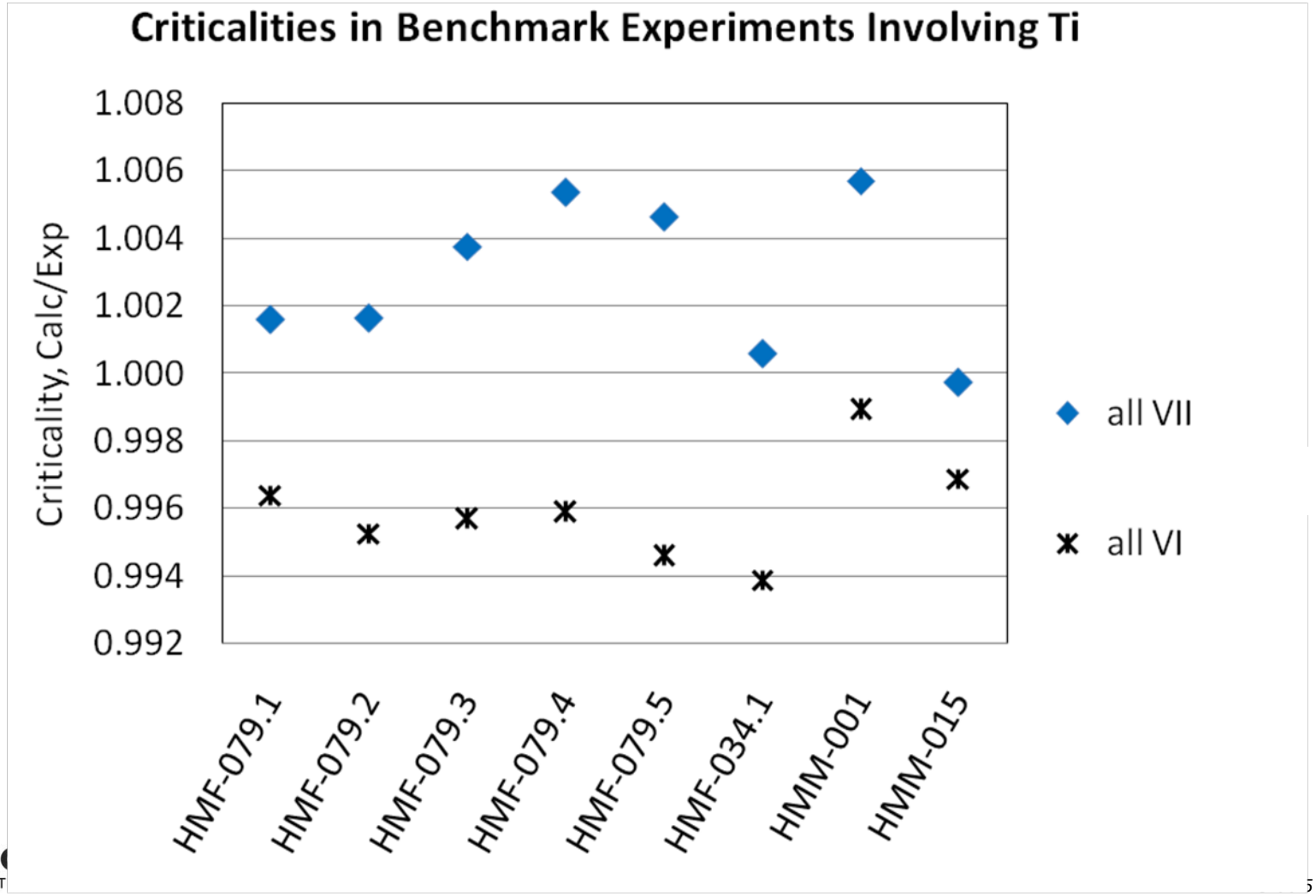
  - thermal fission fraction:

