# DPA Cross Section Calculated with UNF Code

ZHANG Jingshang

*China Institute of Atomic Energy, P.O.Box 275(41)* Beijing *102413*

*e-mail zhangjsh@iris.ciae.ac.cn*

## Introduction

All of the structure nuclear materials have crystal lattice structure. The radiation damage implies the damage in varying degree in their crystal lattice structure, which is account for the changing of internal stress intensity and other properties. In general the radiation damage is measured in three fields: displacement of primary atom; production of the hole in the crystal lattice structure; and helium gas production. On the other hand, various nuclear reactions could provide amount of neutrons and gamma ray. Since their long free-path in the material the main task is radiation protection, besides the secondary reaction induced by them.

In the case of low and middle incident energies the radiation damage mainly caused by elastic scattering and inelastic scattering processes. The damage quantity is estimated by dpa.annal with the unit of b•keV. If the dpa cross sections are obtained with the unit of barn, then multiplying the current of the incident particles, then one can obtain the annual damage quantity.

The energy of the residual nuclei is depleted by three ways:

(1) The energy to get rid of the crystal lattice, which is the threshold energy of the nucleus in the crystal lattice, as the example, some effective threshold energies $E_d$ in the unit of eV of structure materials are given in Table 1.

**Table 1 Effective threshold energy of PKA in unit of eV**

| Material | Al | Ti, Cu | Cr,Fe,Co,Ni | Nb,Mo | W |
|---|---|---|---|---|---|
| $E_d$ / eV | 25 | 30 | 40 | 60 | 90 |

(2) The ionization of the electrons, which only reduce the energies of the residual nucleus, but do not affect the material damage.

(3) Displacement of primary atom in the material causes the hole production in the crystal lattice, which is the main part of the material damage. Only the kinetic energy of the residual nucleus is larger than the threshold energy of the primary knock-on atom (PKA), the displacement of primary atom could be happen.

## 1 Displacement of Primary Atom

The energies used for the electron ionization and displacement of primary atoms are denoted by $\eta(T)$ and $\nu(T)$, respectively. $A_T$ and $Z_T$ refer to the mass number and charge number of the target, respectively. The energy accumulated in the target material can be given by

$$\hat{E}(E_0)=N\int_{E_d}^{E_0}\frac{dx}{dE}dE\int_{E_d}^{T_{max}}T[(\eta(T)+\nu(T)]\frac{d\sigma}{dT}dT \tag{1}$$

where $T$ is the kinetic energy of the residual nucleus, $N$ is the atomic density of the (1/cm$^3$), $E_0$ stands for the incident energy, d$E$/d$x$ is the stopping power of the target material, d$\sigma$/d$T$ is the spectrum of the recoil residual nucleus in laboratory system, which is related sensitively to the type of incident particle and energy.

The spectrum of the recoil residual nucleus can be calculated by UNF code with full energy balance[1], while in JENDL the effective single particle emission approximation is employed. The hole defective caused by the displacement of primary atom $\nu(T)$ can be calculated by Lindhard model[2,3]. In this model the dimensionless primary knock-on energy is defined by $\varepsilon$

$$\varepsilon=\frac{T(\text{keV})}{0.0869\times Z_T^{7/3}}=\frac{T(\text{eV})}{86.931Z_T^{7/3}} \tag{2}$$

The number of the displacement of primary atom caused by per PKA is given by

$$\nu(T)=\frac{1}{2E_d}\frac{T}{1+k_L g(\varepsilon)} \tag{3}$$

Based on the study from Robinson[4], for elastic scattering of atom the number through the displacement of primary atom has the following form

$$\nu(T) = \frac{\beta T}{2E_{\mathrm{d}}} \tag{4}$$

where $\beta$=0.8 is used[3].

