#### Cross sections for neutron capture from Surrogate measurements

Jutta Escher Nuclear Theory & Modeling Lawrence Livermore National Lab



Gamma Strength and Level Density in Nuclear Physics and Nuclear Technology Aug 30 – Sept 3, 2010, Dresden-Rossendorf, Germany

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract DE-AC52-07NA27344.



**UCRL-PRES-452591** 

#### **Overview**

- 1. Compound-nuclear reactions
- 2. Surrogate idea
- 3. Weisskopf-Ewing approximation
- 4. Challenges specific to (n,γ)
- 5. Getting better cross section constraints from Surrogate data
- 6. Summary

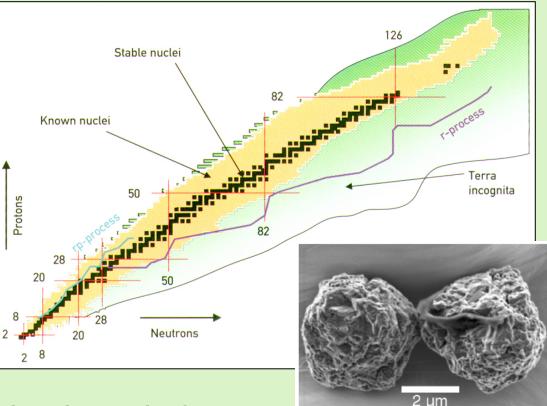
### **Compound-nuclear reactions**

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#### **Compound-nuclear reactions**

Important for understanding astrophysical phenomena and the origin of the elements:

- The s and r processes produce almost all heavy elements
- Processes are linked to stellar evolution
- Abundance patterns predicted by models, require cross section input



#### Important for exploiting nuclear energy in a clean and safe manner:

- Goals are to operate safely, reduce toxic waste, ensure availability of U resource, increase efficiency, and contain costs
- Cross sections are needed for investigating waste transmutation scenarios, explore alternative fuel cycles, simulate reactor designs
- Reactions on actinides, minor actinides, fission fragments, structural materials are of interest.

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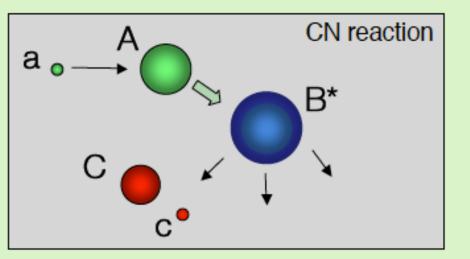
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Presolar grain

#### **Compound-nuclear (CN) reactions**

#### Simplified description:

- A CN reaction proceeds in *two stages*:
  - Formation of the CN via absorption of the projectile by the target nucleus (a series of nucleon-nucleon interactions leading to equilibration)
  - Decay of the CN via particle emission or fission
- Characteristics:
  - CN reactions are slow:  $\sim 10^{-16}$ s (direct reactions  $\sim 10^{-22}$ s )
  - Evaporated particle spectra exhibit characteristic energy spectra and angular distributions
  - The CN forgets how it was produced (but retains memory of conserved quantities!)



#### **Theoretical formulation:**

• Early, simple expression (Weisskopf-Ewing):

 $\sigma_{\alpha\chi}^{WE}(E) = \sigma_{\alpha}^{CN}(E) \cdot \mathcal{G}_{\chi}^{CN}(E)$ 

• Accounting for conservation of angular momentum (Hauser-Feshbach):

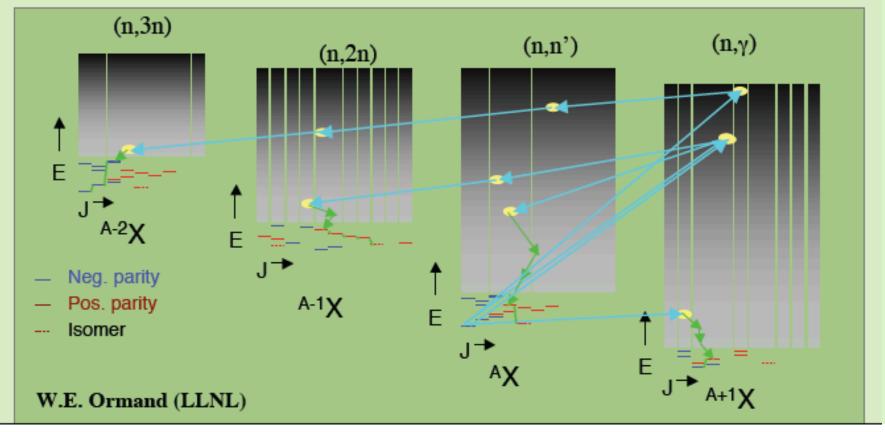
$$\sigma_{\alpha\chi} = \Sigma_{J,\pi} \sigma_{\alpha}^{CN} (E, J, \pi) \cdot G^{CN}_{\chi} (E, J, \pi)$$

#### State-of-the-art: powerful tool to calculate cross sections

Average cross section per unit energy in the outgoing channel:

$$\frac{d\sigma_{\alpha\chi}^{HF}}{dE_{\chi}} = \pi \lambda_{\alpha}^{2} \sum_{J\Pi} \omega_{\alpha}^{J} \sum_{lsl's'l'} \frac{T_{\alpha ls}^{J} T_{xl's'}^{J} \rho_{l'}(U)}{\sum_{x''l''s''}^{Y} T_{x''l''s''}^{J} + \sum_{x''l''s''}^{Y} \int T_{x''l''s''}^{J} (E_{\chi''}) \rho_{l''}(U'') dE_{\chi'}}$$

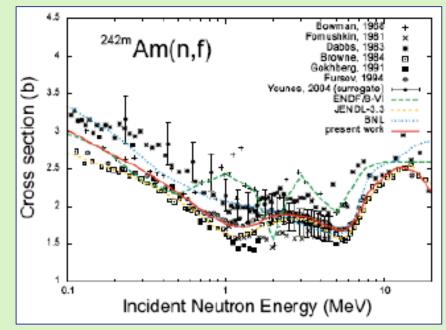
Evaluating this expression requires knowledge of optical potentials and the structure of the nuclei that can be reached in the decay of the CN:



#### State-of-the-art: powerful tool to calculate cross sections

#### **Practice:**

- STAPRE, TALYS, EMPIRE, MCNASH, COH, etc. allow one to calculate cross sections.
- Nuclear physics input is provided by data bases or by the user; input parameters are not unique (art and science)



Chadwick et al, Nucl. Data Sheets 107 (2006) 2931



Available online at www.sciencedirect.com



Nuclear Data Sheets 110 (2009) 3107-3214

www.elsevier.com/locale/nds

#### RIPL – Reference Input Parameter Library for Calculation of Nuclear Reactions and Nuclear Data Evaluations

ScienceDirect

R. Capote,<sup>1\*</sup> M. Herman,<sup>1,2</sup> P. Obložinský,<sup>1,2</sup> P.G. Young,<sup>3</sup> S. Goriely,<sup>4</sup> T. Belgya,<sup>5</sup> A.V. Ignatyuk,<sup>6</sup> A.J. Koning,<sup>7</sup> S. Hilaire,<sup>8</sup> V.A. Plujko,<sup>0</sup> M. Avrigeanu,<sup>10</sup> O. Bersillon,<sup>6</sup> M.B. Chadwick,<sup>3</sup> T. Fukahori,<sup>11</sup> Zhigang Ge,<sup>12</sup> Yinlu Han,<sup>12</sup> S. Kailas,<sup>13</sup> J. Kopeeky,<sup>14</sup> V.M. Maslov,<sup>16</sup> G. Reffo,<sup>16</sup> M. Sin,<sup>17</sup> E.Sh. Soukhovitskii,<sup>16</sup> P. Talou<sup>3</sup> <sup>1</sup> NAPC-Nuclear Data Section, International Atomic Energy Agency, A-1400 Vienna, Austria <sup>2</sup> National Nuclear Data Center, Brookhaven National Laboratory, Upton, NY 11973, USA Los Alamos National Laboratory, Los Alamos, NM 87544, USA <sup>4</sup> Université Libre de Bruzelles, BE 1050 Brussels, Bel Institute of Isotope and Surface Chemistry, Chemical Research Center, H-1525 Budapest, Hungar Institute of Physics and Power Engineering, 249033 Obninsk, Russia <sup>7</sup> Fuels Actinides and Isotopes NRG Nuclear Research and Consultance Group, NL-1755 Petten, The Netherland 8 CEA, DAM, DIF, F-91297 Arpajon, France Taras Shevchenko National University, 03022 Kiev, Ukraine National Institute of Physics and Nuclear Engineering "Horia Hulubet", 077125 Bucharest-Magurele, Romania <sup>11</sup> Japan Atomic Energy Agency, Tokai-mura, Naka-gun, Ibaraki-ken, 319-1195 Japan 12 China Institute of Atomic Energy, Beijing 102413 China <sup>13</sup> Bhabha Atomte Research Center, Trombay, 400085 Mumbat, Indu <sup>14</sup> JUKO Research, NL-1817 Alkmaar, The Netherlands <sup>15</sup> Joint Institute for Power and Nuclear Research – Sosny, BY-220109 Minsk, Belarus Retired in 1998, Ente Nuove Tecnologie, Energia e Ambiente (ENEA), 40129 Bologna, Italy and Nuclear Physics Department, Bucharest University, 077125 Bucharest-Magurele, Romania

(Received July 20, 2009)

We describe the physics and data included in the Reference Input Parameter Library, which is devoted to input parameters needed in calculations of nuclear reactions and nuclear data evaluations. Advanced modelling codes require substantial numerical input, therefore the International Atomic Energy Agency (IAEA) has worked extensively since 1993 on a library of validated nuclear-model input parameters, referred to as the Reference Input Parameter Library (RIPL). A final RIPL coordinated research project (RIPL-3) was brought to a successful conclusion in December 2008, after 15 years of challenging work carried out through three consecutive IAEA projects. The RIPL-3 library was released in January 2009, and is available on the Web through http://www.nds.teac.org/RIPL-3/. This work and the resulting database are extremely important to theoretician involved in the development and use of nuclear reaction modelling (ALCE, EMPIRE, GNASH, UNF, TALYS) both for theoretic and and use of avaluations.