  HMM 01 ~ 23%

  HMM 15 ~ 37%



1.2 Discrepancies in Criticality Benchmarks



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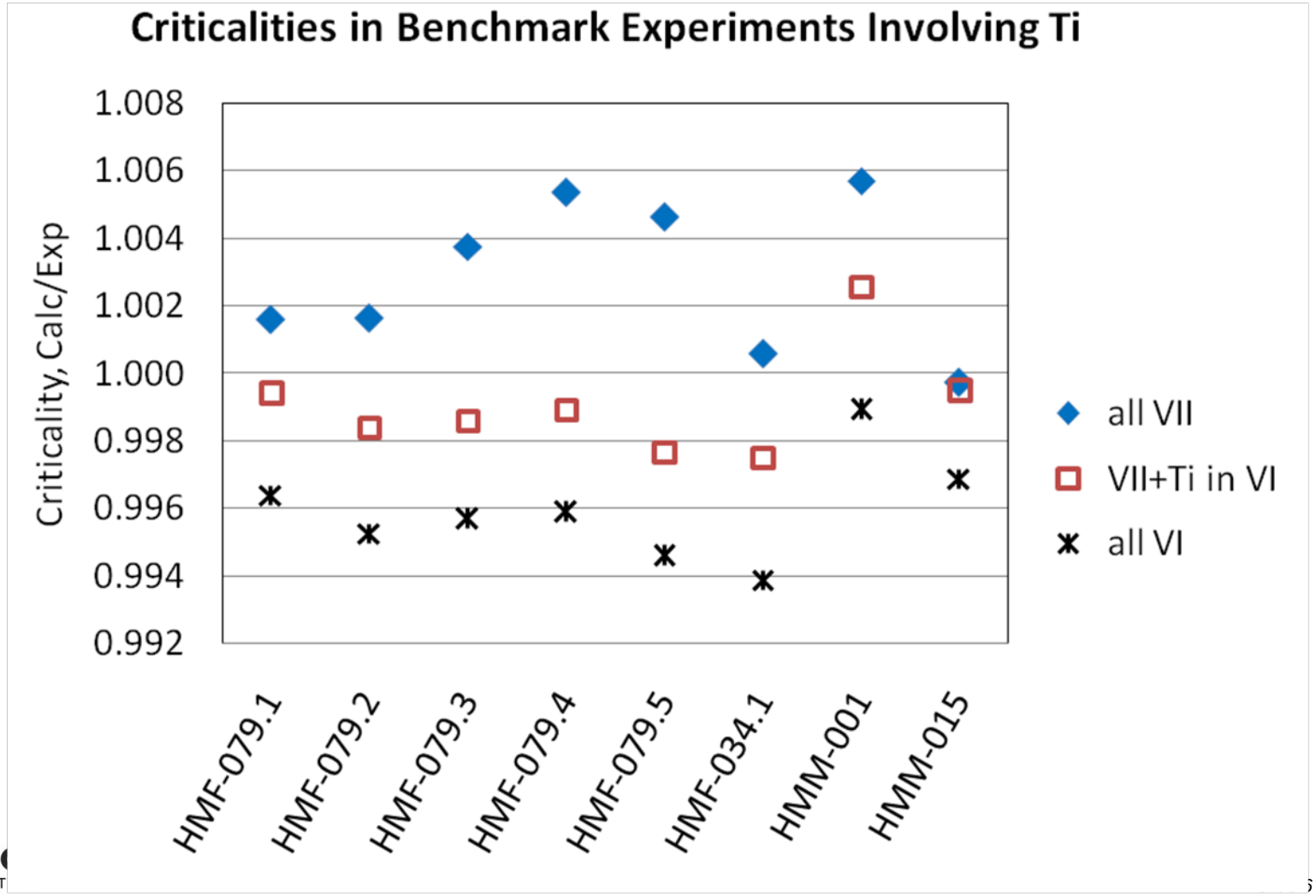
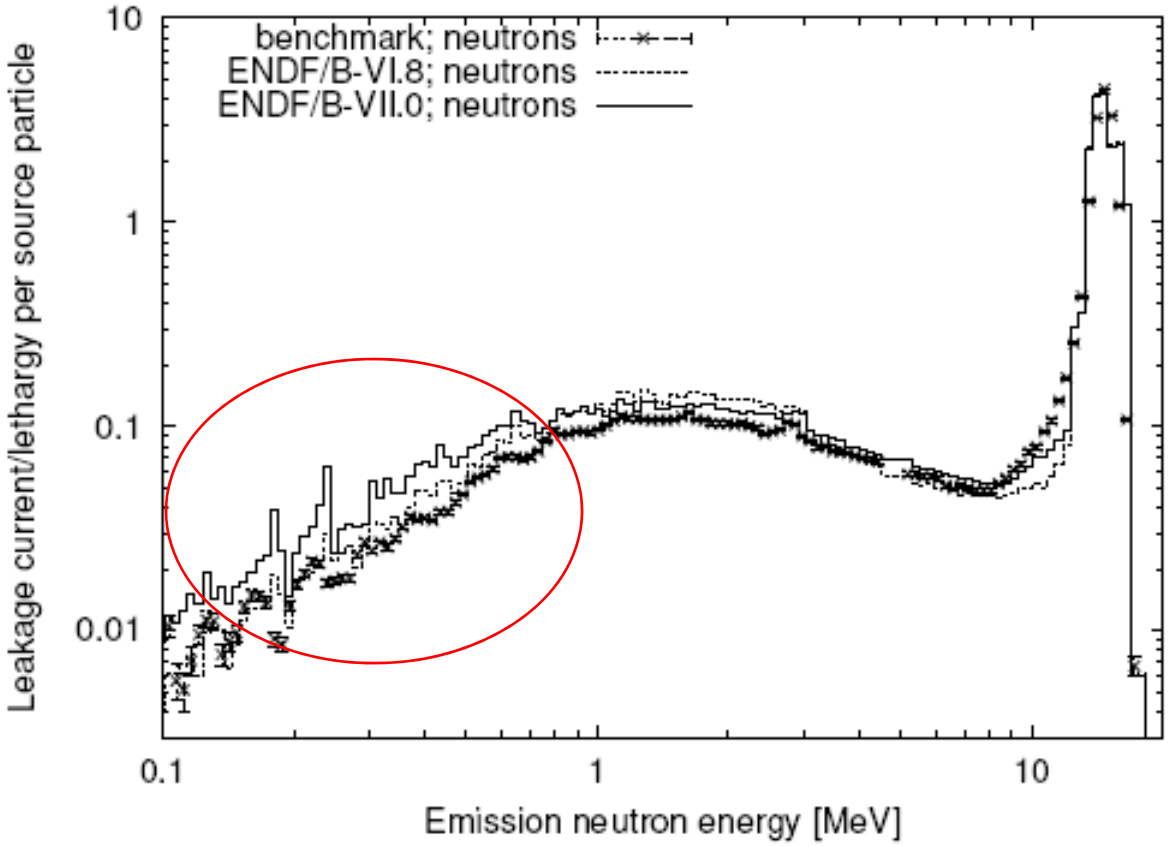
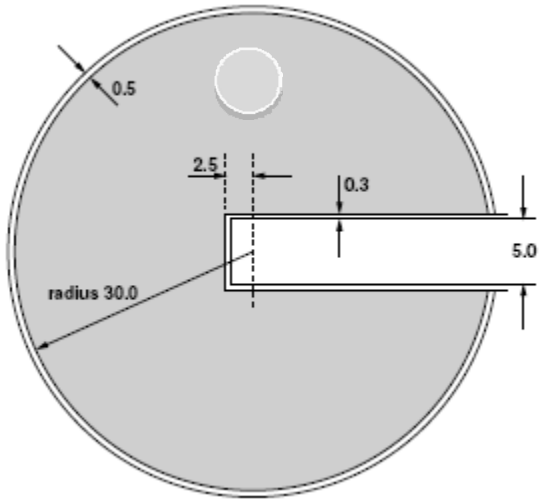


