GRUCON-2017: Reconstruction of Angular Distributions from Resonance Parameters in Blatt-Biedenharn Formalism

Statements of work:

- include to the RXTXS module the possibility of reconstruction the U-collision matrices from RML, SLBW, MLBW, RM and RML resonance parameters;
- develop the module for summing the obtained U-matrices with Wigner geometrical coefficient and preparing the Blatt-Biedenharn coefficients for Legendre polynomial expansion of angular distributions (SXLXA module);
- provide possibility of optimization the energy grid of angular distribution parameters and conversion to required representation for preparing the ENDF MF4 file (AXEXA, ENDF modules);
- provide possibility of preparing the ACE files with obtained data for MC transport codes;
- perform verification of new modules by comparison with results of other codes;
- validate the functionality of the GRUCON package in the neutron leakage spectra calculations by comparison with experiments.

1. The formula and algorithms

Differential cross section in Blatt-Biedenharn formalism [1] for the partition into reaction partners α, the total angular momentum *J*, orbital angular momentum *l*, the s channel spin, for zero Coulomb interaction is given by

$$d\sigma_{\alpha\alpha'}/\,d\Omega = \frac{\lambda_\alpha^2}{(2i+1)(2I+1)}\sum_{s,s'}\sum_{L=0}^{\infty} B_L(\alpha s, a's')P_L(\cos\theta) \tag{1}$$

$$B_L(\alpha s, a's') = \frac{(-1)^{s-s'}}{4}\sum_{J_1,J_2}\sum_{l_1,l_2}\sum_{l_1',l_2'} \overline{Z}(l_1 J_1 l_2 J_2\,|sL)\overline{Z}(l_1' J_1' l_2' J_2'|s'L)$$
$$\times\left(\delta_{\alpha\alpha'}\delta_{l_1 l_1'}\delta_{ss'} - U^{J_1}_{\alpha l_1 s,\alpha' l_1' s'}\right)\left(\delta_{\alpha\alpha'}\delta_{l_2 l_2'}\delta_{ss'} - U^{J_2}_{\alpha l_2 s,\alpha' l_2' s'}\right) \tag{2}$$

$$\overline{Z}(l_1 J_1 l_2 J_2|sL) = \sqrt{(2l_1+1)(2l_2+1)(2J_1+1)(2J_2+1)}\,(l_1 l_2 00|L0)W(l_1 J_1 l_2 J_2|sL) \tag{3}$$

Where $\overline{Z}$ is a Blatt-Biedenharn coefficients, with phase convention for $\overline{Z}$ is that of Ref. [2],
$W(l_1 J_1 l_2 J_2|sL)$ is a Racah coefficients,
$(l_1 l_2 00|L0)$ is a Clebsh-Gordan coefficients of angular momentum coupling,

and $U^{J_1}_{\alpha l_1 s,\alpha' l_1' s'}$ is a collision function.

The form of collision function depends on approximation [3].
In Breight-Wigner approximation, the collision function [2] is expressed as:

$$U_{cc'} = e^{-i(\varphi+\varphi')}\left(\delta_{cc'} + i\sum_{\lambda}\frac{\Gamma_{\lambda c}^{\frac{1}{2}}\omega_{\lambda cc'}\Gamma_{\lambda c'}^{\frac{1}{2}}}{E_\lambda + \Delta_\lambda - E - \frac{i\Gamma_\lambda}{2}}\right) \tag{4}$$

with $\omega_{cc'} = 1$ (SLBW case) or

$$\omega_{\lambda cc'} = 1 + \sum_{\mu \neq \lambda} \left(\frac{\gamma_{\mu c}}{\gamma_{\lambda c}} + \frac{\gamma_{\mu c'}}{\gamma_{\lambda c'}} \right) \frac{\sum_{c''} \gamma_{\lambda c''} L^0_{c''} \gamma_{\mu c''}}{E_\mu + \Delta_\mu - E_\lambda - \Delta_\lambda - i\,(\Gamma_\mu - \Gamma_\lambda)/2} \qquad (5)$$

(MLBW case).

