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ANALYSIS OF (n,α) REACTION BY USE OF MODIFIED TNG CODE

Keiichi Shibata

Japan Atomic Energy Research Institute
Tokai-mura, Naka-gun, Ibaraki-ken 319-11, Japan

and

Kichinosuke Harada

Nuclear Energy Data Center
Tokai-mura, Naka-gun, Ibaraki-ken 319-11, Japan

Abstract: The nuclear-model code TNG is modified to treat alpha-particle emission more physically. Information of the intrinsic wave function of alpha-particle is contained in the formation factor proposed by Iwamoto and Harada. The spectra of alpha-particle emitted from structural materials are calculated and compared with experimental data in order to verify the present modification. Furthermore, activation cross sections for the (n,α) reactions are calculated by using the modified code.

(TNG, nuclear-model code, alpha-particle formation factor, alpha-particle emission spectra, activation cross section)

Introduction

Theoretical calculation plays an important role in nuclear data evaluations. Particularly, the unified Hauser-Feshbach code which includes precompound effects has been widely used in recent evaluations. TNG/1/ is one of the unified Hauser-Feshbach codes developed by Fu, ORNL. It is well-known that the ORNL group has been successful/2-4/ in the evaluations of structural materials using TNG. However, the code is still under development and there are some problems to be overcome. One problem is concerned with treatment of alpha-particles. In the original TNG, alpha-particle is considered one particle without any structure, which is physically unacceptable. The alpha-particle emission process is important for the radiation damage study. Thus, it is desired to treat the alpha-particle emission more realistically.

In this work, we incorporate the alpha-particle formation factor of Iwamoto and Harada/5/ into TNG. The formation factor contains information of the intrinsic wave function of alpha-particle. The calculated alpha-particle spectra are presented for structural materials to verify the modification of TNG. Furthermore, (n,α) activation cross sections are calculated for several nuclei by using the modified TNG code.

Modification of TNG

Alpha-Particle Emission Rate

In the original code/1/, the alpha-particle emission rate from a state with p particles and h holes is given by

$$W_\alpha(p,h,\varepsilon) = \frac{1}{\pi^2\hbar^3}\,\mu\varepsilon\sigma(\varepsilon)\,\frac{\omega(p-1,h,U)}{\omega(p,h,E)} \quad ,$$

where μ is the reduced mass, ε the outgoing energy, σ(ε) the inverse reaction cross section, U the excitation energy of the residual nucleus and E the excitation energy of the compound nucleus. The state density ω is calculated from Williams' formula/6/ with proper pairing corrections/7/. On the other hand, Iwamoto and Harada /5/ proposed a new expression for alpha-particle emission:

$$W_\alpha(p,h,\varepsilon)= \frac{1}{\pi^2\hbar^3}\,\mu\varepsilon\sigma(\varepsilon)\sum_{\ell+m=4} F_{\ell m}(\varepsilon)\,\frac{\omega(p-\ell,h,U)}{\omega(p,h,E)}.$$

The formation factor $F_{\ell m}(\varepsilon)$ stands for the probability that the composite particle of an energy ε is composed of ℓ particles above the Fermi level and m particles below. It is expressed by the overlap between the alpha-particle wave function and four particles' wave functions. The formation factor was proved/8/ to be independent of the orbital angular momentum of alpha-particle, and it can be applied to nuclear-model codes without any difficulty. In practical calculation, we used the polynomial expressions for the formation factor which were found by Iijima/9/ using the least-squares fitting. The expressions are given as follows:

$$F_{13}(\varepsilon)=0.28144-0.01113\varepsilon+1.34\times10^{-4}\varepsilon^2,$$

$$F_{22}(\varepsilon)=0.61409+1.96\times10^{-3}\varepsilon-1.74\times10^{-4}\varepsilon^2,$$

$$F_{31}(\varepsilon)=0.10408+9.39\times10^{-3}+1.61\times10^{-5}\varepsilon^2,$$

$$F_{40}(\varepsilon)= \begin{array}{l} 0.0 \text{ if } \varepsilon < 8 \text{ MeV}, \\ 4.31\times10^{-4}-2.27\times10^{-4}\varepsilon+2.31\times10^{-5}\varepsilon^2 \\ \quad \text{if } \varepsilon \geq 8 \text{ MeV}, \end{array}$$

where ε is given in MeV units. Figure 1 shows the calculated alpha-particle emission rate in the case of the $n+^{56}Fe$ reaction.