1.3 Discrepancies in Shielding Benchmarks

- **Oktavian with Ti shield**

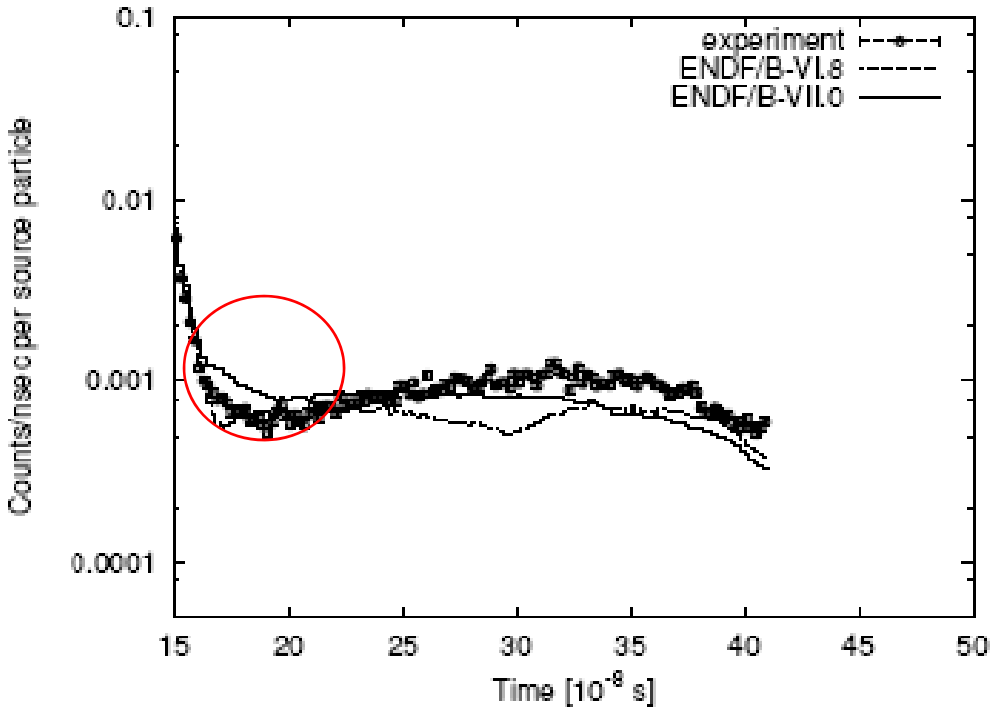




	energy range [MeV]	C/E
Ti	0.0–0.1	1.16 ± 0.11
Ti	0.1–1.0	1.51 ± 0.01
Ti	1.0–5.0	1.16 ± 0.01
Ti	5.0–10.0	1.07 ± 0.01
Ti	10.0–20.0	1.18 ± 0.01

1.3 Discrepancies in Shielding Benchmarks (cont.)

- **LLNL Pulsed Source with Ti shields**



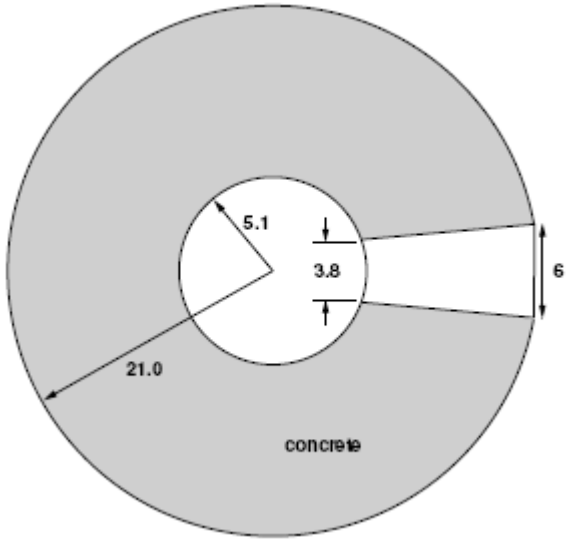


FIG. 122: Neutron spectrum for the LLNL Pulsed Sphere, Ti (1.2 mfp) benchmark, angle=39°.

1.4 Status of Evaluated Files of Ti

- ENDF/B-VII.0 (dist. 2006)
  - Adopted JENDL-3.3 (with minor modification)
- JENDL-3.3 (dist. 2002)
  - JENDL-fusion, -activation,… + Re-evaluation by Asami in 2000
  - Isotopic files for all natural isotopes (Ti-46, 47, 48, 49, and 50)
  - Resonance parameters from Mughabghab 1981;
    Model calculations (CASTHY, EGNASH, …) + Experiments
- JEFF-3.1 (dist. 2005)
  - 0.2 ~ 20 MeV, new evaluation by Tagesen & Vonach in 2004;
    < 0.2 MeV, adopted ENDF/B-VI (total and capture CS's for Ti-nat.)
  - Isotopic files for all natural isotopes
  - Model calculations (TALYS) + Experiments (GLUCS)

2. Evaluation Method

- We focused on the high energy region.
  - Hundred keV ~ 20 MeV
  - Model calculations: GNASH, CoH, KALMAN
  - Adjusting model parameters based on experiments:

    - the germanium array for neutron induced excitations (GEANIE) at LANSCE, and
    - other (*n*,*p*), (*n*,α), … experiments

- We adopted new resonance parameters and thermal CSs.
  - "Atlas of Neutron Resonances" (Mughabghab 2006)
  - Resolved resonances up to hundred keV
  - Some adjustments were needed.