In Reich-Moore approximation, the collision function can be written in form

$$U_l = e^{-i2\varphi_l} \left(1 + \frac{2iR_l P_l}{1 - R_l L^0_l} \right) \qquad (6)$$

with R_l defined as

$$R_l \equiv \sum_\lambda \frac{\gamma^2_{\lambda l}}{E_\lambda - E - \frac{i\Gamma_{\lambda a}}{2}} \qquad (7)$$

The formulae (4-7) have been implemented in the RXTXS module to calculate optionally (in addition to cross sections) the (1-U) function for each spin group. The option is controlled by the RXTXS command parameter IOPT=0 or 1 (cross sections or 1-U function).

Reconstruction of angular distribution parameters (Blatt-Biedenharn coefficients) requires the geometrical Clebsh-Gordan and Racah coefficients are needed. To prepare Racah coefficients, the algorithm for calculation of Wigner 6j coefficients, described in the Ref. [5], was used. A general formula for Wigner 6j coefficients is

$$\begin{Bmatrix} j_1 & j_2 & j_3 \\ j_4 & j_5 & j_6 \end{Bmatrix} = \Delta(j_1 j_2 j_3)\Delta(j_1 j_5 j_6)\Delta(j_4 j_2 j_6)\Delta(j_4 j_5 j_3)$$

$$\times \sum_z \left[\frac{(-1)^z (z+1)!}{(z - j_1 - j_2 - j_3)!\,(z - j_1 - j_5 - j_6)!\,(z - j_2 - j_4 - j_6)!} \right.$$
$$\left. \times \frac{1}{(z - j_3 - j_4 - j_5)!\,(j_1 + j_2 + j_4 + j_5 - z)!\,(j_2 + j_3 + j_5 + j_6 - z)!\,(j_1 + j_3 + j_4 + j_6 - z)!} \right] \qquad (5)$$

where

$$\Delta(abc) = \left[\frac{(a+b-c)!\,(a-b+c)!\,(-a+b+c)!}{(a+b+c+1)!} \right]^{1/2} \qquad (6)$$

The Racah W-coefficient is obtained from the relation

$$W(j_1 j_1 l_2 l_1 | j_3 l_3) = (-1)^{j_1+j_2+l_1+l_2} \begin{Bmatrix} j_1 & j_2 & j_3 \\ l_1 & l_2 & l_3 \end{Bmatrix} \tag{7}$$

For the Wigner 3j coefficients the corresponding formula is used

$$\begin{aligned} \begin{Bmatrix} j_1 & j_2 & j_3 \\ l_1 & l_2 & l_3 \end{Bmatrix} = {} & \delta_{l_1+l_2+l_3,0}(-1)^{j_1-j_2-l_3} \\ \times & \left[\frac{(j_1+j_2-j_3)!\,(j_1-j_2+j_3)!\,(-j_1+j_2+j_3)!}{(j_1+j_2+j_3+1)!}\right]^{1/2} \\ \times & \left[(j_1+l_1)!\,(j_1-l_1)!\,(j_2+l_2)!\,((j_2-l_2)!\,(j_3+l_3)!\,(j_3-l_3)!\right]^{1/2} \\ \times \sum_z & \frac{(-1)^z}{z!\,(j_1+j_2+j_3-z)!\,(j_1-l_1-z)!\,(j_2+l_2-z)!\,(j_3-j_2+l_1+z)!\,(j_3-j_1-l_2+z)!} \end{aligned} \tag{8}$$

The Clebsh-Gordan coefficient is evaluated via its relation to Wigner 3j coefficients:

$$(j_1 l_1 j_2 l_2 | j_3 l_3) = (-1)^{j_1-j_2+l_3}\sqrt{2j_3+1} \begin{Bmatrix} j_1 & j_2 & j_3 \\ l_1 & l_2 & -l_3 \end{Bmatrix} \tag{9}$$

The algorithms of calculation the Wigner 6j coefficients has been tested by comparison with tables from Ref.[6].
The calculation of the Blatt-Biedenharn coefficients by summing the U collision functions with geometrical coefficients performs the SXLXA module. Optionally obtained coefficient can be inserted to the angular distribution parameters extracted from the ENDF MF4 file. If the last are represented as the p(μ) tables, obtained coefficients will be preliminary converted to the same representation.