Master Equation

As seen in Fig. 1, if the alpha-particle formation factor is applied to TNG without any other change, the calculated (n,α) cross section will be decreased, being inconsistent with experimental data. In the original TNG, the master equation is divided into three parts, each of which corresponds to a particle-type, i.e., neutron, proton and alpha-particle. The set of master equations is solved with different initial conditions. This treatment, however, competes with inclusion of the formation factors. Therefore, we decided to adopt the conventional single master equation which includes the Q factors of Kalbach/10/.

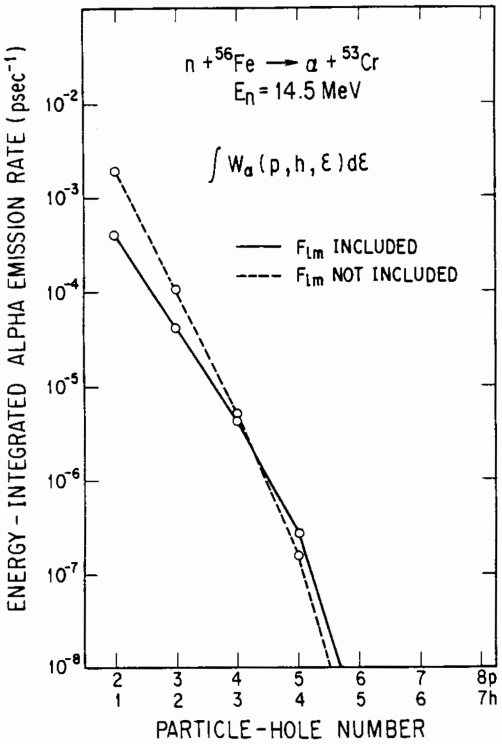

Fig. 1 Alpha-particle emission rate for ${}^{56}Fe(n,\alpha){}^{53}Cr$

Equilibration Time

In the original TNG, the equilibration time T is obtained from the relation

$$\frac{P(\bar{p},\bar{h},T)}{P(\bar{p}+1,\bar{h}+1,T)} \leq \frac{\omega(\bar{p},\bar{h},E)}{\omega(\bar{p}+1,\bar{h}+1,E)} ,$$

where P is the occupation probability, and $\bar{p}$ ($\bar{h}$) the most probable particle (hole) number which gives the maximum ω value. This relation comes from the condition that the time-derivative of the occupation probability at T should be zero. According to this definition, T depends on the exciton number and cannot be determined uniquely. On the other hand, Agassi et al./11/ estimated T by using the nucleon-nucleon collision probability of Kikuchi and Kawai/12/:

$$T = \sum_{n=3}^{\bar{n}} \frac{(n+1)}{2\lambda(E)} ,$$

where $\bar{n}$ is the most probable exciton number. The collision probability $\lambda(E)$ is expressed by

$$\lambda(E) = [1.6\times10^{21}(E/\text{MeV})-6.0\times10^{18}(E/\text{MeV})^2] /4.8 \text{ sec}^{-1},$$

where a factor of 4.8 was introduced to reproduce experimental data. In the present work, we adopted the equilibration time of Agassi et al., because it has a clear physical meaning and is uniquely obtained.

The time-integral of the occupation probability P from T to infinity is calculated as

$$\int_T^\infty P(p,h,t)dt = \frac{\hbar\omega(p,h,E)}{\sum_{p,h}\Gamma_{p,h}\omega(p,h,E)} e^{-qT/\hbar}$$

where the symbols $\Gamma_{p,h}$ and q are defined as follows:

$$\Gamma_{p,h} = \hbar\sum_b \int_0^{\varepsilon_{max}} W_b(p,h,\varepsilon)d\varepsilon$$

and

$$q = \sum_{p,h} \Gamma_{p,h}\, \omega(p,h,E)/\sum_{p,h}\omega(p,h,E).$$

Alpha-Particle Emission Spectra

The alpha-particle emission spectra were calculated for several nuclei using the modified code. Input data to TNG were taken from the ORNL evaluations. The k factor for the residual two-body matrix elements was changed from 400 MeV^3 to 600 MeV^3 in order to reproduce neutron emission spectra, because we adopted the single master equation and the Q factor of Kalbach.

The calculated results are shown in Figs. 2-6 together with experimental data. The solid line is the calculation with the modified code, while the dashed one stands for that with the original code. The difference between the two lines is small in the nuclei near iron. In these nuclei, the alpha-particle emission induced by 14 MeV neutrons is dominated by the compound process. On the contrary, in the case of ${}^{93}Nb$, the high-energy part of the spectrum is enhanced by including the formation factor, because in this reaction the precompound process plays a dominant role above outgoing energies of 8 MeV.