The numerical data and computer codes included in RIPL-3 are arranged in seven segments: MASSES contains ground-state properties of nuclei for about 9000 nuclei, including three theoretical predictions of masses and the evaluated experimental masses of Audi et al. (2003). DISCRETE LEVELS contains 117 datasets (one for each element) with all known level schemes, electromagnetic and  $\gamma$ -ray decay probabilities available from ENSDF in October 2007. NEUTRON RESONANCES contains average resonance parameters prepared on the basis of the evaluations performed by Ignatyuk and Mughabghab. OPTICAL MODEL contains 495 sets of phenomenological optical model parameters defined in a wide energy range. When there are insufficient experimental data, the evaluator has to resort to either global parameterizations or microscopic approaches. Radial density distributions to be used as input for microscopic calculations are stored in the MASSES segment. LEVEL DENSITIES contains phenomenological parameterizations based on the modified Fermi gas and superfluid models and microscopic calculations which are based on a realistic microscopic single-particle level scheme. Partial level densities formulae are also recommended. All tabulated total level densities are consistent with both the recommended average neutron resonance parameters and discrete levels. GAMMA contains parameters that quantify giant resonances, experimental gar functions and methods for calculating gamma emission in statistical model codes. The experimental GDR parameters are represented by Lorentzian fits to the photo-absorption cross sections for 102 nuclides ranging from  $^{51}V$  to  $^{239}Pu$ . FISSION includes global prescriptions for fission barriers and nuclear level densities at fission saddle points based on microscopic HFB calculations constrained by experimental fission cross sections

\*) Corresponding author, electronic address: r.capotenoy@iaea.org; roberto.capote@yahoo.com

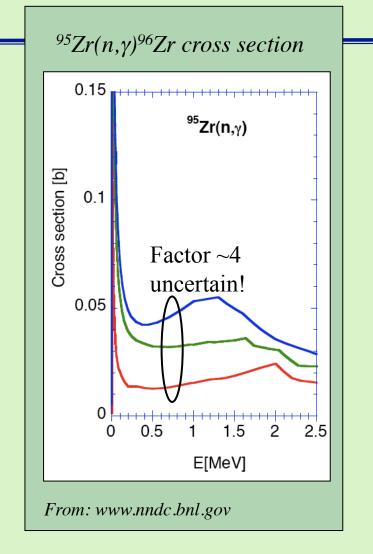
Capote et al, Nuclear Data Sheets 110 (2009) 3107 23 authors, 108 pages, many years...

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#### **Constraining the input**

#### **Constraints for models and parameters:**

- γSF: total radiative width,...
- Level densities: discrete low-lying levels, neutron resonance spacings at S<sub>n</sub>,...
- Microscopic calculations for γSF and LDs
- Global systematics
- Local systematics
- Complementary/competing cross sections
- Measured cross sections of the reaction of interest, possibly near the energy of interest



Lack of cross section constraints can lead to large differences between evaluations

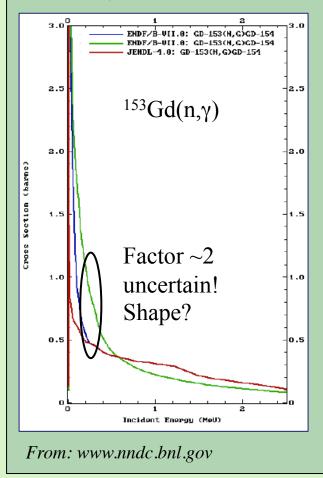
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#### **Constraining the input**

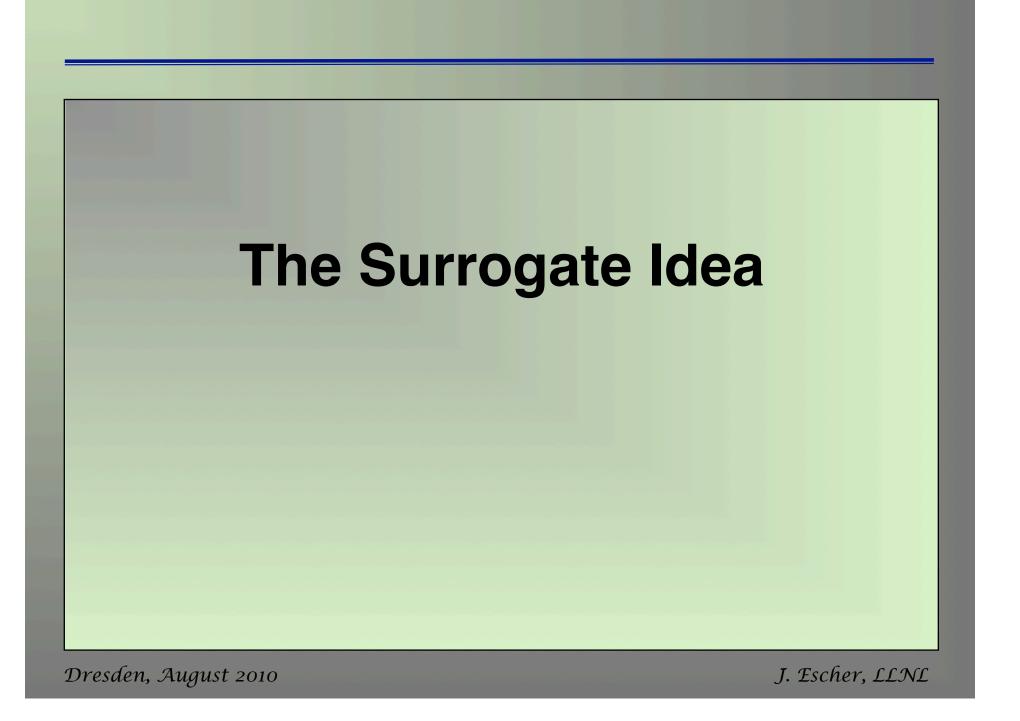
#### **Constraints for models and parameters:**

- γSF: total radiative width,...
- Level densities: discrete low-lying levels, neutron resonance spacings at S<sub>n</sub>,...
- Microscopic calculations for γSF and LDs
- Global systematics
- Local systematics
- Complementary/competing cross sections
- Measured cross sections of the reaction of interest, possibly near the energy of interest

#### $^{153}Gd(n,\gamma)^{154}Gd$ cross section

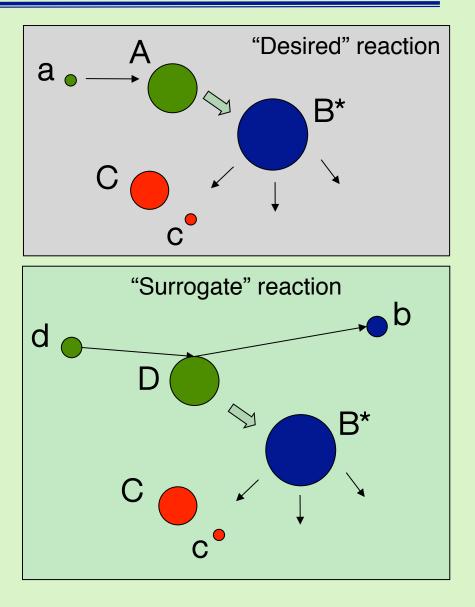


Measurements of cross sections are very important to constrain calculations. Where these are not feasible, we explore using Surrogate reactions to determine meaningful constraints.



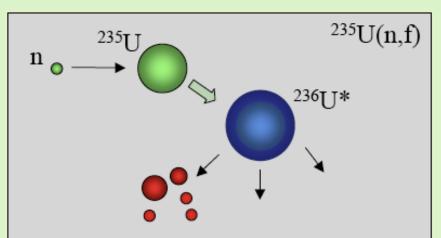
#### The Surrogate Idea - schematically

The Surrogate Nuclear Reactions approach combines theory and measurements to determine cross sections of compound-nuclear reactions that are difficult/ impossible to measure directly.

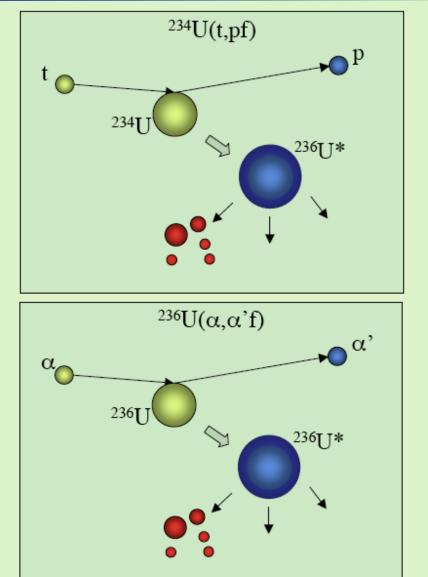


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#### **The Surrogate Idea - examples**



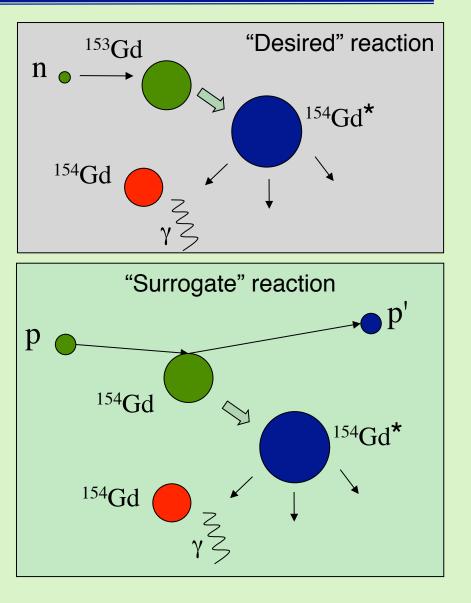
Various direct-reaction mechanisms can be employed to create the compound nucleus of interest.



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#### **The Surrogate Idea - examples**

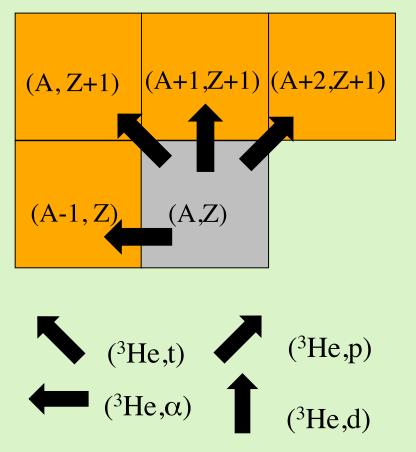
Different types of compoundnuclear decays can be considered.