Angular distributions, prepared by RXTXS and SXLXA modules, usually contain excess of energy points. To optimize the energy greed, the AXEXA module with a thinning function is added to the package. Parameters of angular distribution (*A* structures) can be converted to the ENDF format by the ENDF module or included to the ACE file by the ACE module.

2. Calculation Task

Here is an example of input deck for preparing ENDF MF4 file with angular distributions, restored from resonance parameters. Command parameter &1 for RXTXS module point at collision function calculation. Command parameter &20 for the SXLXA module means, that reconstructed angular parameters should be joint with taken from the original ENDF data, registered at the 20-th catalogue string.

```
! Reconstruction of Angular Distributions
! from Resonance Parameters
,,,init,1,0,10000
,in                 ! enter input parameters
,in,1,endf          !
,in,2,rxtxs         !
,in,3,sxlxa         !
,in,4,axexa         !
,in,5,endf          !
,1,20,ra            ! read *r* and *a* structures  from mf2 and mf4 endf files
20,2&1,21,s         ! calculate collision function
21,3&20,22,a        ! reconstruct angular distributions
22,4,23,a           ! remove excess of points in the  energy grid
23,5                ! write to the mf4 endf file
,,,end
!-------------------------------------------------
!    local parameters
*mt:2,
*de:1.e-5,150.e6,
*eps:0.001
!-------------------------------------------------
!    control parameters
*endf:ntape=20,nmat=0,nmf=2,nmt=0,mf=2,4
*r/t-s:nfor=0,nt=1,*de,*eps,tem=0.
*s/l-a:nl=0,ns=1,*mt,*de,*eps
*a/e-a:lap=-1,lct=-1,na=0,*eps
*endf:ntape=21,nmat=0,nmf=1,nmt=0,mf=4
```

At the Fig.1(a-c) are shown calculation results, obtained in the task for Fe-56 (WPEC/CIELO test evaluation) , namely, the Re (1-U) and Im(1-U) components of the U-collision function; the Legendre polynomial coefficients, reconstructed from resonance parameters.