In Lindhard model, for a single constituent rather than an alloy in Eq.(3)

$$k_{\mathrm{L}} = 0.1334 Z_{\mathrm{T}}^{2/3} / A_{\mathrm{T}}^{1/2} \tag{5}$$

$$g(\varepsilon) = \varepsilon + 0.40244\varepsilon^{3/4} + 3.4008\varepsilon^{1/6} \tag{6}$$

For an alloy ($A_1$, $Z_1$, and $A_2$, $Z_2$ ), $A_1$, $Z_1$ are the mass number and charged number of recoil residual nucleus; $A_2$, $Z_2$ are that of the matrix atoms, Eq.(5) becomes

$$k_{\mathrm{L}} = \frac{(0.0793) Z_1^{2/3} Z_2^{1/2} (A_1 + A_2)^{3/2}}{(Z_1^{2/3} + Z_2^{2/3})^{3/4} A_1^{3/2} A_2^{1/2}} \tag{7}$$

From the study of Robinson[4], for pure iron, chromium and nickel, the difference of calculated results from pure and alloy is only 1%.

The dpa cross section is defined by

$$\sigma_{\mathrm{dpa}} = \int_{E_{\mathrm{d}}}^{T_{\max}} \frac{\mathrm{d}\sigma}{\mathrm{d}T} \nu(T) \mathrm{d}T \tag{8}$$

The rate of displacement of primary atom is given by

$$K_{\mathrm{d}} = \sigma_{\mathrm{dpa}} \times \Phi \tag{9}$$

where $\Phi$ is the particle current, while for single atom $\Phi$ is the bombard frequency of the incident particle.

## 2 Calculation of DPA Cross Sections

Based on the formula mentioned above, the function to calculate the dpa cross section can be executed by UNF code. Since the energy spectrum calculated is in CMS, while in the dpa calculation of $\mathrm{d}\sigma/\mathrm{d}T$ is in LS, so the transformation from the CMS to the LS need to be performed in UNF code.

For elastic scattering process, the recoil energy of the target nucleus in CMS is obtained by

$$T_{\mathrm{el}}^{\mathrm{c}} = \frac{m_{\mathrm{n}} M_{\mathrm{T}}}{M_{\mathrm{c}}^2} E_{\mathrm{n}}, \tag{10}$$

the recoil energy of the target nucleus in LS is

$$T_{\mathrm{el}}^{1} = 2T_{\mathrm{el}}^{\mathrm{c}} (1 - \cos\theta_{\mathrm{c}}) \tag{11}$$

where $M_{\mathrm{n}}$, $M_{\mathrm{T}}$, $M_{\mathrm{c}}$ are the masses of incident neutron, target and compound nucleus, respectively. Thus, the dpa cross section in elastic scattering channel is obtained by

$$\sigma_{\mathrm{dpa}}(el) = \int_{E_{\mathrm{d}}}^{E_{\mathrm{c,max}}} \frac{\beta}{2E_{\mathrm{d}}} T_{\mathrm{el}}^{1} \frac{\mathrm{d}\sigma}{\mathrm{d}\,\Omega_{\mathrm{c}}} \delta(T_{\mathrm{el}}^{\mathrm{c}} - \frac{m_{\mathrm{n}} M_{\mathrm{T}}}{M_{\mathrm{c}}^2}) \mathrm{d}T_{\mathrm{el}}^{\mathrm{c}} \mathrm{d}\,\Omega_{\mathrm{c}}$$

$$= \sigma_{\mathrm{el}}(E_{\mathrm{n}}) \frac{\beta}{E_{\mathrm{d}}} \frac{m_{\mathrm{n}} M_{\mathrm{T}}}{M_{\mathrm{c}}^2} (1 - f_1^{\mathrm{el}}(\mathrm{c})) E_{\mathrm{n}}, \tag{12}$$

where $f_1^{\mathrm{el}}(\mathrm{c})$ is the Legendre coefficient of the elastic scattering angular distribution with the partial wave $l$=1 in CMS.

