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NUCLEAR CROSS SECTION CALCULATIONS WITH A SIMPLIFIED-INPUT VERSION OF ELIESE-GNASH JOINT PROGRAM

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Abstract: To calculate the nuclear cross sections with a statistical and preequilibrium model as efficiently and easily as possible, a simplified-input version of ELIESE-GNASH joint program has been developed. The program has a simple input-format and a set of global optical model potential parameters. Using the present version, neutron cross sections for 25 nuclides covering the range from ^{27}Al to ^{109}Ag were calculated up to 20 MeV. The 50 MeV neutron induced reaction for copper, and the proton and alpha-particle induced reactions for ^{58}Ni were also calculated. As the result of general agreements with experimental data for wide mass range, the availability of the present version of joint program is proved.

(cross section, statistical model, preequilibrium model, global optical potential, neutron, proton, alpha-particle, calculation)

Introduction

Nuclear cross section calculations with a statistical and preequilibrium model are usually troublesome. Particle transmission coefficients for neutron, proton, alpha-particle and other particles have to be calculated using appropriate optical model potential parameters. Suitable level density parameters and factors for preequilibrium process are selected. The preparation of discrete levels data takes much time. Because there are many parameters, the input-format of calculation code becomes so complicate, that the change of those parameters to improve the calculated results of cross sections is not easy.

Although the global neutron optical model potential is rarely used, recently, in the accurate cross section calculation, if there is a set of the global potential parameters, which can be applied in the wide mass region, the procedure for calculation of the particle transmission coefficients becomes simpler. The GNASH code[1] is able to automatically determine the nuclear temperature, if the discrete levels and Fermi-gas level density parameter "a" were inputted. Then by using this method, the number of parameters to be inputted can be decreased.

In order to efficiently execute many cross section calculations, it is necessary to simplify and standardize the procedures of calculations. An ELIESE-GNASH joint program has been developed to satisfy the requirements. The function of calculation of transmission coefficients was quoted from the program ELIESE-3[2] and global optical model potential parametrization was accepted, and the program has been combined with a simplified-input version of GNASH.

The discrete levels data were prepared from Evaluated Nuclear Structure Data File (ENSDF) after correction and input-format conversion. Direct inelastic scattering cross sections were calculated with the DWUCK4[3] code, which was also simplified in the input-format.

The joint program has new functions: (1) The double differential cross sections can be calculated using the output of DWUCK4 for direct reaction process and the systematics of Kalbach and Mann[4] for equilibrium and preequilibrium processes. (2) The transmission coefficients of each decaying channel in the multi-step nuclear reactions can be prepared. This option is useful for the calculation of charged particle induced reaction cross sections.

The calculated results of neutron induced reactions for from aluminium to silver, and proton and alpha-particle induced reactions for ^{58}Ni are compared with experimental data to show the wide applicability of the new version.

Simplified Input and Programmed Optical Model Potential

An input-format of new version is very simple. Flags for control of calculation are arranged in a line. Physical quantities, which are inputted in the minimum, are (1) atomic and mass numbers of incident particle, (2) atomic and mass numbers of nuclei which decay in the multi-step nuclear reactions, and the number of decay channels, (3) incident particle energy and energy bin for calculation, (4) level density parameter "a" for each nuclus, (5) parameters for preequilibrium process. In addition, radiative widths at neutron separation energy are recommended to input. Other many variables or parameters are set at the defaulted value or calculated in the program.

In the statistical nuclear model calculation, the angular momentum dependent particle transmission coefficients are calculated by optical model parameters. In the present program, optical potential parameters are predetermined and programmed in the code.

For neutron, Walter and Guss[5] potential is used. But, since their potential was parametrized for 10<E<80 MeV, the surface imaginary potential below 20 MeV has been assumed to be

$$W_s = 5.0 - 14.94\cdot(N-Z)/A + 0.271\cdot E_{lab},$$

for $0<E_{lab}<10$ MeV,

$$W_s = 7.71 - 14.94\cdot(N-Z)/A,$$

for $10<E_{lab}<20$ MeV. Their determinations were referred to the experimental nonelastic cross sections of a few elements and some results of cross section calculations. Above 20 MeV, the potential well is the same as the original.

Perey[6], Lemos[7], and Lohr and Haeberli[8] potentials are cited for proton, alpha-particle, and deuteron, respectively. For triton and ^{3}He, Becchetti,Jr and Greenlees[9] potential parameters are programmed. Transmission coefficients are calculated using these parameters before the calculations of nuclear decaying processes.