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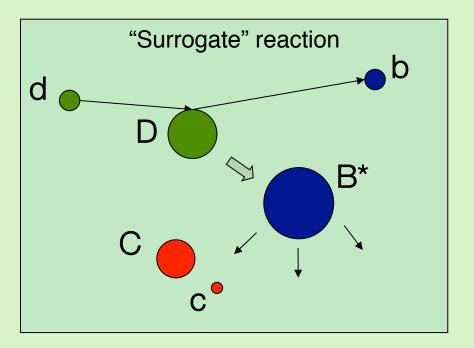
#### The Surrogate Idea

One experiment can be used to determine several cross sections:



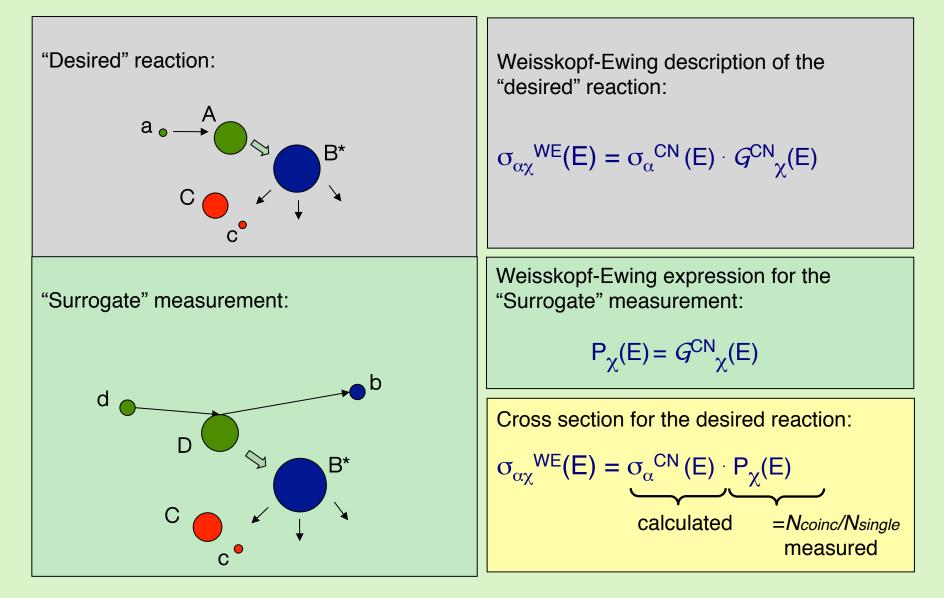
A Surrogate measurement with fixed beam energy can be used to probe the desired cross section for a range of energies:

For fixed beam energy  $E_d$ , the CN can be produced at various excitation energies



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#### Simple Weisskopf-Ewing (WE) description

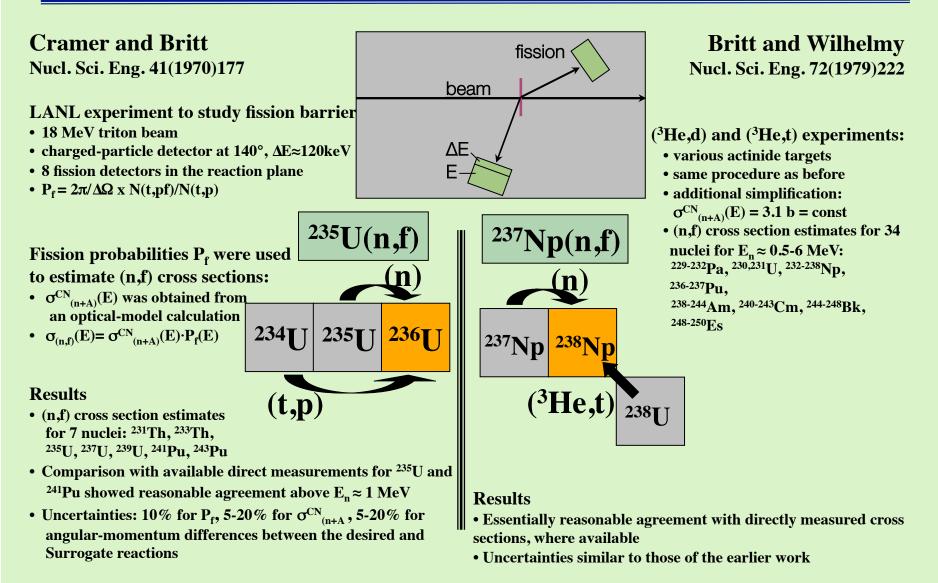


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## WE applications to (n,f) reactions

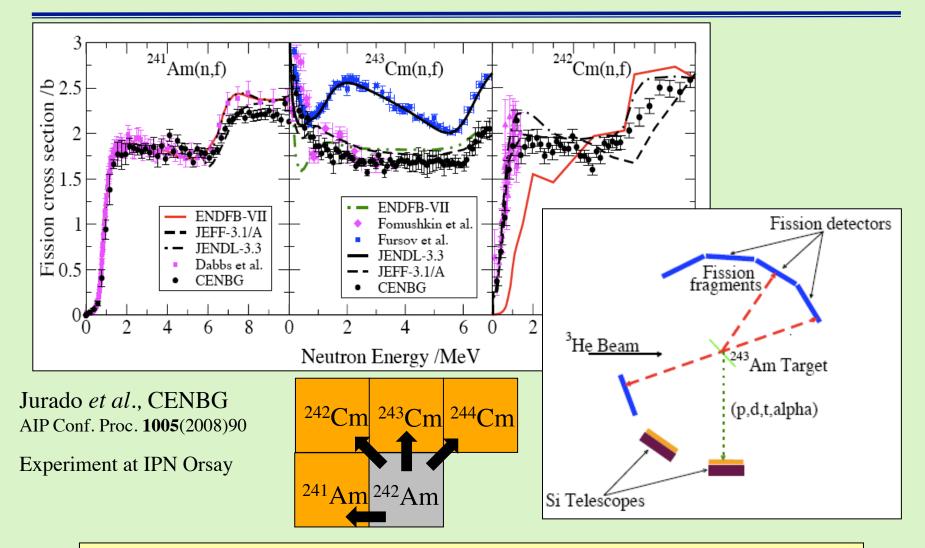
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#### Early Surrogate work in the WE limit



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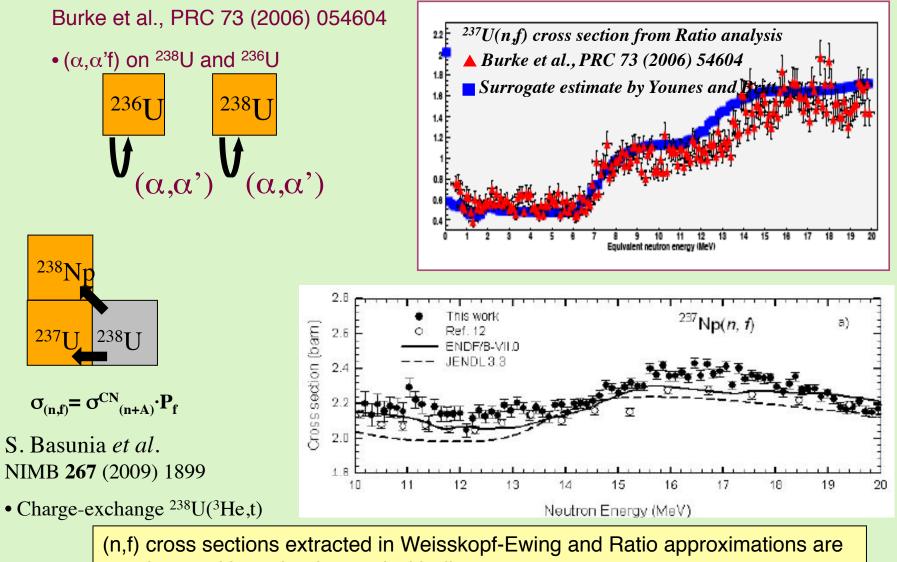
#### **Results from CENBG collaboration**



(n,f) cross sections extracted in Weisskopf-Ewing approximation are consistent with direct measurement, able to resolve controversies and extend range of data.

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#### **Results from the STARS/LiberACE collaboration**



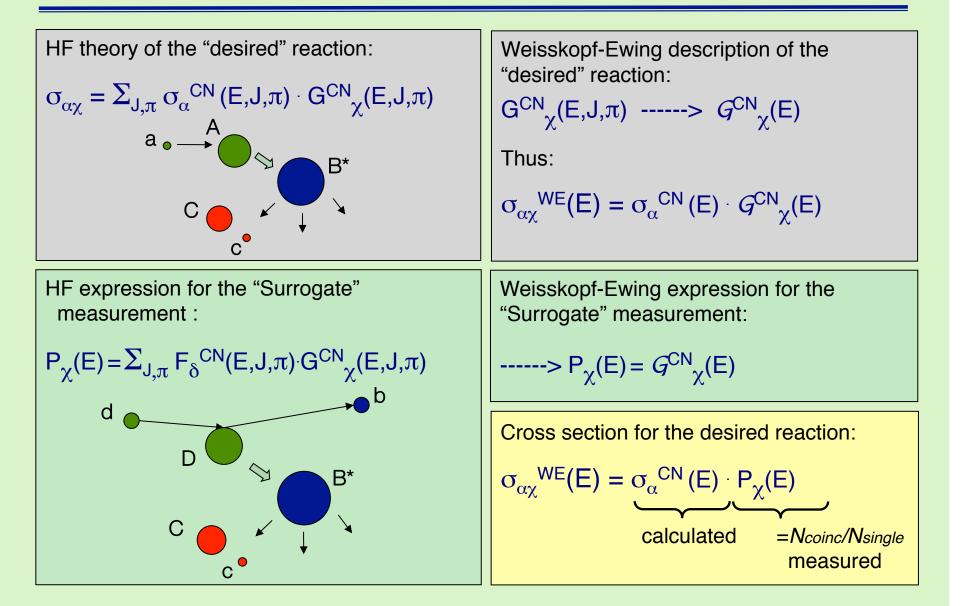
consistent with each other and with direct measurements