For the first particle emission from compound nucleus to discrete levels, the recoil nucleus has definite energy in CMS.

$$E_k^{\mathrm{c}}(M_1) = \frac{m_1}{M_{\mathrm{c}}} (E^* - B_1 - E_{k_1}), \tag{13}$$

where $m_1$ ,$M_1$ are the masses of the first emitted particle and its residual nucleus; $B_1$ is the binding energy of $m_1$ in the compound nucleus; $E_{k_1}$ is the level energy of residual nucleus. The energy of $M_1$ in LS reads[1]

$$E_k^{l}(M_1) = \frac{m_{\mathrm{n}} M_1}{M_{\mathrm{c}}^2} E_{\mathrm{n}} + E_k^{\mathrm{c}}(M_1)_{\mathrm{c}} + \frac{2}{M_{\mathrm{c}}} \sqrt{m_{\mathrm{n}} M_1 E_{\mathrm{n}} E_k^{\mathrm{c}}(M_1)} \cos\theta \tag{14}$$

where $\theta_{\mathrm{c}}$ is the outgoing angle of recoil residual nucleus $M_1$ in CMS. Averaged by the angular distribution of recoil residual nucleus $M_1$, the dpa cross section has the form as

$$\sigma_{\mathrm{dpa}}(M_1)_k = \int_{E_{\mathrm{d}}}^{E_{l,\max}} \frac{\mathrm{d}\sigma}{\mathrm{d}E_k^1} \nu(E_k^1) \mathrm{d}E_k^1$$

$$= \int \mathrm{d}\,\Omega_{M_1}^{\mathrm{c}} \frac{\mathrm{d}\sigma}{\mathrm{d}\,\Omega_{M_1}^{\mathrm{c}}} \nu(E_k^1(M_1)) \tag{15}$$

In the case of continuum final states, including the emissions from compound nucleus to continuum states or the sequential multi-particle emissions. The double-differential cross section is represented in the Legendre expansion form in CMS

$$\frac{\mathrm{d}^2\sigma}{\mathrm{d}\varepsilon^{\mathrm{c}} \mathrm{d}\,\Omega^{\mathrm{c}}} = \frac{\sigma}{4\pi} \sum_l (2l+1) f_l^{\mathrm{c}}(\varepsilon^{\mathrm{c}}) \mathrm{P}_l(\cos\theta^{\mathrm{c}}) \tag{16}$$

The dpa cross section of the recoil nucleus with the mass $M_2$ can be obtained by

$$\sigma_{\mathrm{dpa}} = \int_{E_{\mathrm{d}}}^{E_{l,\max}} \frac{\mathrm{d}\sigma}{\mathrm{d}E^1} \nu(E^1) \mathrm{d}E^1 = \iint \frac{\mathrm{d}^2\sigma}{\mathrm{d}E^1 \mathrm{d}\,\Omega^1} \nu(E^1) \mathrm{d}E^1 \mathrm{d}\,\Omega^1$$

$$= \iint \frac{\mathrm{d}^2\sigma}{\mathrm{d}E^{\mathrm{c}} \mathrm{d}\,\Omega^{\mathrm{c}}} \nu(E^1) \mathrm{d}E^{\mathrm{c}} \mathrm{d}\,\Omega^{\mathrm{c}} \tag{17}$$

where

$$E^1 = E^c(1+2\gamma\cos\theta_c+\gamma^2) \quad (18)$$

and
$$\gamma = \frac{\sqrt{m_n M_2}}{M_c}\sqrt{\frac{E_n}{E^c}} \quad (19)$$

The relation $E^1 \geq E_d$ must be held in the Eq.(17).

As an example, the calculations of dpa cross sections of n+$^{56}$Fe have been performed with UNF code. Since the resonance region is below 0.8 MeV, so the model calculation only performed at the energies from 1 MeV to 20 MeV. The dpa cross section caused by gamma ray emissions is small enough to be neglected. The comparison of the calculated result and measured data is shown in Fig.1 for the total dpa cross section. The calculations indicate that elastic scattering channel is the dominant term. Therefore, the key point is to fit the measured elastic scattering data well on the cross section and angular distribution as far as possible in the model calculation. The dpa cross sections of elastic scattering channel have very different values from different evaluated neutron data files. The calculated dpa cross section with the related evaluated data in eq.(12) taken from ENDF/B-6, Jendl-3.2 and CENDL-2 from $E_n$=1 MeV to 20 MeV are shown in Table 2. From this table one can see that the results are very different from each other.