Comparisons between Calculated and Experimental Cross Sections

Neutron cross section calculations in the energy range from 1 MeV to 20 MeV were performed for 25 nuclides; ^{27}Al, ^{59}Co, ^{58,60}Ni, ^{63,65}Cu, ^{64,66,67,68,70}Zn, ^{90,91,92,94}Zr, ^{93}Nb, ^{92,94,95,96,97,98,100}Mo, and ^{107,109}Ag. It is possible to extend the energy region to about 50 MeV, and a calculation of isotope production cross sections for neutron bombarding on copper was carried out as a test of the performance. The charged particle induced reaction cross sections can also be calculated.

Several results are presented below with experimental data, as examples of many cross sections calculated with the joint program. Fig. 1 shows the ^{27}Al(n,α) cross section which is often used as standard. Except above 17 MeV, the calculated result agrees well with experimental data within errors. The calculated cross sections of ^{58}Ni(n,p) and ^{58}Ni(n,xp), shown in Fig. 2, agree fairly well with Paulsen et al.[10], Pavlik et al.[11], Grimes et al.[12], and Graham et al[13]'s data. But, Smith et al.'s measurement[14] have a different shape of cross section between 5 and 10 MeV. An excellent agreement with Santry et al.'s measurement[15] was obtained for ^{64}Zn(n,p) cross section in almost whole energy region, as shown in Fig. 3, but Smith et al.'s data[14] showed lower values.

For the nuclei of large mass number, we have many isomer-state productions in the nuclear reactions. The cross section of isomer production can be calculated with the ground state production if the discrete level data were inputted. As an example, the production cross section of ^{93}Nb(n,2n)^{92m}Nb reaction is shown in Fig. 4 with total (n,2n) cross section. Both cross sections reproduced well experimental data, which means that the discrete levels of ^{92}Nb were correctly treated. The ^{107}Ag(n,2n) isomer production and the ^{107}Ag(n,3n) total production cross sections are calculated with the joint program and shown in Fig. 5. In this case, agreements between the calculated and the experimental cross sections are also satisfactory up to 30 MeV, although we have slightly higher calculated values in the threshold regions.