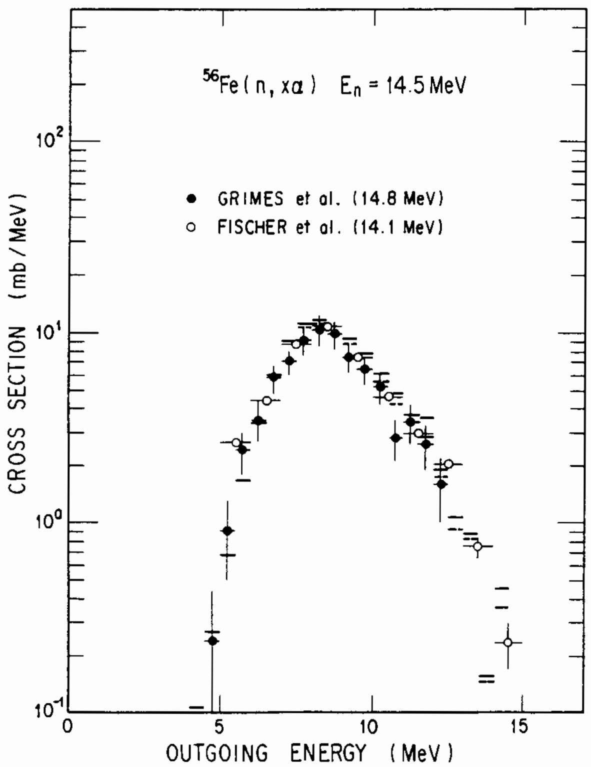

Fig. 2 Alpha-particle emission spectra from 14.5-MeV neutrons on ${}^{56}Fe$

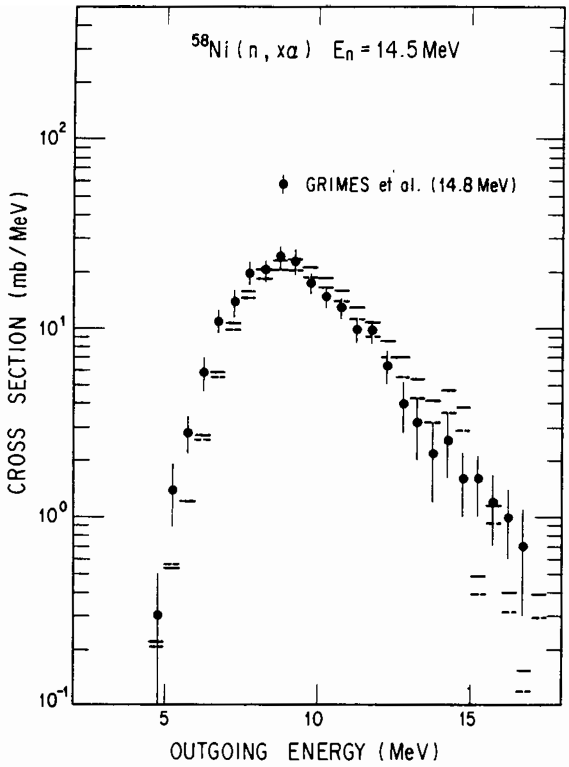

Fig. 3 Alpha-particle emission spectra from 14.5-MeV neutrons on ^{58}Ni

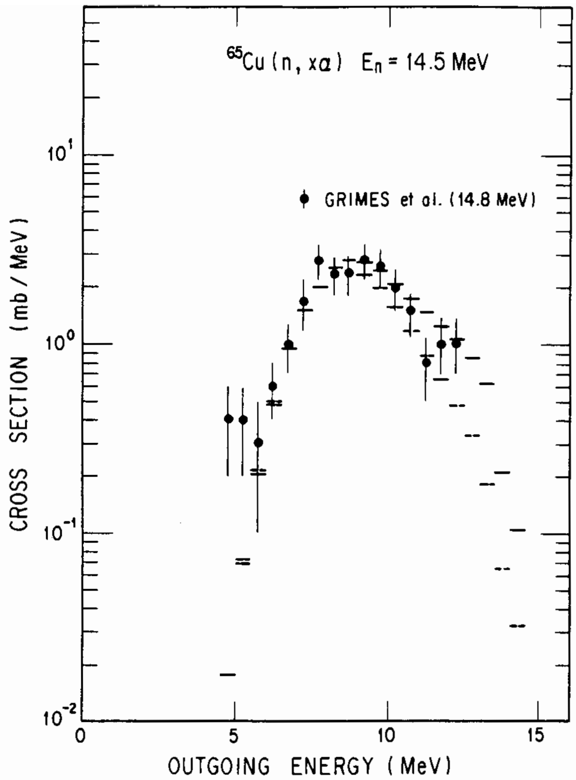

Fig. 5 Alpha-particle emission spectra from 14.5-MeV neutrons on ^{65}Cu

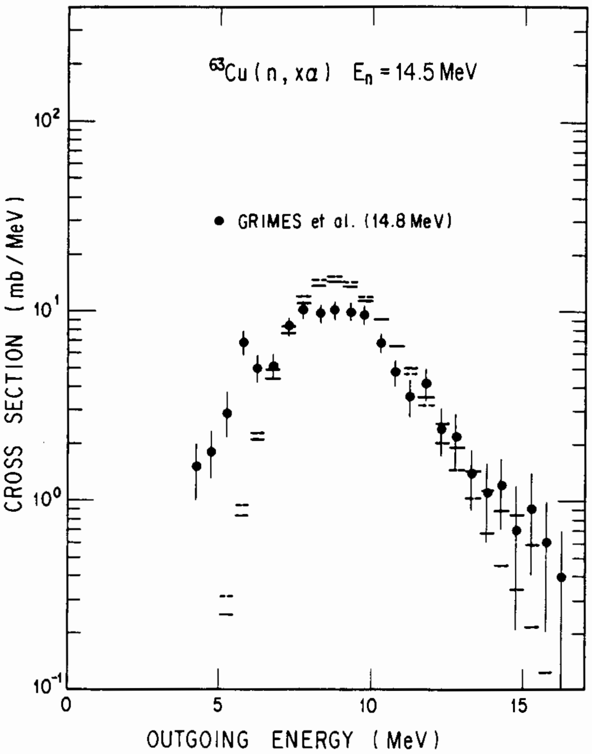

Fig. 4 Alpha-particle emission spectra from 14.5-MeV neutrons on ^{63}Cu