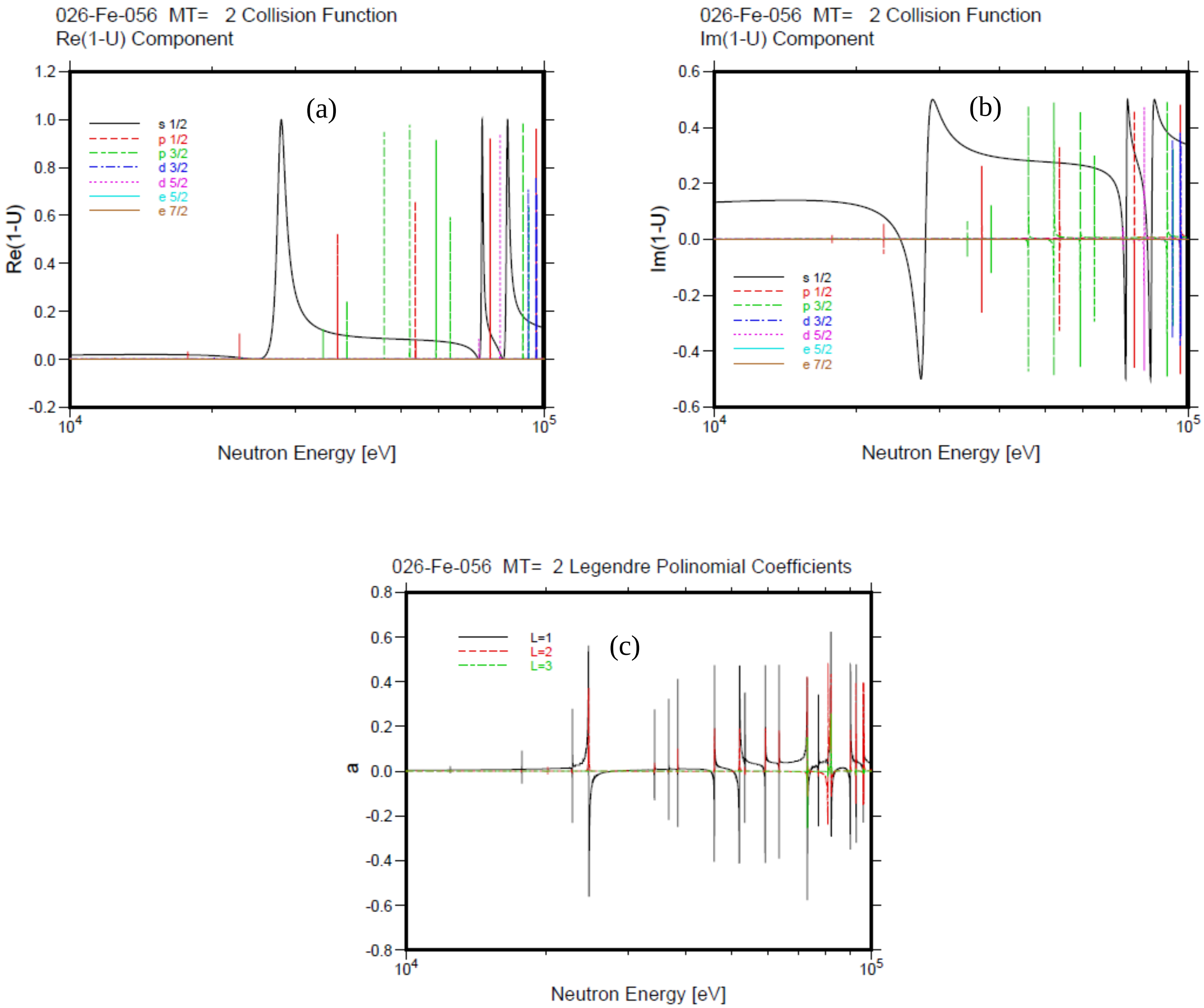

Fig.1 Collision function (a),(b) and Legendre polynomial coefficients (c), reconstructed from resonance parameters of Fe-56 (CIELO)

3. Verification and Validation

New modules of the GRUCON package have been tested by comparison with angular distributions, restored from resonance parameters by the NJOY-2016 processing code (to prepare angular distribution, the value **Want_Angular_Dist=.false.** in the RECONR module was changed to **Want_Angular_Dist=.true.**). Results of comparison elastic and inelastic angular distributions, obtained from the Fe-56 file (WPEC/CIELO test evaluation) are shown on Fig.2. The MF4 curve corresponds to data, taken from original ENDF file.