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## Weisskopf-Ewing Approximation: Ignoring spin effects

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#### The Weisskopf-Ewing (WE) limit



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#### **Reduction of Hauser-Feshbach to Weisskopf-Ewing**

$$\frac{d\sigma_{\alpha\chi}^{HF}}{dE_{\chi}} = \pi \lambda_{\alpha}^{2} \sum_{J\Pi} \omega_{\alpha}^{J} \sum_{lsl's'l'} \frac{T_{\alpha ls}^{J} T_{x'l's'}^{J} \rho_{l'}(U)}{\sum_{x''l''s''}^{i} T_{x''l''s''}^{J} + \sum_{x''l''s''}^{j} \int T_{x''l''s''}^{J} (E_{\chi''}) \rho_{l''}(U'') dE_{\chi''}}$$

#### WE limit valid when:

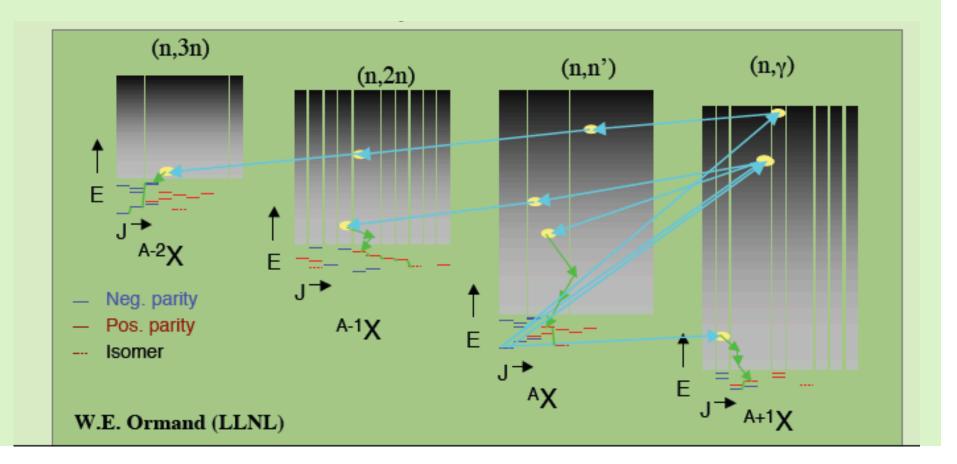
- Decay channels are dominated by integrals over the level density.
- Width fluctuations are negligible.
- Transmission coefficients T associated with available exit channels are independent of spin of states reached.
- Level densities in available channels are independent of parity and dependence on spin I has the form ~(2I+1)

$$\sigma_{\alpha\chi} = \Sigma_{J,\pi} \sigma_{\alpha}^{CN} (E, J, \pi) \cdot G^{CN}_{\chi} (E, J, \pi) \rightarrow \sigma_{\alpha\chi}^{WE} (E) = \sigma_{\alpha}^{CN} (E) \cdot G^{CN}_{\chi} (E)$$

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#### **Reduction of Hauser-Feshbach to Weisskopf-Ewing**

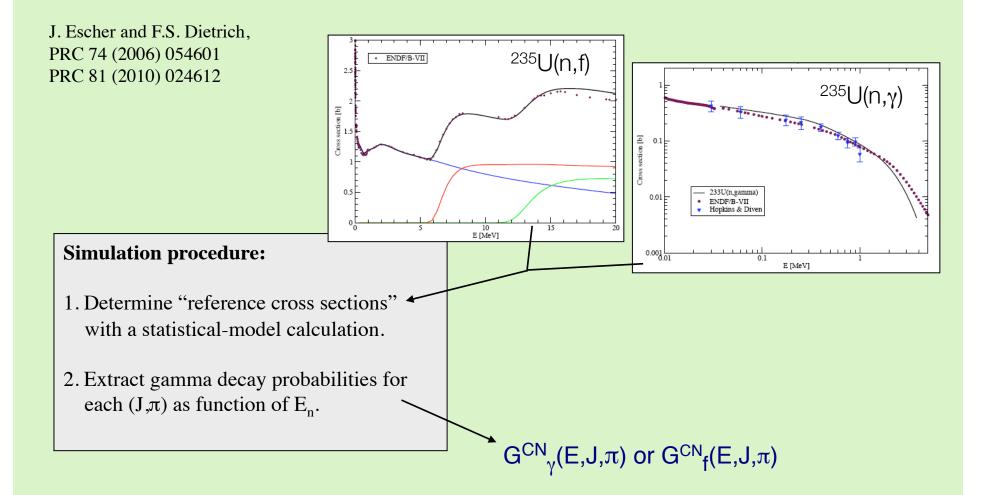
$$\frac{d\sigma_{\alpha\chi}^{HF}}{dE_{\chi}} = \pi \lambda_{\alpha}^{2} \sum_{J\Pi} \omega_{\alpha}^{J} \sum_{lsl's'l'} \frac{T_{\alpha ls}^{J} T_{xl's'}^{J} \rho_{l'}(U)}{\sum_{x''l''s''}^{i} T_{x''l''s''}^{J} + \sum_{x''l''s''}^{j} \int T_{x''l''s''}^{J} (E_{\chi''}) \rho_{l''}(U'') dE_{\chi''}}$$



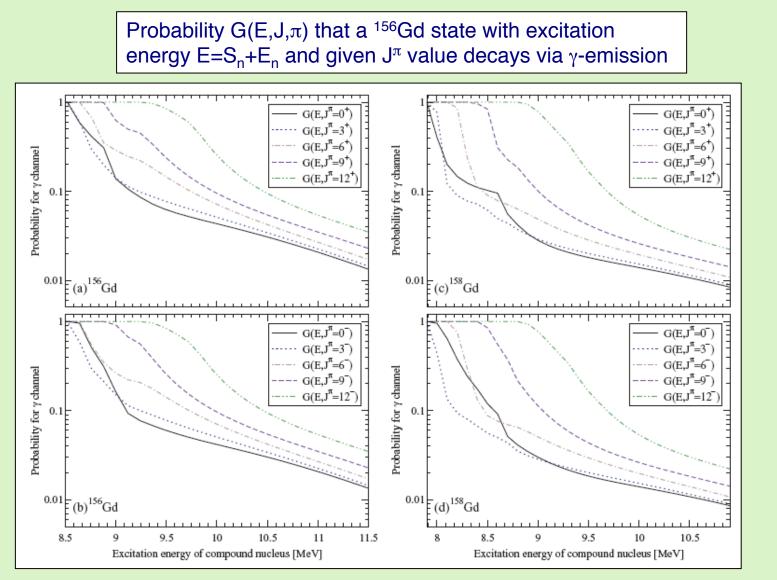
## **Testing the WE approximation for (n,γ)**

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#### **Testing the WE approximation....**



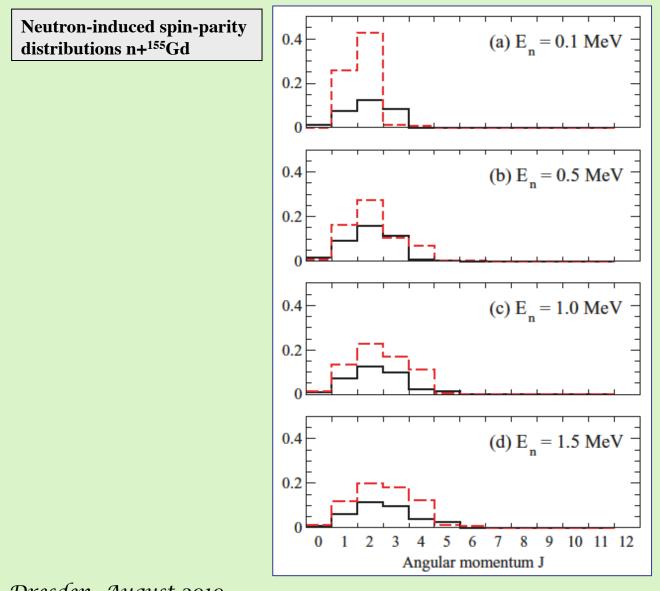
#### **Case 3:** $(n,\gamma)$ reactions for rare-earth targets



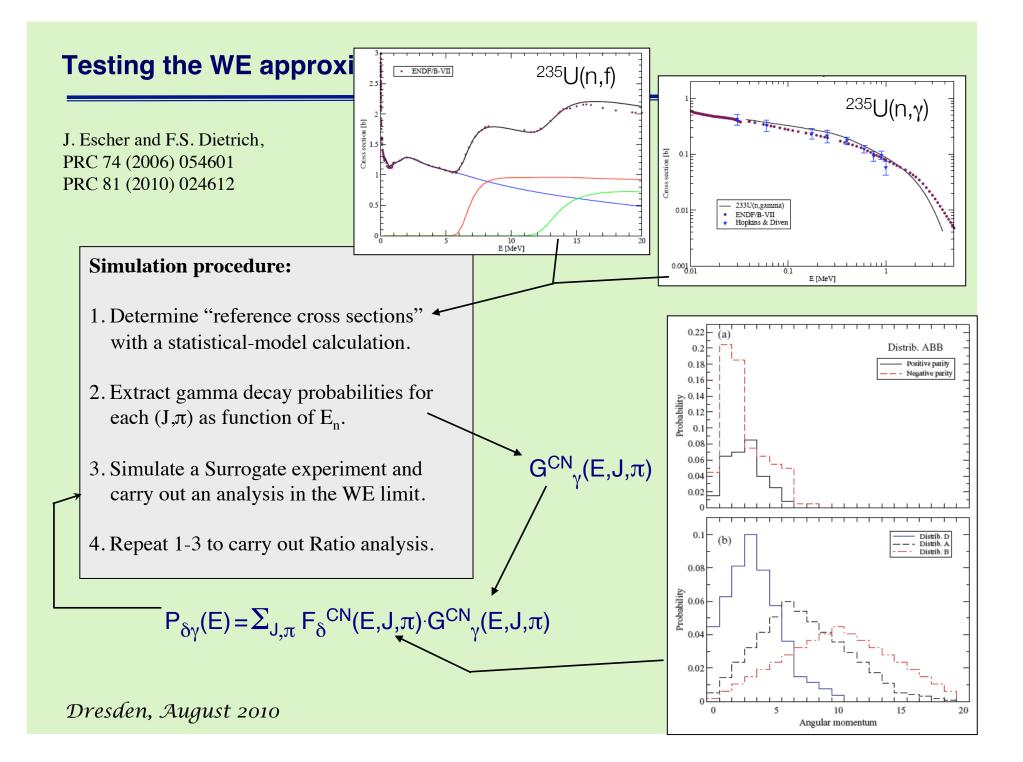
J. Escher and F.S. Dietrich, PRC 81 (2010) 024612