2.1 Evaluation Plan

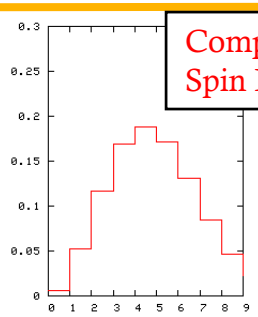
■ Resonance Parameters (MF=2)	Mughabghab 2006
■ Neutron Cross Sections (MF=3)	
• Total	CoH
• Elastic Scattering	Total - Sum of Partial CSs
• Threshold Reactions: (n,2n), (n,n'), (n,p),…	GNASH
• Capture	CoH + DSD
■ Angular Distribution (MF=4)	
• (n,n), (n,n')_discrete	CoH
■ Energy-Angle Distribution (MF=6)	
• (n,2n), (n,n')_continuum, (n,nα), (n,np)	GNASH
■ Covariance of Neutron CSs (MF=33)	GNASH or CoH + KALMAN

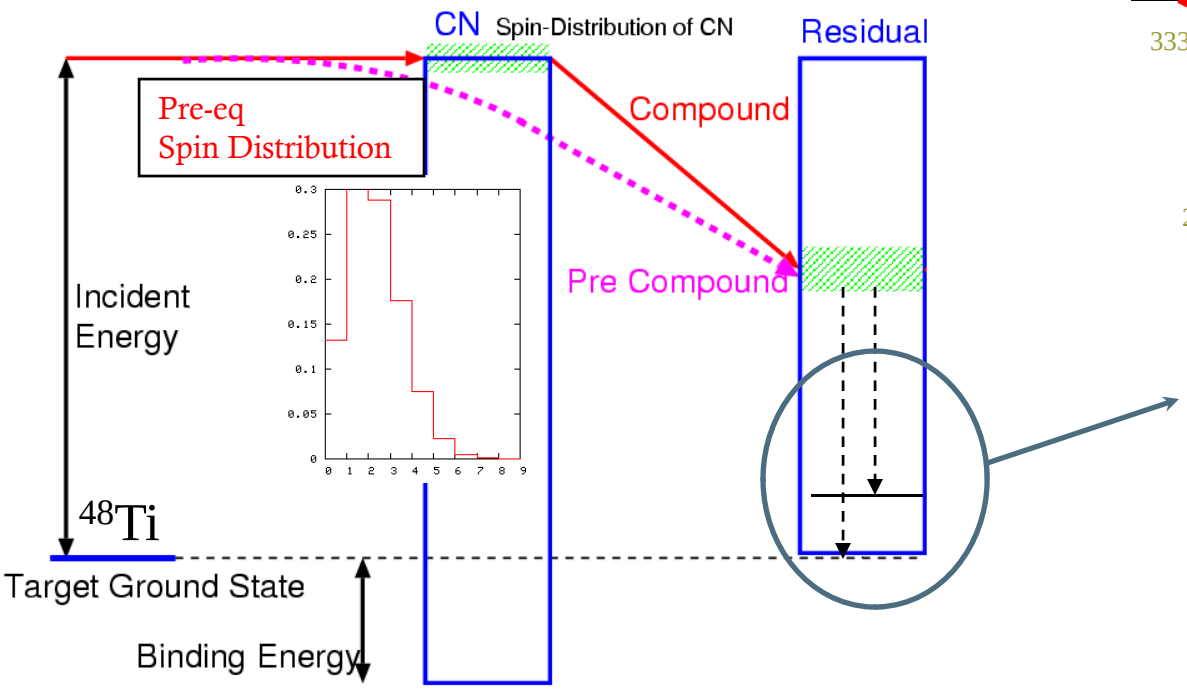
2.2 GNASH Modeling (1)