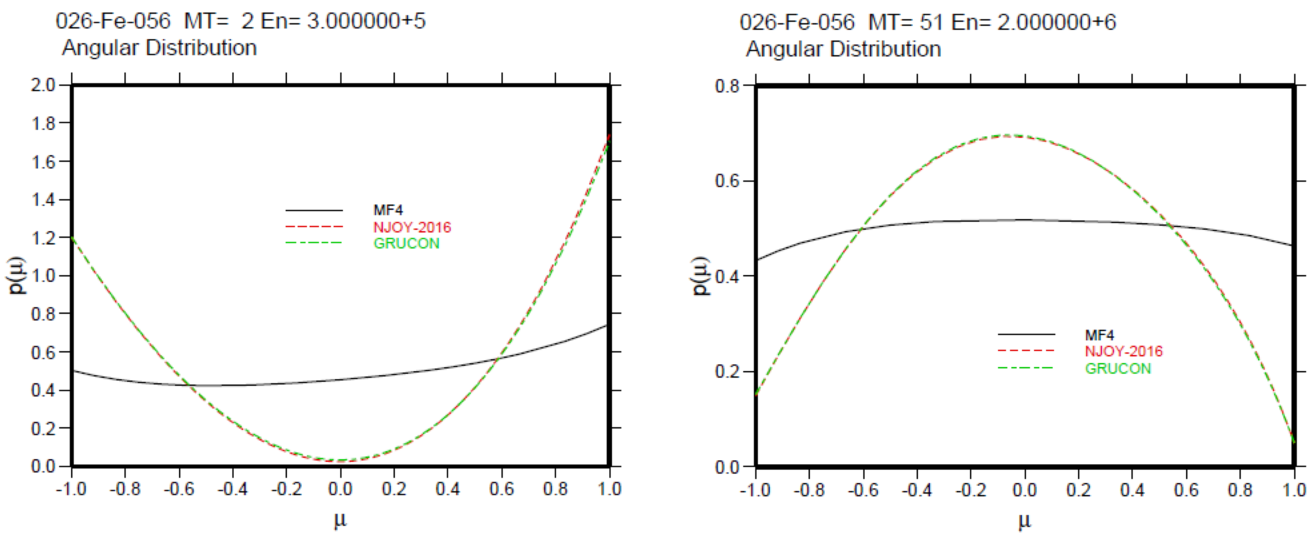

Fig.2 Angular distributions for elastic (a) and inelastic (b) scattering, calculated for Fe-56 by GRUCON and NJOY codes from resonance parameters (MF=2) and taken from the original ENDF file MF=4.

Validation of the functionality of GRUCON-2017.6 has been performed in calculations of neutron leakage spectra for iron shells. Benchmark experiments with 14MeV neutron source, described in the SINBAD radiation shielding data base [5], were used for comparison with calculation results:

- iron shell No. 1 (r= 4.5 cm, wall thickness = 2.5 cm),
- iron shell No. 2 (r=12.0 cm, wall thickness = 7.5 cm),
- iron shell No. 3 (r=12.0 cm, wall thickness =10.0 cm),
- iron shell No. 4 (r=20.0 cm, wall thickness =18.1 cm),
- iron shell No. 5 (r=30.0 cm, wall thickness =28.0 cm)

The ACE file have been prepared for Fe-56 CIELO evaluation with angular distributions, restored from resonance parameters (RML formalism) and original data, taken from original MF4 data file. Other materials were taken from ENDF/B-VII.1 library with original angular distributions.

The results of comparison are shown at the Fig.3(a-e).

