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ESTIMATION OF PARAMETERS IN NUCLEAR MODEL FORMULA FOR NUCLIDES OF STRUCTURAL MATERIALS

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Abstract: Optical model parameters and level density parameters for Hauser-Feshbach model calculations have been estimated systematically for Z = 22 to 28 nuclei by using Bayesian method. The experimental data for the estimation are total, (n,p), (n,α), and (n,2n) cross sections, and energy distribution of proton and α-particles emitted by neutron induced reactions. The prior optical model parameters of neutron, proton, and α-particles are taken from Beccetti-Greenlees', Menet et al.'s, and Huizenga-Igo's values, respectively. The prior level density parameters are taken from Gilbert-Cameron's values. The optical model and level density parameters estimated in the present work have been found to be reasonable comparing with the other works. The cross sections calculated with posterior parameters have been improved more than those done with prior ones.

(Baysian Method, Level density parameter, Optical parameter, V, Cr, Mn, Fe, Co, Ni)

Introduction

Nuclear reaction model calculations have been utilized for nuclear data evaluations, in which the nuclear reaction model parameter should be selected to reproduce available experimental cross sections. Calculated neutron cross sections almost correlate each other because of their competition so that the parameters in the model formula cannot be determined for an only single type of cross sections. The determination is very complicated work.

The optical model and Hauser-Feshbach model calculations are utilized for the nuclear data evaluations. The optical model and level density parameters are essential for these model calculations.

The optical model parameters and level density parameters have been evaluated and compiled in many works. They are shown as systematic variations for the atomic and mass number. They are evaluated to represent simultaneously cross sections and level data in the wide mass range. Their parameters are uncertain for the individual nucleus. The level density parameters have been determined by using level data. They express the level density fairly well. They, however, are uncertain for the precise calculations of cross sections. On the other hand, The optical model and Hauser-Feshbach model are believed to be ambiguous. In order to use these parameters to more precise evaluations, they need to be modified.

The modifications have been performed intuitively by ascertaining qualitatively the reproducibility of calculated cross sections. This conventional procedure is too unsystematic to expect for the determined parameters to reproduce many kinds of reaction cross sections for many target nuclei. The abundant experiences and intuition for nuclear reaction models are required for the determination. In spite of the efforts, it is not guaranteed that ones can fined the optimal parameters.

We have tried to estimate optical model parameters and level density parameters used in spherical optical model and Hauser-Feshbach model and presented elsewhere[1,2,3]. The present work was performed quantitatively by using Bayesian method.

In the present work, ^{51}V, $^{50,52-54}$Cr, ^{55}Mn, $^{54,56-58}$Fe, ^{59}Co, and ^{58,60}Ni were taken as target nuclei. These elements are structural materials of nuclear fission and fusion reactors and the precise evaluations are expected. Since their reaction chains are overlapped, it is difficult to find the parameters reproducing experimental cross sections. Therefore, they are suitable for the application of the present method.

The experimental data are available total, (n,p), (n,α), (n,2n) cross sections, and energy distribution of proton and α-particles emitted by 14.8 MeV neutron induced reactions. The prior optical model parameters of neutron, proton, and α-particles were taken from Beccetti-Greenlees[4], Menet et al.[5], and Huizenga-Igo's[6] values, respectively. The prior level density parameters were taken from Gilbert-Cameron's values. The optical model parameters were estimated within the several percent of prior ones. The overestimation was found in the obtained level density parameters.

Parameter Estimation

A brief description on the method is shown here because of presenting in detail in the previous works[1,2,3].

The posterior parameters are given by

$$p = p_0 + X_0A_0{}^t\Phi^t(\Phi A_0X_0A_0{}^t\Phi^t + V)^{-1}(y - \Phi\theta_0), \quad (1)$$

where the superscripts t and -1 denote transposed and inverse matrix, respectively. The vector p_0 is a set of prior parameters and X_0 covariance matrix of them. The vector y and matrix V are a set of experimental data and covariances, respectively. The vector θ_0 is a set of cross sections calculated in the interval of 2 MeV in the neutron energy range from the about 5 MeV to 20 MeV using prior parameters. The matrix A_0 is the sensitivity of θ_0 to the parameters. The elements of matrix Φ are calculated by spline function.

The computer code ELIESE-3[8] and GNASH[9] was used for the optical model and Hauser-Feshbach model calculations, respectively.