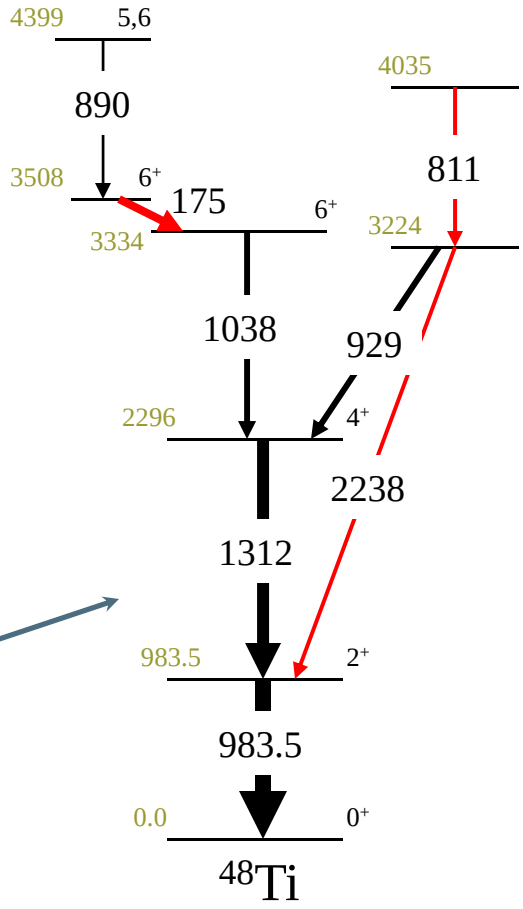
- GNASH
  - Statistical Hauser-Feshbach theory + Preequilibrium model
  - From keV up to hundred MeV region
- Transmission coefficients calculation
  - Koning and Delaroche global optical potentials for *n* and *p*
  - Avrigeanu, Hodgson, and Avrigeanu potentials for α
- Use/Adjustments of model parameters
  - Spin distribution of pre-equilibrium reaction
    - calculated using the Feshbach-Kerman-Koonin theory
    - different from the distribution of compound nucleus
  - Adjustments of model parameters (^{48}Ti)
    - level density parameter of ^{48}Sc
    - γ branching ratios of some discrete levels

2.2 GNASH Modeling (2)

The γ-ray cascade in the residual nucleus is sensitive to the fraction of pre-equilibrium emission.







2.2 GNASH Modeling (3)

- Inclusion of direct reaction cross sections (^{48}Ti)
  - Coupled channel and DWBA calculations
  - Direct inelastic scattering for 0+, 2+, 4+, 6+ rotational band members
  - Coupled channel potential is assumed to be similar to the spherical potential of Koning and Delaroche with proper deformation parameters.

See details in

Dashdorj et al., Phyical Review C 75, 054612 (2007)

3. Evaluation Results

3.1 Thermal neutron (2200 m/s) cross sections

- Capture CSs (upper) and capture resonance integrals (lower) (b)

Isotope (nat. abd.)	ENDF/B-VII	Present	Mughabghab 2006
22-Ti-46 (8.25%)	0.58 0.32	0.61 0.35	0.59 +- 0.18 0.30 +- 0.09
22-Ti-47 (7.44%)	1.71 1.40	1.58 1.26	1.63 +- 0.04 1.5 +- 0.2
22-Ti-48 (73.72%)	7.86 3.70	8.34 3.73	8.32 +- 0.16 3.9 +- 0.2
22-Ti-49 (5.41%)	1.84 0.88	1.87 0.92	1.87 +- 0.04 1.2 +- 0.2
22-Ti-50 (5.18%)	0.18 0.087	0.18 0.087	0.179 +- 0.003 0.083 +- 0.006