Dresden, August 2010

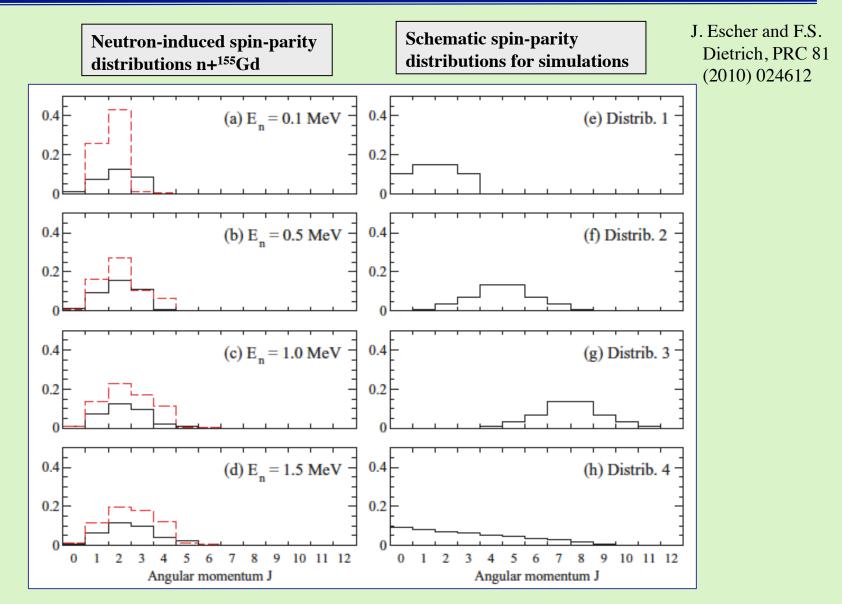
#### **Case 3: (n,** $\gamma$ **) reactions for rare-earth targets**



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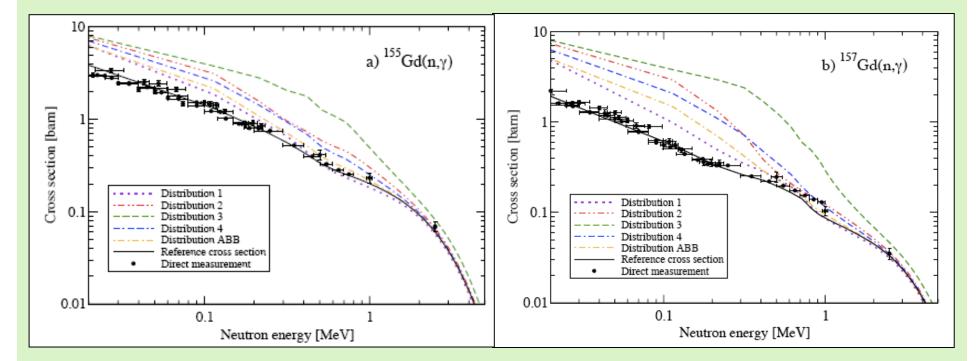
#### Case 3: $(n,\gamma)$ reactions for rare-earth targets



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#### $(n,\gamma)$ reactions for rare-earth targets

Cross sections extracted from simulated Surrogate observables



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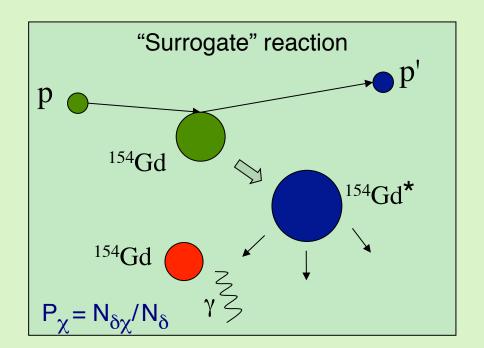
#### Inelastic p scattering on <sup>154,156,158</sup>Gd at STARS/LiBerACE



Silicon

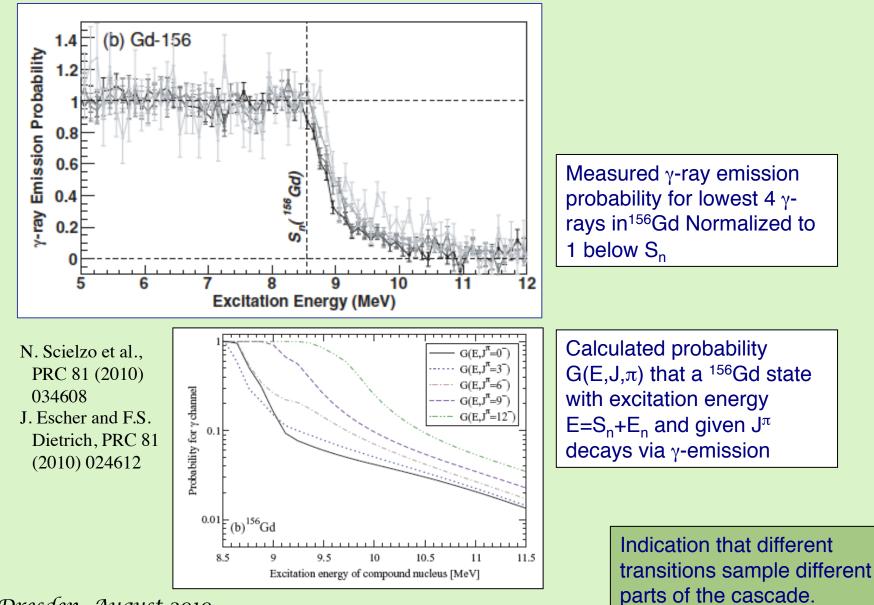
Array

Telescope



#### N. Scielzo et al., PRC 81 (2010) 034608

Measurements of <sup>154,156,158</sup>Gd(p,p' $\gamma$ ) with with E<sub>p</sub>=22 MeV. Goal: determine the <sup>153,155,157</sup>Gd(n, $\gamma$ ) cross sections -- two cross sections are known, can provide tests, one is an unknown cross section of interest to astrophysics.



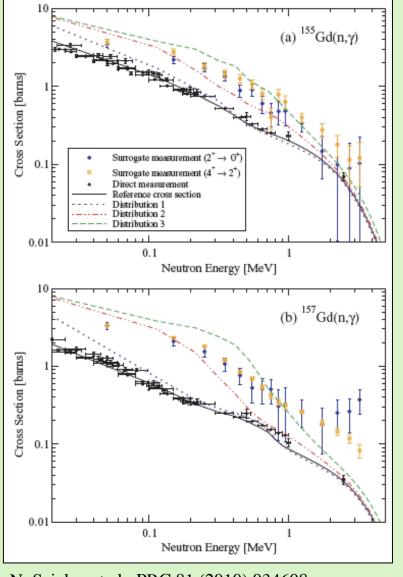
#### <sup>156</sup>Gd decay following excitation by inelastic p scattering

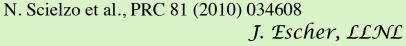
#### <sup>155,157</sup>Gd(n,γ) cross sections from WE analysis

Extracted <sup>155</sup>Gd(n,γ) cross section compared to reference cross section and Surrogate simulations

The WE approximation gives results roughly within a factor of 2-5 of the expected cross section.

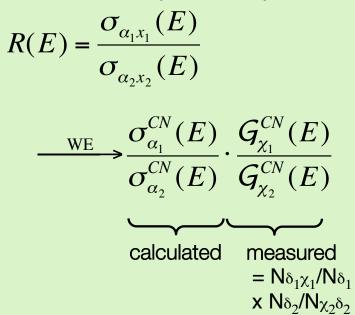
More work is needed to obtain cross sections to better than a factor of two.





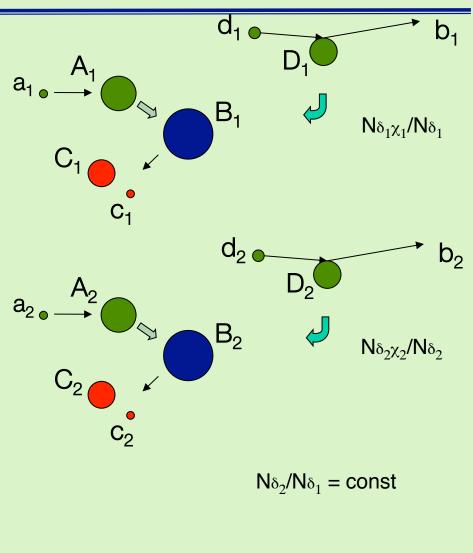
#### The Surrogate Ratio approach

Goal: Determine experimentally



#### Advantages of the Ratio approach:

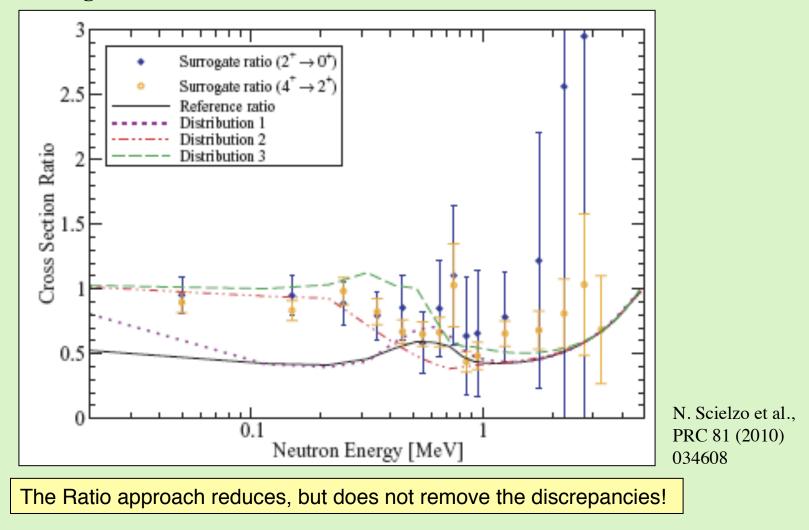
- Eliminates need to measure direct-reaction "singles" events in *Ncoinc/Nsingle*
- Small systematic errors or violations of assumptions underlying a Surrogate WE analysis might cancel