The sequential multi-particle emission processes give relative large recoil effect to the single particle emission. Meanwhile, the heavier emitted particle yields stronger recoil effect. Of course, dpa cross sections are also proportionally dependent on the reaction cross sections.

**Table 2 The dpa cross sections of elastic scattering calculated with the data from ENDF/B-6, JENDL-3.2 and CENDL-2 at $E_n$=1 to 20 MeV**

| $E_n$ / MeV | CENDL-2 | JENDL-3.2 | ENDF/B-6 |
|---|---|---|---|
| 1.0 | 657.2 | 633.6 | 491.0 |
| 3.0 | 1272.7 | 1282.0 | 1236.7 |
| 5.0 | 1146.4 | 1168.2 | 1061.0 |
| 7.0 | 1040.4 | 1033.9 | 980.7 |
| 9.0 | 910.5 | 945.4 | 996.6 |
| 11.0 | 883.4 | 969.3 | 1044.4 |
| 13.0 | 919.1 | 1033.0 | 1099.5 |
| 15.0 | 1011.0 | 1116.1 | 1396.5 |
| 17.0 | 1087.2 | 1188.8 | 990.3 |
| 20.0 | 1283.7 | 1283.1 | 1165.5 |

The dpa cross sections calculated by UNF code are listed in Table 3. The dpa cross sections induced by $^3$He and triton emissions are not included due to very small.

**Table 3 The dpa cross sections of each reaction channel and the total dpa cross section calculated by UNF code**

| $E$ | in-el | n,p | n,$\alpha$ | n,d | n,2n |
|---|---|---|---|---|---|
| 1.0 | 0. | 0.024 | 0 | 0 | 0 |
| 2.02 | 403.4 | 9.85 | 0 | 0 | 0 |
| 4.0 | 719.3 | 251.9 | 1.19 | 0 | 0 |
| 6.5 | 746.7 | 714.9 | 70.4 | 0 | 0 |
| 8.0 | 750.9 | 631.0 | 166.3 | 0 | 0 |
| 10. | 685.1 | 433.9 | 136.1 | 1.31 | 0 |
| 12. | 561.2 | 189.3 | 63.0 | 6.90 | 0 |
| 14. | 514.9 | 40.7 | 22.1 | 7.62 | .014 |
| 16. | 596.4 | 24.4 | 8.0 | 5.05 | 12.7 |
| 18. | 682.8 | 17.5 | 3.32 | 3.18 | 54.7 |
| 20. | 760.7 | 13.7 | 1.64 | 2.06 | 100.9 |

| $E$ | n,np | n,n$\alpha$ | n,2p | elas. | Total |
|---|---|---|---|---|---|
| 1.0 | 0 | 0 | 0 | 620.2 | 620.2 |
| 2.02 | 0 | 0 | 0 | 626.4 | 1040. |
| 4.0 | 0 | 0 | 0 | 653.9 | 1632. |
| 6.5 | 0 | 0 | 0 | 694.7 | 2231. |
| 8.0 | 0 | 0 | 0 | 749.1 | 2297. |
| 10. | 0 | 0 | 0 | 1089. | 2344. |
| 12. | 50.0 | 0 | 0.43 | 1697. | 2568. |
| 14. | 285.6 | 0.62 | 3.70 | 1961. | 2836. |
| 16. | 484.3 | 29.6 | 14.5 | 1848. | 3023. |
| 18. | 570.9 | 149.2 | 38.9 | 1641 | 3160. |
| 20. | 578.5 | 296.3 | 62.9 | 1384. | 3200. |

The results indicate that the radiation damage mainly caused by elastic scattering and inelastic scattering processes. Meanwhile, the sequential particle emissions from (n,np) and (n,n$\alpha$) channels give large contribution to the dpa cross section due to large reaction cross sections at high energies.