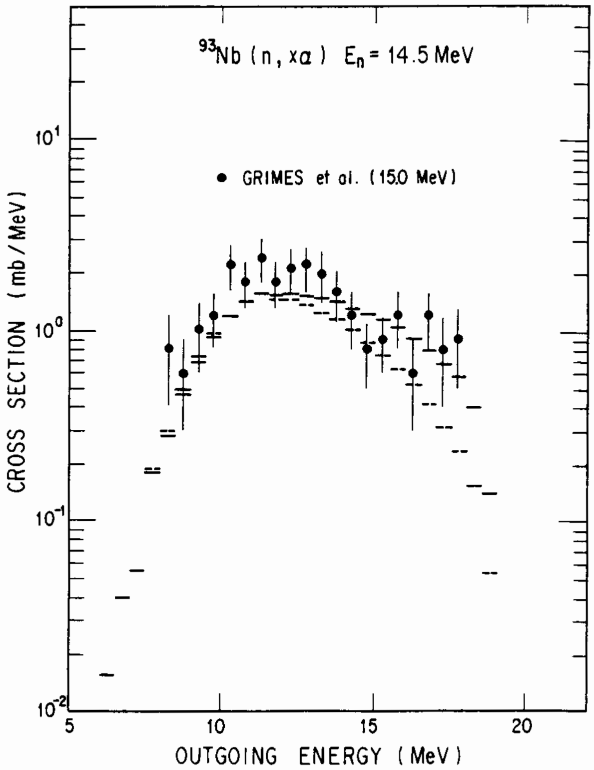

Fig. 6 Alpha-particle emission spectra from 14.5-MeV neutrons on ^{93}Nb

(n,α) Activation Cross Section

The activation cross sections for the (n,α) reactions were calculated by using the modified code. The results are shown in Figs. 7-9. In the case of ^{55}Mn, the calculation is in good agreement with experimental data. The calculation of activation cross sections for other nuclei was performed for the JENDL special purpose data file.