Table I. Experimental Cross Sections Used in the Present Estimation

	^{51}V	^{50}Cr	^{52}Cr	^{53}Cr	^{54}Cr	^{55}Mn	^{54}Fe	^{56}Fe	^{57}Fe	^{58}Fe	^{59}Co	^{58}Ni	^{60}Ni
Total	y		y	y		y					y		y
(n,p)	y		y	y	y	y	y	y	y	y	y	y	y
(n,α)	y	y				y	y				y	y	
(n,2n)		y				y	y	y			y	y	
Proton-Spectrum												y	y
α-Spectrum												y	y

The symbols y, in the table denote the reaction used in the present work.

The prior covariance matrix X_0 was obtained by assuming fractional standard deviation of thirty percent for diagonal elements and correlation coefficient of null for non-diagonal elements.

The experimental data used in the present work are shown in the Table. I.

Result and Discussions

The optical model parameters are shown in the Table II. The level density parameters, *a*, are done in Figures 1, and 2. The prior cross sections:, cross sections calculated with prior parameters, and posterior cross sections are compared with the experimental data in Figures 3 to 9 as the examples of the calculated cross sections. The references of the experiments are not shown because of a limited space.

The posterior optical parameters are shown in Table II. Those of neutron were underestimated relative to prior ones, except for the radius parameters of real potential. These underestimations were caused by the measured total cross sections smaller than those predicted by the prior parameters. The total cross sections increase with these four neutron optical parameters estimated in the present work. As shown in Figure 3, the total cross sections decrease with the changes of these parameters. The underestimations of neutron optical parameters are resulted from the prior total cross sections different from experimental data. The miner changes are found in the optical parameters for proton and α-particle.

The *a* for Mn, Fe, Co, and Ni almost became larger than the prior values. They are those of residual nuclei formed through Fe, Co, Ni(n,x) reactions. These prior cross sections almost are discrepant from their experimental data. The ^{56}Fe(n,p) cross sections are shown in Figures 4. In the present estimation, the larger *a* for residual nuclei of (n,n') and (n,p) reactions resulted from the decreasing (n,p) cross sections.

On the contrary, the *a* for Sc, Ti, V, and Cr decreased. They are the parameters of residual nuclei formed through V, Cr, and Mn(n,x) reactions. These underestimations almost were caused by the estimation of level density parameters for ^{54}Fe reactions. As the typical description, the underestimations of *a* for ^{50,52}Cr, ^{49}V, and ^{47}Ti are explained as follows.

The *a* for ^{54}Fe similar to prior value resulted from the estimation of *a* for ^{58}Ni reactions. The ^{54}Fe(n,p) prior cross sections are larger than the experimental data as shown in Figure 5. The a for ^{54}Mn, which is the residual nucleus of ^{54}Fe(n,p), decreased to obtain small (n,p) cross sections. The decrease of *a* for ^{54}Mn ,however, caused the increase of (n,α) and (n,2n) cross sections. The ^{54}Fe(n,α)^{51}Cr and (n,2n)^{53}Fe prior cross sections, however, agree with experimental data. The *a* for ^{51}Cr and ^{53}Fe, therefore, decrease. To decrease ^{54}Fe(n,p) cross sections, the *a* of ^{53}Mn, which is a residual nucleus of (n,pn) reaction, increased. This increase caused the decrease of (n,2n) cross sections. Since the thresholed of ^{54}Fe(n,2n) reaction is higher than that of ^{54}Fe(n,np), the sensitivity of (n,2n) cross sections to ^{53}Fe is

Table II. Optical Model Parameters for Neutron, Proton, and α-particle. The numerals enclosed parentesis are fractional standard deviations: square roots of posterior variances

	Radius				Potential			
	Real		Imaginary		Real		Imaginary	
	Prior	Posterior	Prior	Posterior	Prior	Posterior	Prior	Posterior
Neutron	1.17	1.17 (1.0%)	1.26	1.16 (1.5%)	56.30	53.69 (1.2%)	13.00	9.84 (2.1%)
Proton	1.16	1.18 (2.3%)	1.37	1.34 (2.2%)	49.90	48.46 (4.2%)	4.20	4.19 (5.0%)
α-particle	1.17	1.18 (1.0%)	1.17	1.39 (3.0%)	50.00	48.91 (5.0%)	10.26	10.45 (4.9%)