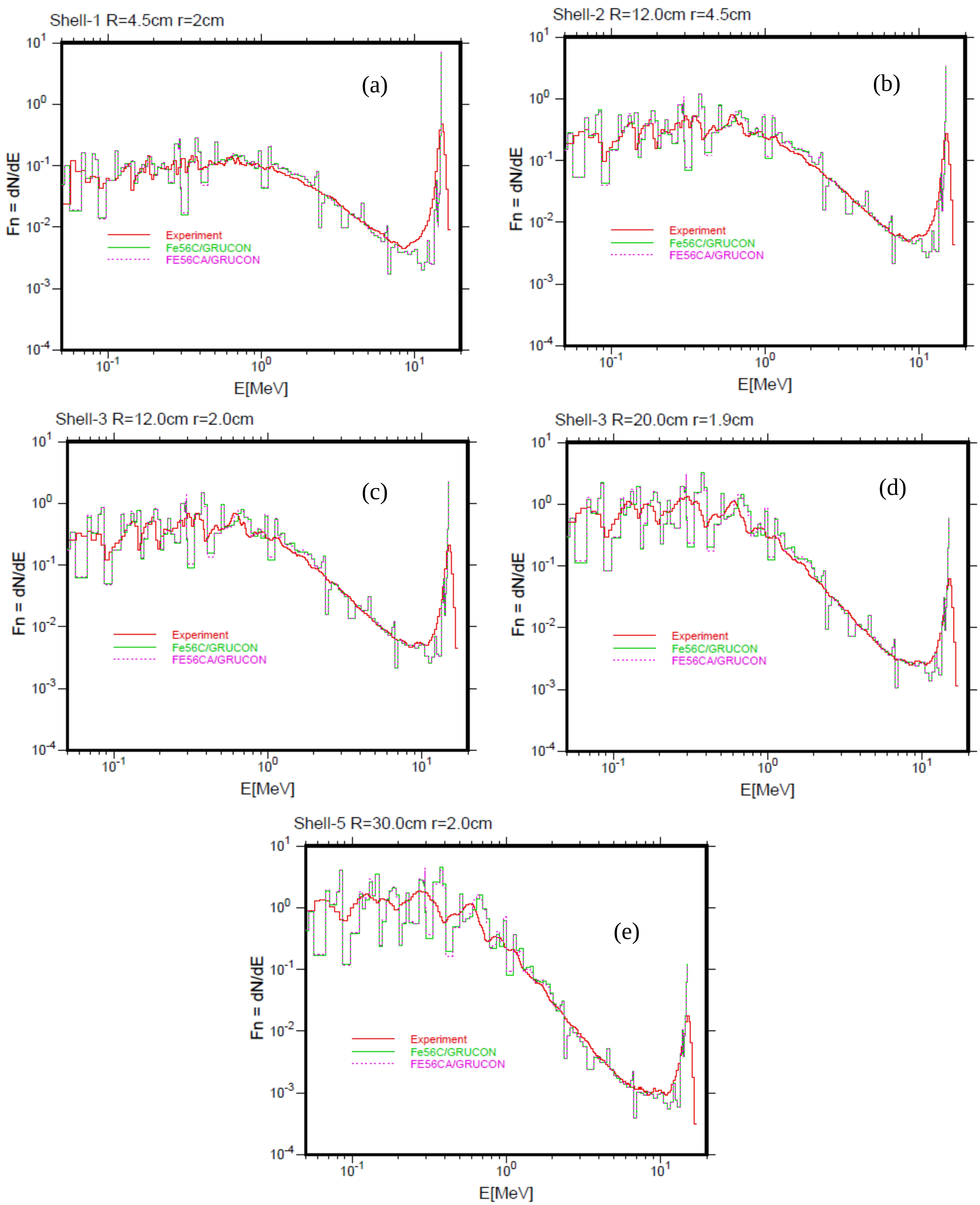

Fig.3 Comparison leakage spectra, calculated with original (Fe56C) and reconstructed (Fe56CA) angular distributions with measured in benchmark experiments for iron shells.

Conclusion

The functionality of the GRUCON-D code package is extended to provide possibility of

- reconstruction the U-collision matrices, used in the ENDF file and preparation of the Legendre polynomial expansion of angular distributions for different ENDF representations of resonance parameters
- conversion of obtained angular distributions to the ENDF MF4 formatted file;
- preparing of the ACE file for MC transport calculations.

This functionality is verified and validated by comparison with NJOY-2016 calculations, and by comparison MCNP-4C2 leakage spectra calculations with results of benchmark experiments.

Acknowledgments

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References

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   S.P. Simakov, B.V. Devkin, M.G. Kobozev, V.A. Talalaev (Inst. of Physics and Power Engineering, Obninsk),U. Fischer, U. von Moellendorff (Forschungszentrum Karlsruhe), Radiation shielding and dosimetry experiments database (SINBAD) , IPPE Fe shells Experiment and Analysis.