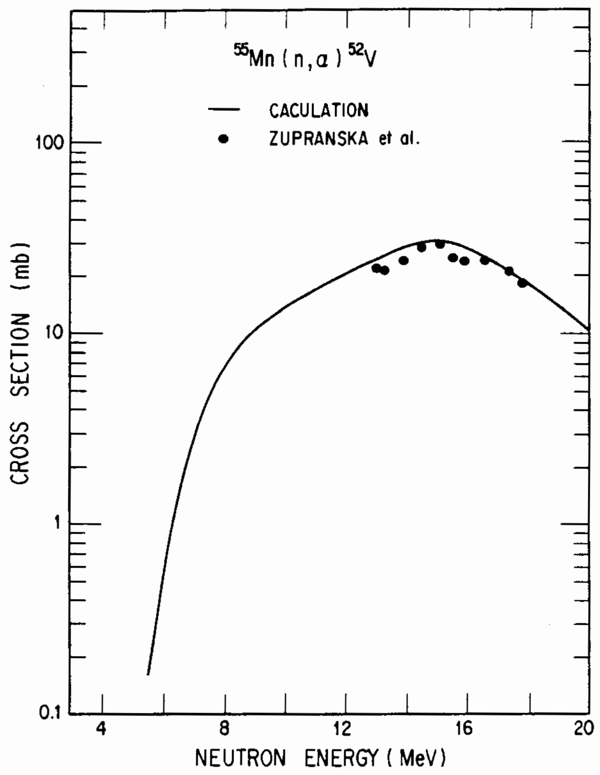

Fig. 7 $^{55}Mn(n,\alpha)$ activation cross section

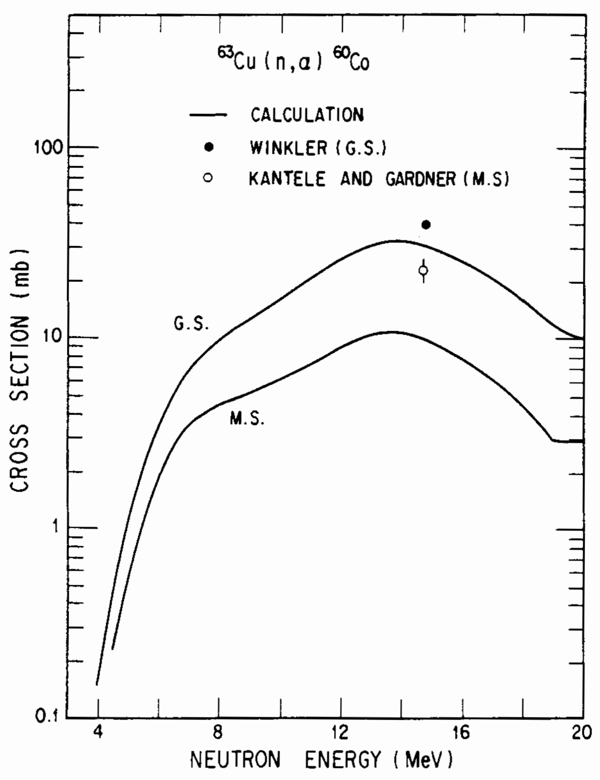

Fig. 8 $^{63}Cu(n,\alpha)$ activation cross section

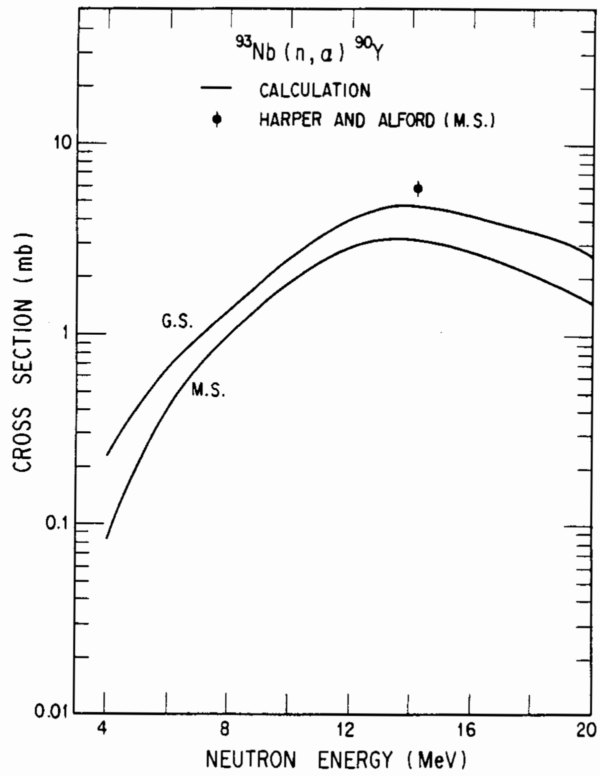

Fig. 9 $^{93}Nb(n,\alpha)$ activation cross section

Concluding Remarks

The alpha-particle formation factor of Iwamoto and Harada was incorporated into the TNG nuclear model code. The master equation and derivation of the equilibration time were also modified to make the physical meaning clear. The inclusion of the formation factor led to an improvement of the alpha-particle emission spectra from ^{93}Nb, in which the precompound process is dominant. In the nuclei near iron, the present calculation is consistent with that obtained using the original code.

The calculation of activation cross sections was performed for the JENDL special purpose data file.

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