- Most significant revision of Ti-48 capture CS

→ 6% increase in Ti-element thermal capture CS

3. Evaluation Results

3.1 Thermal neutron (2200 m/s) cross sections (cont.)

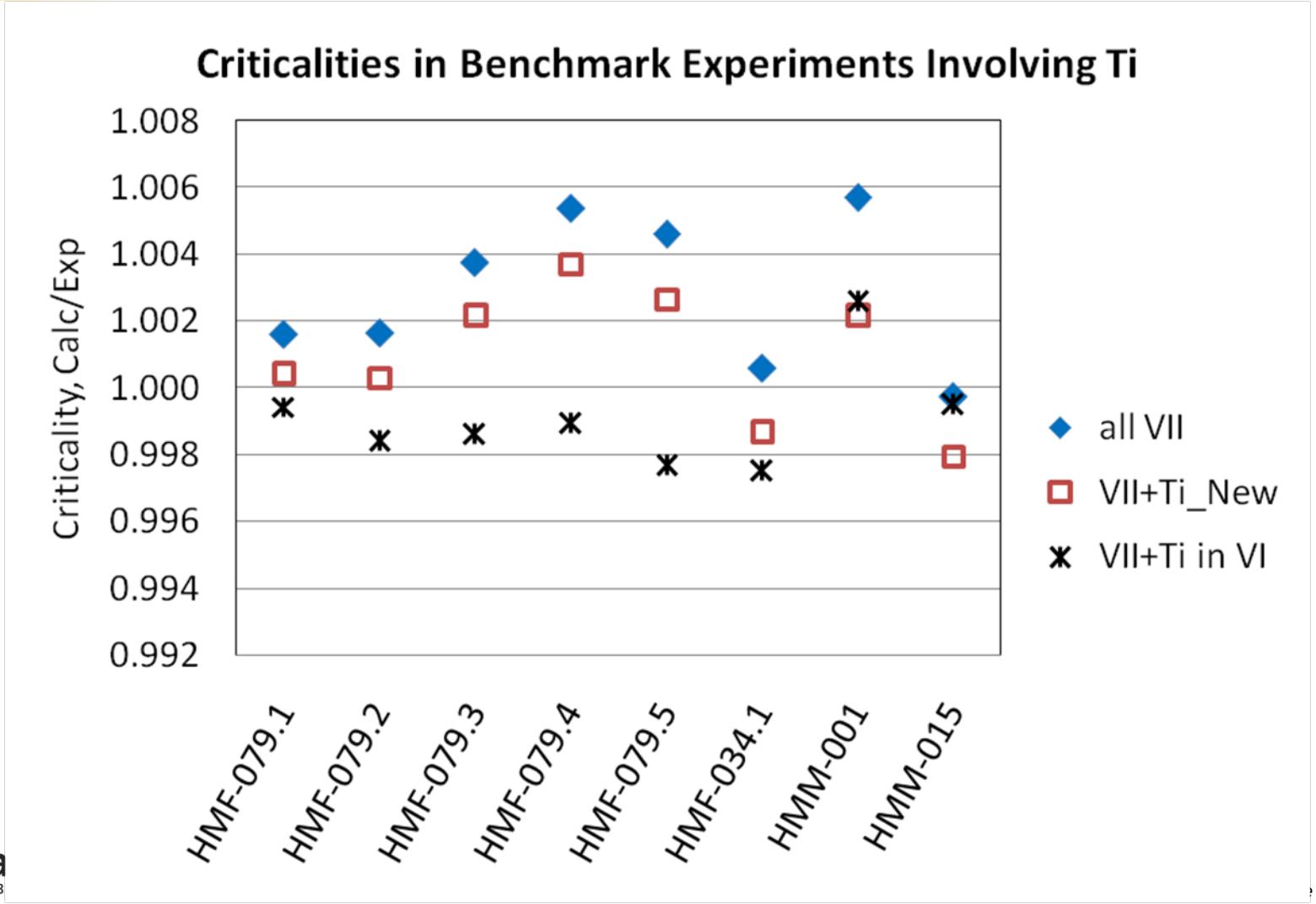
- Elastic scattering cross sections in barn

Isotope (nat. abd.)	ENDF/B-VII	Present	Mughabghab 2006
22-Ti-46 (8.25%)	3.72	2.73	2.72 +- 0.06
22-Ti-47 (7.44%)	3.13	3.50	3.1 +- 0.2
22-Ti-48 (73.72%)	4.37	4.35	4.1 +- 0.2
22-Ti-49 (5.41%)	0.70	0.28	0.7 +- 0.3
22-Ti-50 (5.18%)	3.78	4.30	3.7 +- 0.3

- Rather big changes in elastic CSs, but not in elemental level
- Needs revisit scattering lengths (R' and b_coh)

3. Evaluation Results

3.2 Results of Criticality Benchmark Calculations



3.3 Discussion on the Benchmark Results

- New evaluation resulted in 0.1 ~ 0.4 %Δk decrease in both hard spectrum experiments (HMF 079 series and HMF 034) and soft spectrum cases (HMM 001 and 015).
- The decrease in calculated criticalities is the result of combined effects of
  - Revised resonances (about 0.2 %Δk decrease in HMM 001 and 015) and
  - Reduced elastic scattering cross sections above hundred keV (0.1 ~ 0.2% Δk in HMF series)
- The effect of inelastic scattering cross sections have not been investigated thoroughly yet.

4. Future Work

- The evaluation has not been completed.
- Resonance region
  - Revisiting scattering lengths
- High energy region
  - Adjustment or justification of the reaction model parameters for Ti isotopes other than Ti-48
  - Evaluation of the covariance of the cross sections
  - Making complete files in ENDF-6 format, and so on