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#### Ratio method for $^{157}Gd(n,\gamma) / ^{155}Gd(n,\gamma)$

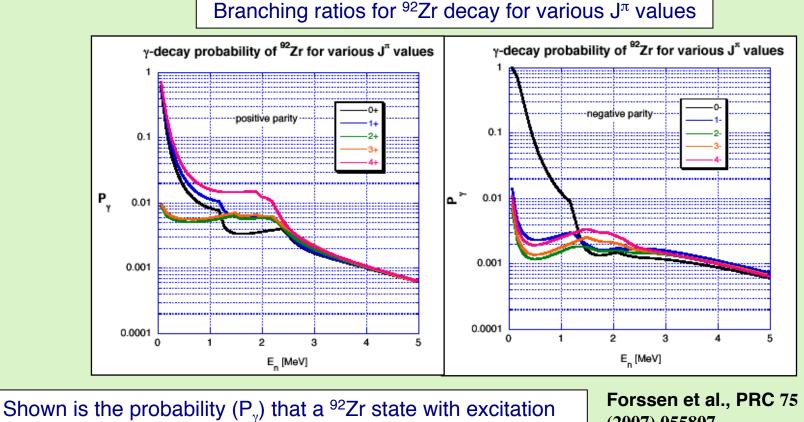
**Comparing ratio of extracted cross sections to ratios of reference cross sections and ratios of Surrogate simulations:** 



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# **Other mass regions** J. Escher, LLNL

### Case 1: WE for $(n,\gamma)$ reactions for near-spherical nuclei?



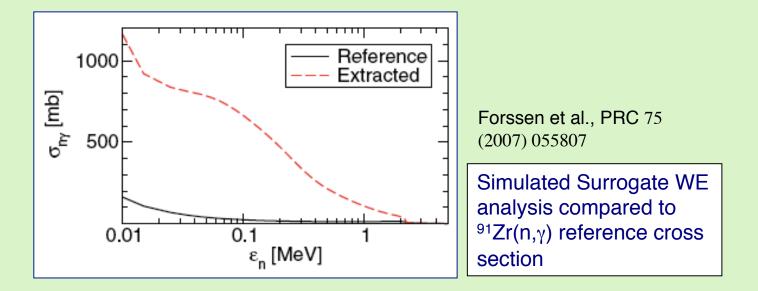
energy  $E=S_n+E_n$  and given  $J^{\pi}$  value decays via  $\gamma$ -emission.  $S_n$  is the neutron separation energy in <sup>92</sup>Zr.

(2007) 055807

At small energies, the branching ratios are VERY sensitive to CN  $J^{\pi}$ values!

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### WE is worse for (n,γ) reactions for near-spherical nuclei

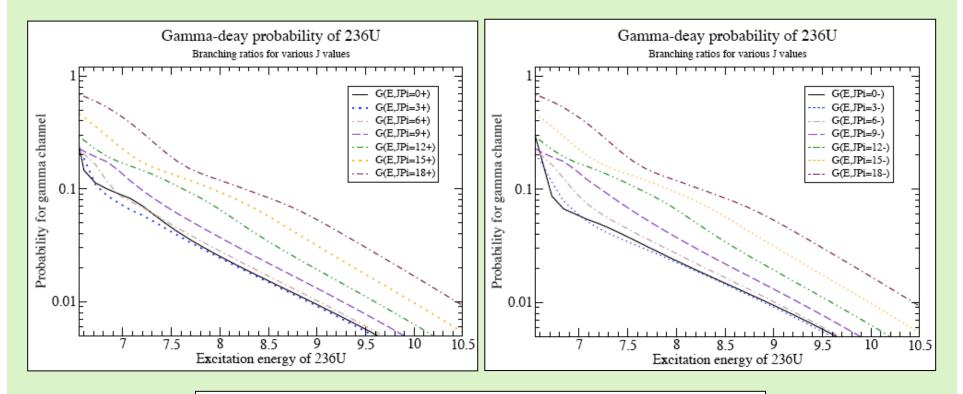


Weisskopf-Ewing analysis does not work here!

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### **Case 2: (n, y) reactions for actinide targets**

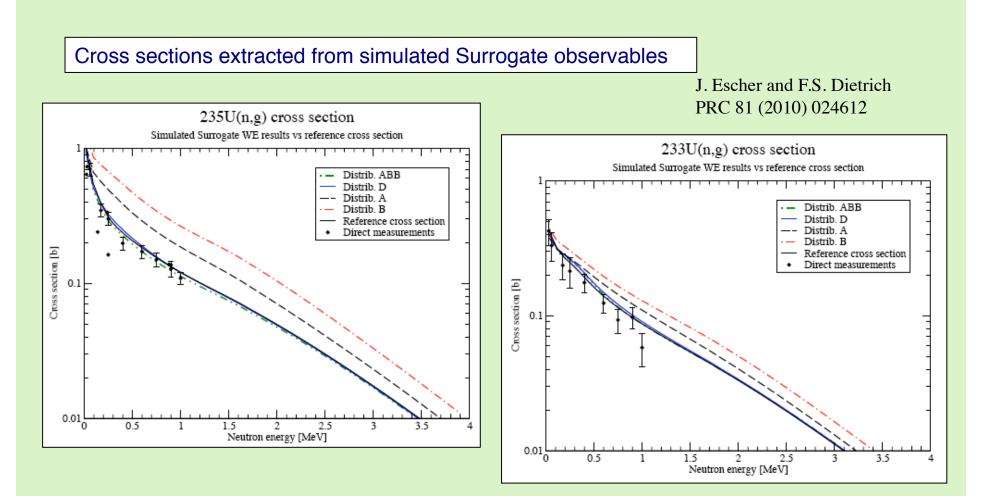
### J. Escher and F.S. Dietrich, PRC 81 (2010) 024612



Probability  $G(E,J,\pi)$  that a <sup>236</sup>U state with excitation energy  $E=S_n+E_n$  and given  $J^{\pi}$  value decays via  $\gamma$ -emission.

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### **Case 2: (n, y) reactions for actinides - Weisskopf-Ewing limit**

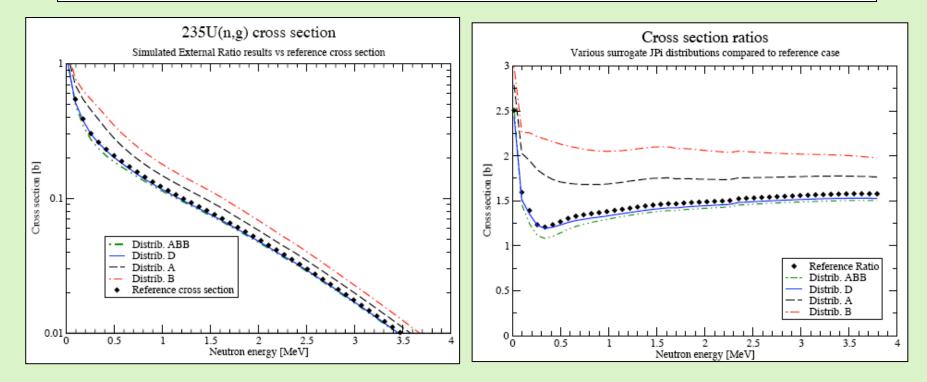


The WE limit may or may not work for  $(n,\gamma)$  cross sections. Knowledge of  $J^{\pi}$  would be very helpful!

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### **Case 2: (n, y) reactions for actinides - External Surrogate Ratio**

### Cross section and cross section ratio extracted from simulated Surrogate observables



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The Ratio approach yields some improvements.

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# Challenges specific to (n, y)

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### Detecting the $\gamma$ channel

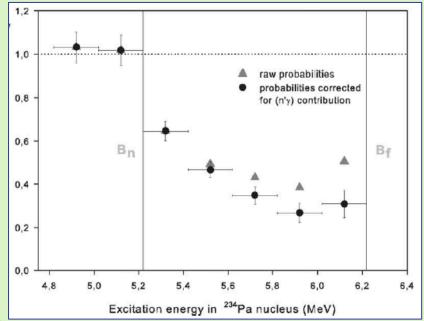
### **Considering some options:**

 Most experiments gate on individual γ rays in the residual nucleus instead of determining the appropriate sum of γ rays

-> need to account for portion of gamma cascade not seen

-> correction depends on the CN spin distribution Additional spin dependence!