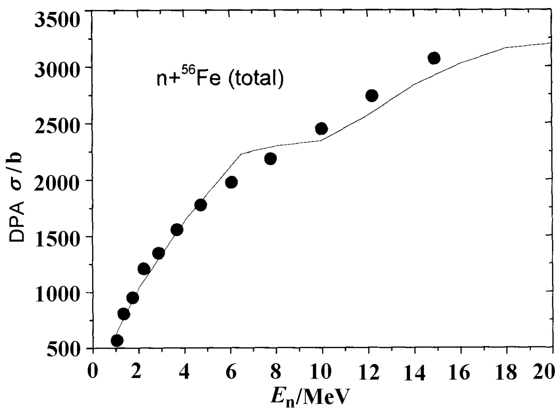


Fig.1 The total dpa cross section of n+$^{56}$Fe calculated by UNF code. The data are taken from Ref. [5]

## Reference


[1] ZHANG Jingshang. Commou. Nucl. Data. CNIC-01475 CNDC-0027 INDC(CPR)0050/L 23,18 (2000)

[2] J. Lindhard et al., Mat. Pys. Medd. Dan. Vid. Selsk., 33, 10 (1963)

[3] D. G. Doran, Nucl. Sci. Eng., 49,130,(1972)

[4] M. T. Robinson, Phil. Mag., 17, 639 (1968)

[5] D. G. Doran and N. J. Graves, HEDL-TME 7670, Hanford Engineering Development Laroratory, 1976


# The Production and Transmission of Covarience in the Evaluation Processing of Fission Yield Data


LIU Tingjin

*China Nuclear Data Center, CIAE, P.O.box 275(41) Beijing, 102413*

*e-mail tjliu@iris.ciae.ac.cn*



**【abstract】** *The production and transmission of correlation in the evaluation processing of fission yield data, including average with weight, ratio and sum consistence adjusting, are researched. The variation of the averaged and adjusted yields and/or rations with the correlation coefficient of the input data are investigated. The results obtained are reasonable in physics.*


## Introduction

The error, as traditionally given, is only the diagonal elements of the covariance matrix and only describes the total error of the data, nothing about the systematical error or the correlation of the data. The systematical error is more important for the engineering applications, because the statistical one can be counteracted in the calculation by using large amount of data, but the systematical one could not be. For evaluators and experimenters, the information is given completely, only in the case of the covariance matrix is given out.

As well known that the correlation describes the systematical error or medium and long range error[1] in the experiment, for example, due to calibration of detector efficiency, multiple scattering correction and measurement geometry, sample quantification, normalization etc. All of these depend on the experimental conditions. Also the correlation can be produced in the data evaluation processing, which is not only from the mathematical restriction condition, for example, the curve must be smooth in the curve fitting by using least-square method, but also from physical restrictive condition, for instance, the total must be the sum of all partials, absolute cross section or fission yield should be consistent with their concerned ratios measured etc.

For fission yield data, the main processing in the evaluation is

a. average with weight;

b. the consistency adjusting between the absolutely measured yields and the ratios concerned;

c. the consistency adjusting between the sum and its partials, e.g. cumulative yield and its independent yields concerned.

All of these processing can be done by using code ZOTT[2], with the different form of the sensitivity matrix. ZOTT is a general partitioned least squares method code, using for adjusting a combined set of data $Y(I)$ of differential and integral quantities with covariance $CY(I,J)$ to new values $Y'(I)$ with covariance $CY'(I,J)$, which are minimum variance linear unbiased estimator of the true values and satisfy the physical relationship prescribed by the sensitivity matrix $S(K,L)$, where $I$ or $J$ is the total number of differential plus integral quantities, $K$ is the number of the integral quantities and $L$ is the number of differential quantities.

In this paper, the production and transmission of the covariance in the fission yield data evaluation processing, as listed above, are investigated. The first section is for the average with weight, and the second one is for ratio adjusting, the third one is for sum adjusting, a practical example is given in the section