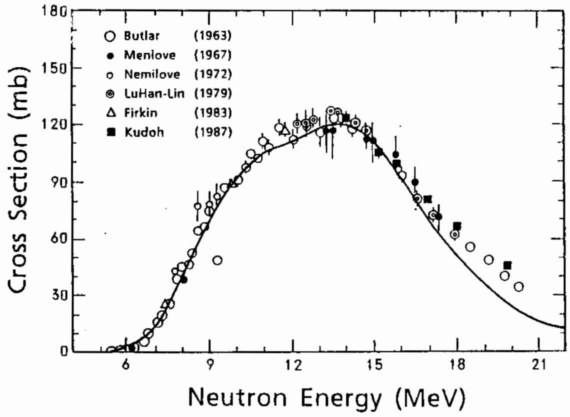

Fig.1 ^{27}Al(n,α)^{24}Na Reaction Cross Sections

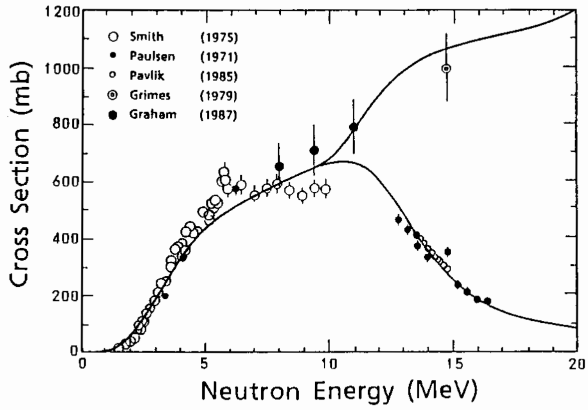

Fig.2 ^{58}Ni(n,p)^{58}Co and ^{58}Ni(n,xp) Reaction Cross Sections

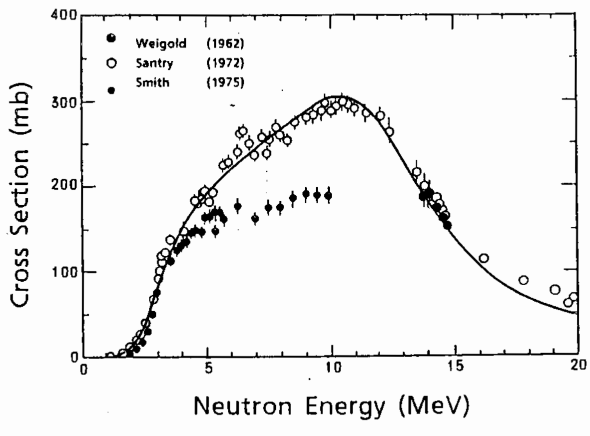

Fig.3 ^{64}Zn(n,p)^{64}Cu Reaction Cross Sections

Charged particle emission spectra in the neutron induced reactions were measured by several authors. By the comparisons between the calculations and experiments, it is possible to examine the contribution of equilibrium and preequilibrium processes.

Proton, alpha-particle, and deuteron emission spectra in reactions of 15 MeV neutrons with ^{63}Cu are calculated and compared with the Grimes et al.'s[12] measurements. Fig. 6 shows good agreements in proton and alpha-particle spectra, resulted in showing the adequate contribution of preequilibrium process. For deuteron , the calculated spectrum is shown to be harder, though the cross section agrees each other.

Calculated helium production cross sections by 15 MeV neutrons for 14 isotopes and 3 natural elements are compared with Kneff et al.'s data[16] in Table 1. The agreements between calculation and experiment are very good, except natural zirconium. Since (n,α) cross sections for zirconium isotopes are rarely measured, level density parameters of daughter nuclei, strontium, are not correctly given. But, it is easy to improve, because the input of present version of joint program is simple.

Cross section calculations for charged particle induced reactions have been attempted to confirm the availability of the present version of joint program. With some modifications of formula for knock-out process of alpha-particle, the generally good results are obtained for ^{58}Ni in case of proton or alpha-particle bombardments. Fig. 7 and Fig.8 show the calculated cross section of ^{58}Ni(p,2p)^{57}Co and of ^{58}Ni(α ,p)^{61}Cu plus ^{58}Ni(α ,n)^{61}Zn reactions, respectively, with experimental data. In the calculation, the transmission coefficients for each decaying channel were used, which is one of new functions of the present program. However, there are some cross sections which heavily disagree with experimental values. Several points remain to be investigated.

Summary

A simplified input version of ELIESE-GNASH joint program has been developed. In the program, the global optical model potential parametrization is accepted. Neutron cross sections up to 20 MeV for aluminium to silver were calculated and compared with experimental data to examine the applicability of the present version of joint program. Good agreements between the calculations and the experiments are obtained for almost all neutron cross sections. It can be expected, then, that the calculations using the present program predict the cross sections, which were not accurately determined by experiments or evaluations up to date, for the mass region from 20 to 120.

The extension of bombarding neutron energy to about 50 MeV is executed and the calculation for copper has been performed. And the charged particle induced reactions for ^{58}Ni are also calculated to test the usefulness of the present program. Although there are some cross sections which disagree with experiments, generally good results are obtained up to about 40 MeV incident energy. It is necessary to clear up the causes of disagreement.