- Alternative: detecting the complete gamma cascade:
  - -> better statistics
  - -> 'contamination' from other γ sources, such as γ following n evaporation require corrections
  - -> does not resolve the spin mismatch issue



Gamma probability for decay of <sup>234</sup>Pa following (3He,p) S. Boyer *et al*. NPA 775 (2006) 175

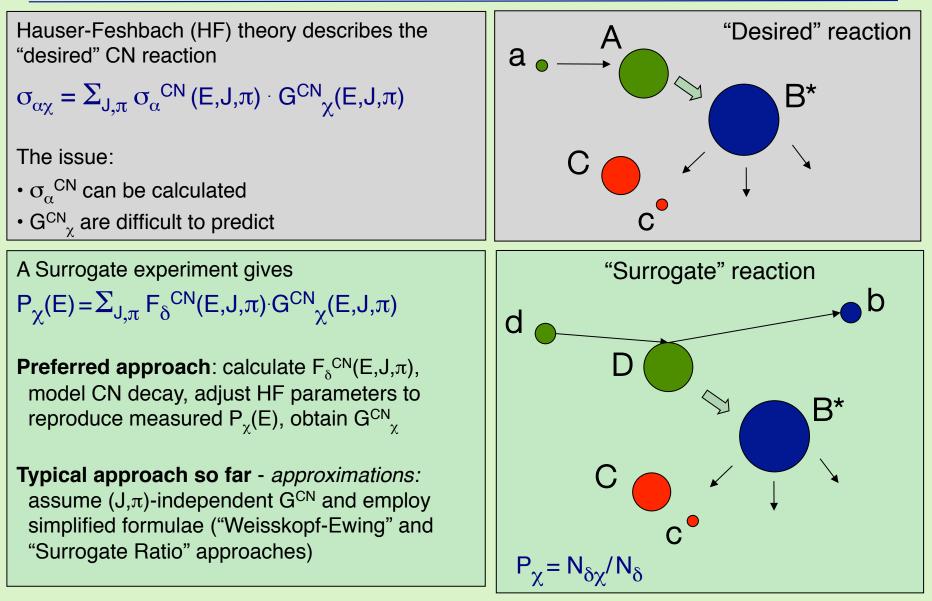
(n,γ) cross sections pose new challenges

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# Getting better cross section constraints from Surrogate data

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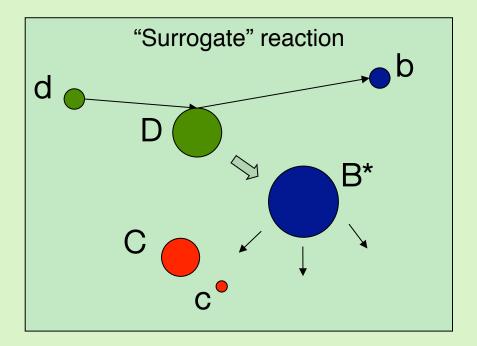
### The Surrogate Idea - Formalism



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J. Escher, LLNL

### **Predicting compound-nuclear spin-parity distributions**



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### **Predicting compound-nuclear spin-parity distributions**

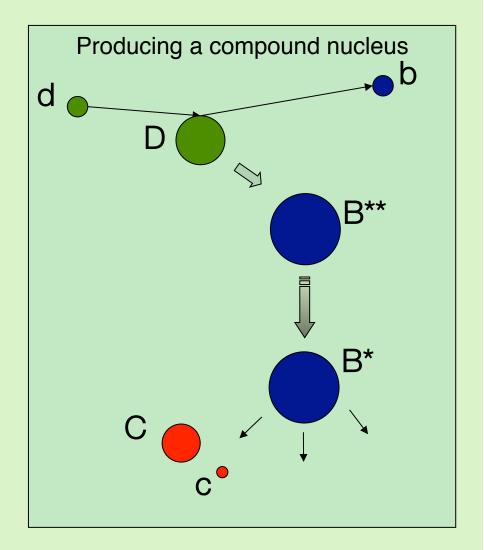
# Formation of a highly excited nucleus in a direct reaction

- inelastic scattering, pickup, stripping reactions
- various projectile-target combinations
- resonances, quasi-bound states

# Damping of the excited states into a compound nucleus

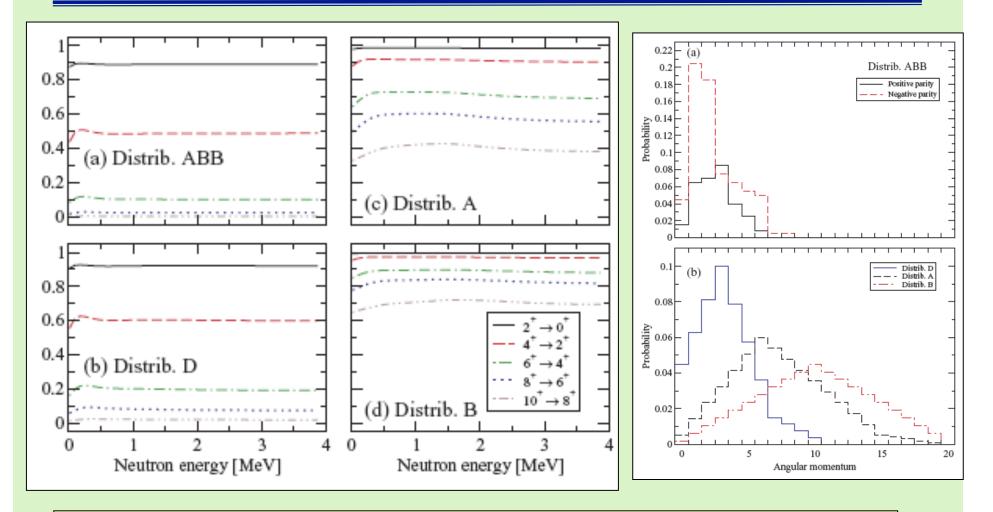
- competition between CN formation and non-equilibrium decay (particle escape)
- dependence on  $J^{\pi}$

### Width fluctuation correlations



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### $\gamma$ -rays as a signature of the CN spin-parity distributions: actinide case



 $\gamma$ -ray intensities are sensitive to the J<sup> $\pi$ </sup> distribution of the decaying CN nucleus. The 'collector' transition (2<sup>+</sup>->0<sup>+</sup>) accounts for 90-100% of the intensity.

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# Summary

The Surrogate nuclear reaction approach is potentially very valuable. It is the only indirect method for obtaining CN reaction cross sections.

### We have observed:

- $\bullet(n,\gamma)$  reactions are very sensitive to angular-momentum effects
- •Cross sections extracted from Surrogate experiments in the WE approximation do, in general, not give satisfactory results. Conclusion is based on theoretical considerations, calculations, and Gd experiments.
- •Nuclei near closed shells present a special challenge due to the low level densities, actinides seem somewhat less sensitive to spin effect.
- •Individual  $\gamma$  transitions contain valuable information. A combination with measurements of the complete  $\gamma$ -cascade is potentially very useful.

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### Collaborators

Theory:

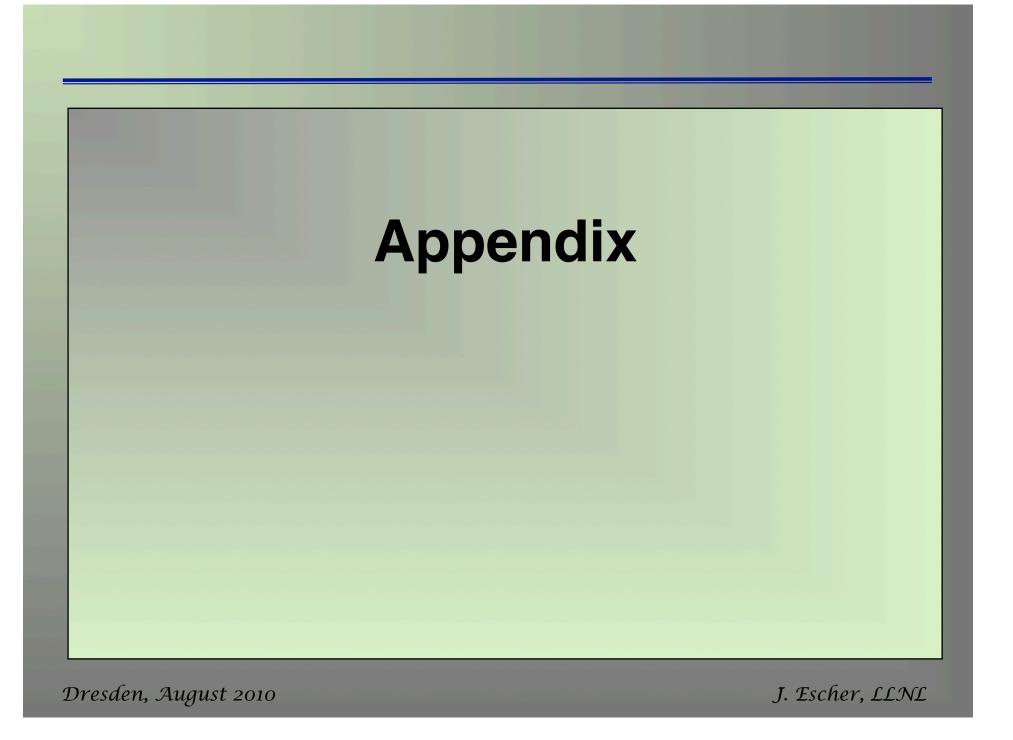
**F.S. Dietrich**, D. Gogny, R. Hoffman, I.J. Thompson, W. Younes *(LLNL)* C. Forssén (*Chalmers University*) A.K. Kerman (*MIT/ORNL*)

### Experiment:

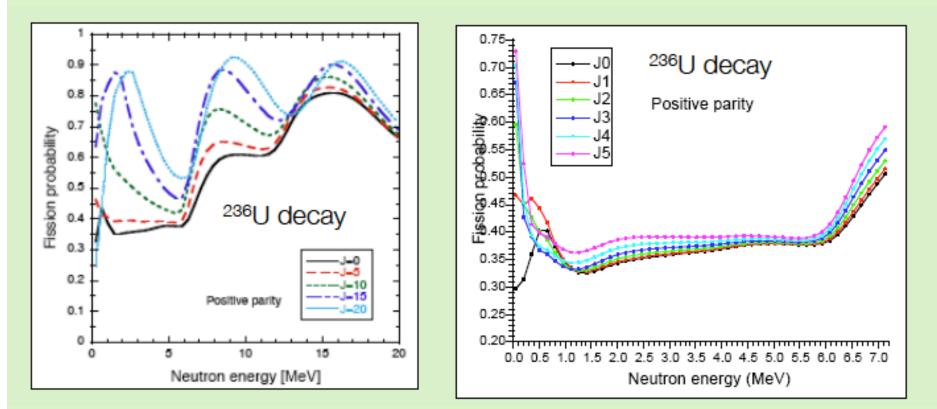
The STARS/LIBERACE collaboration, in particular:
J. Burke, L. Bernstein, S. Lesher, J.J. Ressler, N. Scielzo (LLNL)
R. Hatarik, S. Basunia, L.W. Phair (LBNL)
B. Lyles/Goldblum (LLNL/UC Berkeley)
C. Beausang (University of Richmond)

J. Cizewski, W. Peters (Rutgers/ORNL)

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### <sup>236</sup>U fission probabilities: dependence on $J^{\pi}$

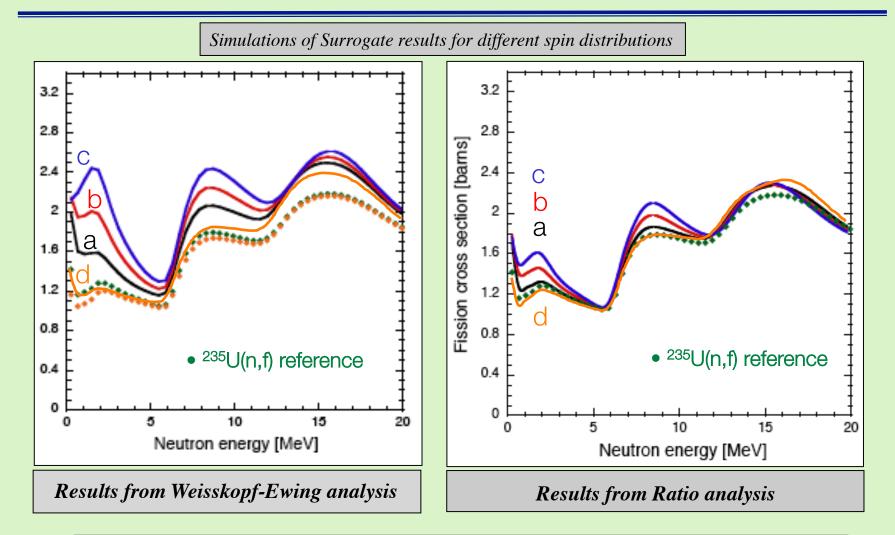


### **Insights:**

- It is not a priori obvious whether the WE approximation applies. The validity of the approximation depends on the energy and the range of  $J^{\pi}$  populated.
- Note the range of spins and the linear scale.

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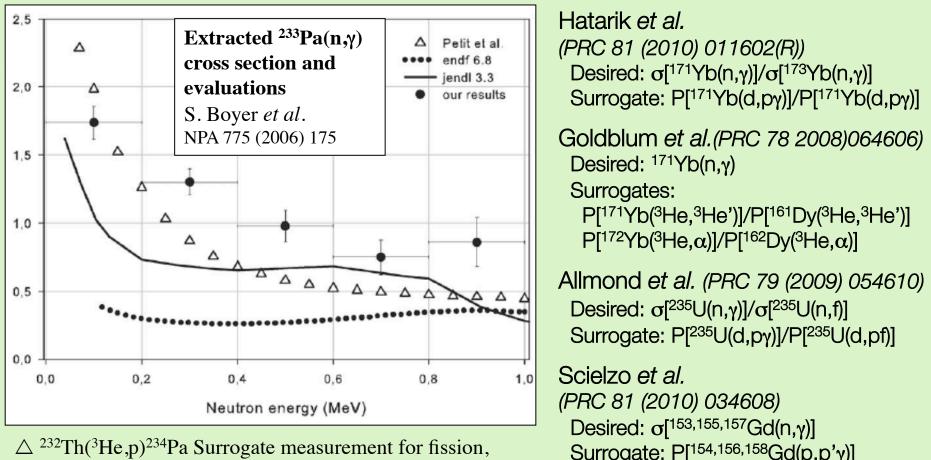
### **Theory tests of WE and Ratio approximations**



Calculations illustrate the level of agreement that can be expected from (n,f) cross sections extracted in Weisskopf-Ewing and Ratio approximations.

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### Surrogate approach for (n,y) cross sections



used to adjust HF calculation of  $(n,\gamma)$  cross section

<sup>232</sup>Th(<sup>3</sup>He,p)<sup>234</sup>Pa Surrogate measurement for γ exit channel, analyzed in WE approximation

Surrogate measurements for  $(n,\gamma)$  are now being considered.

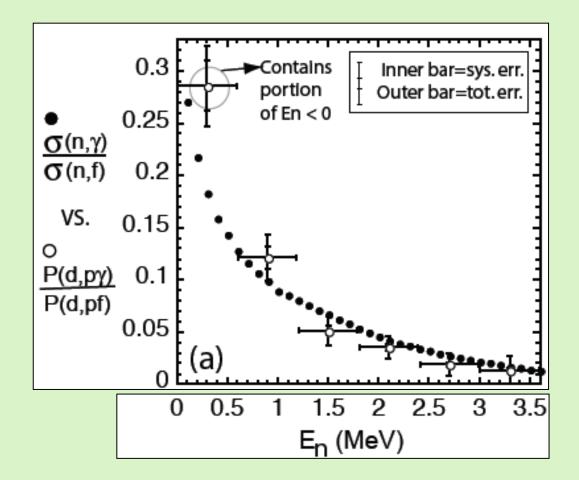
### Minimizing effects of the spin-parity mismatch: ratio results for <sup>235</sup>U(n,γ)

### J.M Allmond et al. (PRC 79 (2009) 054610)

Deduced the  ${}^{235}U(n,\gamma)$  cross section from a Surrogate Internal Ratio, using  ${}^{235}U(d,p\gamma)$ and  ${}^{235}U(d,pf)$  with  $E_d=21MeV$ 

Work assumes that 34% of the gamma cascade proceeds through the 1- -> 2+ (642keV) transition.

Result is in agreement with evaluated cross section.

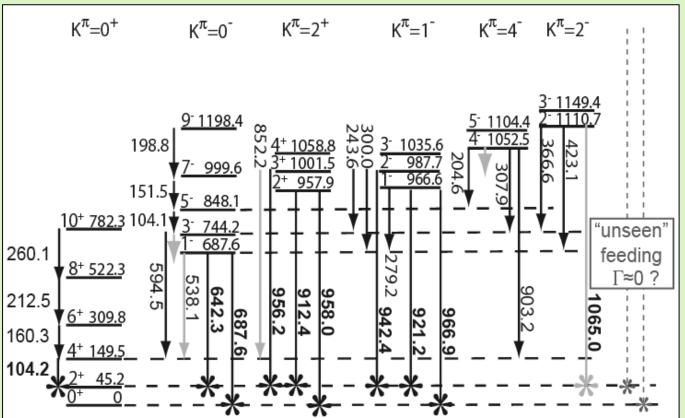


### Minimizing effects of the spin-parity mismatch: ratio results for <sup>235</sup>U(n,γ)

### J.M Allmond et al. (PRC 79 (2009) 054610)

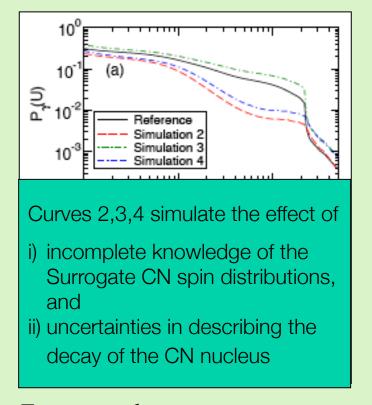
Goal: deduce the  ${}^{235}U(n,\gamma)$ cross section from a Surrogate Internal Ratio, using  ${}^{235}U(d,p\gamma)$ and  ${}^{235}U(d,pf)$  with  $E_d=21MeV$ 

Work makes use of the assumption that 34% of the gamma cascade proceeds through the 1- -> 2+ (642keV) transition.



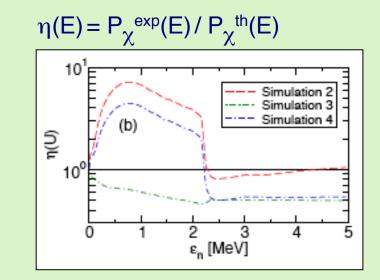
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### Normalizing calculated cross sections with Surrogate data



Forssen et al. Phys. Rev. C 75 (2007) 055807

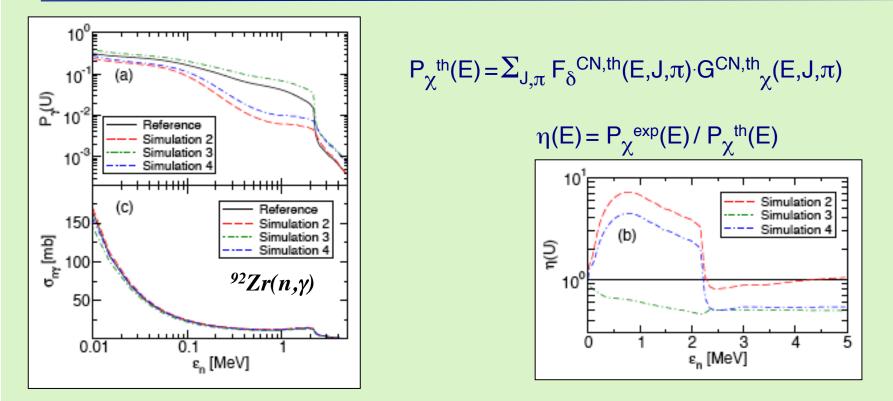
$$\mathsf{P}_{\chi}^{\text{th}}(\mathsf{E}) = \sum_{\mathsf{J},\pi} \mathsf{F}_{\delta}^{\mathsf{CN},\mathsf{th}}(\mathsf{E},\mathsf{J},\pi) \cdot \mathsf{G}^{\mathsf{CN},\mathsf{th}}_{\chi}(\mathsf{E},\mathsf{J},\pi)$$



 $\sigma_{n\gamma}^{\text{extr}}(\mathsf{E}) = \eta(\mathsf{E}_{s}) \Sigma_{\mathsf{J},\pi} \sigma_{n}^{\text{CN,th}}(\mathsf{E},\mathsf{J},\pi) G^{\text{CN,th}}(\mathsf{E},\mathsf{J},\pi)$ 

### Dresden, August 2010

### Normalizing calculated cross sections with Surrogate data



Forssen et al. Phys. Rev. C 75 (2007) 055807

$$\sigma_{n\gamma}^{\text{extr}}(\mathsf{E}) = \eta(\mathsf{E}_{s}) \Sigma_{\mathsf{J},\pi} \sigma_{n}^{\text{CN,th}}(\mathsf{E},\mathsf{J},\pi) G^{\text{CN,th}}(\mathsf{E},\mathsf{J},\pi)$$

Surrogate experiments may help constrain models at higher energies and improve calculations in the desired energy range - **even for very challenging cases**!

Dresden, August 2010