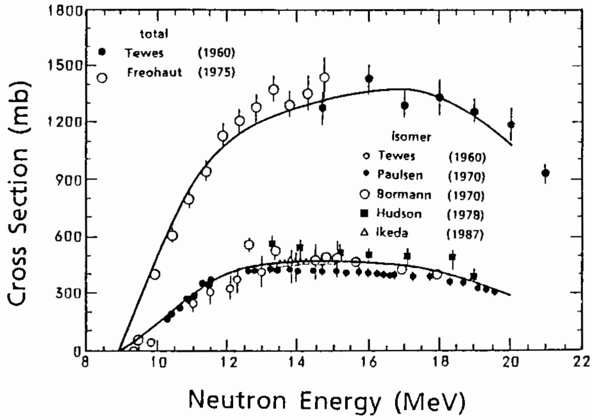

Fig.4 ^{93}Nb(n,2n)^{92}Nb and ^{93}Nb(n,2n)^{92m}Nb Reaction Cross Sections

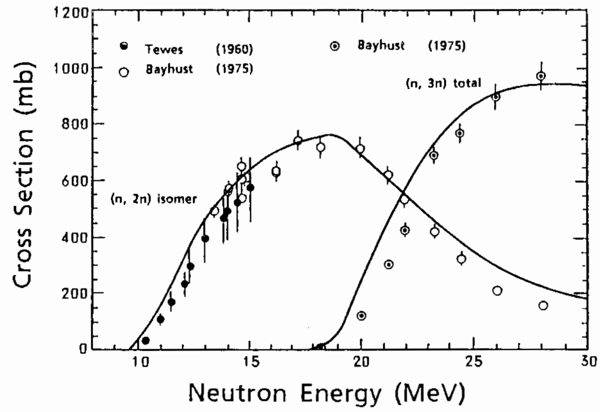

Fig.5 ^{107}Ag(n,2n)^{106m}Ag and ^{107}(n,3n)^{105}Ag Reaction Cross Sections

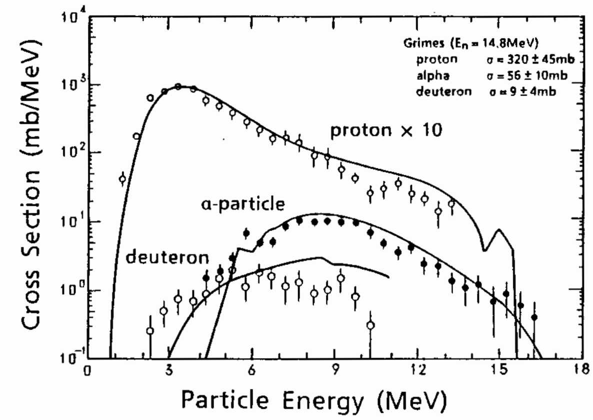

Fig.6 Proton, α-particle, and Deuteron Emission Spectra in Reactions of 15 MeV Neutrons with ^{63}Cu

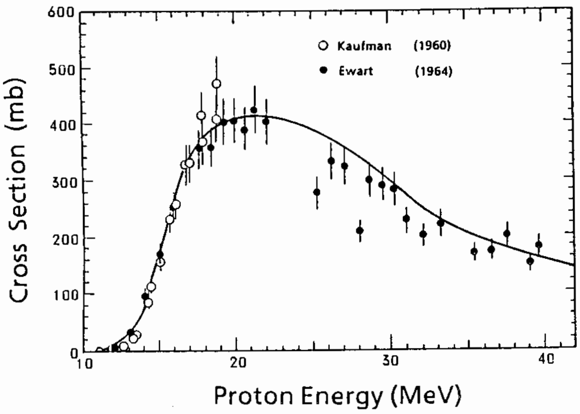

Fig.7 $^{58}Ni(p,2p)^{57}Co$ Reaction Cross Sections

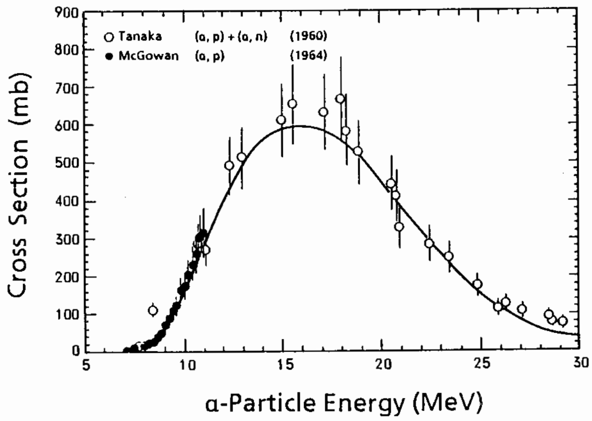

Fig.8 Sum of $^{58}Ni(\alpha,p)^{61}Cu$ and $^{58}Ni(\alpha,n)^{61}Zn$ Reaction Cross Sections

Table 1. Helium Production Cross Sections by 15 MeV Neutrons (mb)

Nuclide	Experiment	Calculation
^{27}Al	143 ± 7	143
^{59}Co	40 ± 3	39.2
^{58}Ni	121 ± 8	120
^{60}Ni	79 ± 5	73.2
^{63}Cu	65 ± 4	64.6
^{65}Cu	17 ± 1	17.8
^{93}Nb	14 ± 1	11.2
^{92}Mo	31 ± 2	27.5
^{94}Mo	22 ± 2	22.1
^{95}Mo	17 ± 1	19.4
^{96}Mo	12 ± 1	10.2
^{97}Mo	10 ± 1	11.6
^{98}Mo	6.7 ± 3.2	6.74
^{100}Mo	3.8 ± 0.3	3.49
Zr	10.1 ± 0.7	18.8
Mo	14 ± 1	14.0
Ag	7.6 ± 0.6	7.83

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