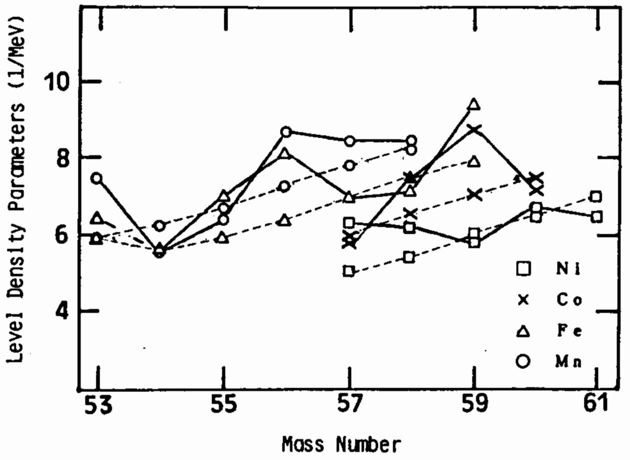

Figure 1 Comparisons of level density parameters for Mn, Fe, Co, and Ni. The dashed and solid lines indicate prior and posterior parameters, respectively.

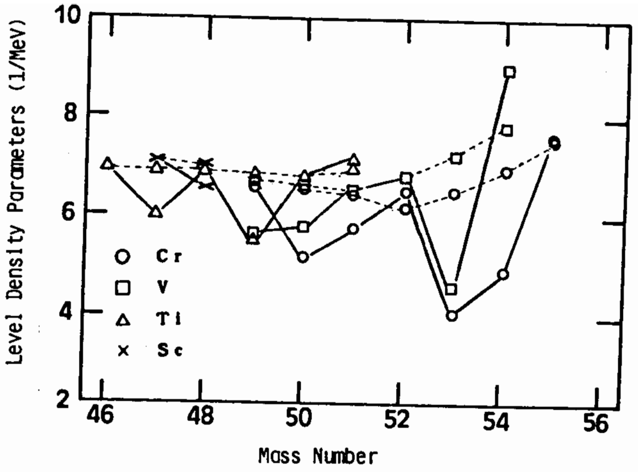

Figure 2 Comparisons of level density parameters for Sc, TI, V, and Cr. The dashed and solid lines indicate prior and posterior parameters, respectively.

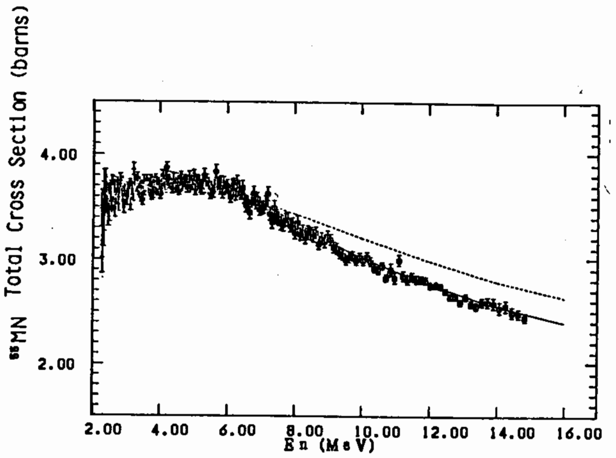

Figure 3 Comparisons of calculated and experimental ^{55}Mn total cross sections. Dashed and solid lines indicate the cross sections calculated using prior and posterior parameters, respectively.

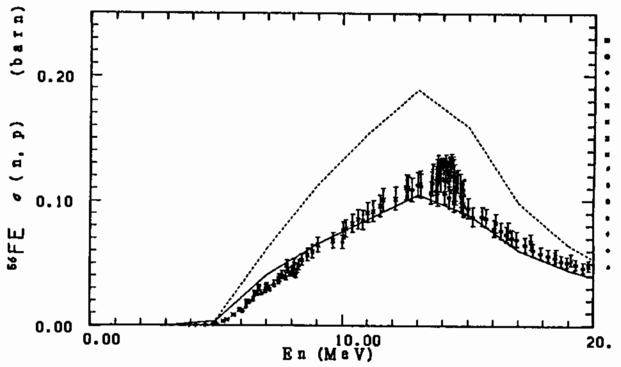

Figure 4 Comparisons of calculated and experimental ^{56}Fe(n,p) cross sections. Dashed and solid lines indicate the cross sections calculated using prior and posterior parameters, respectively.

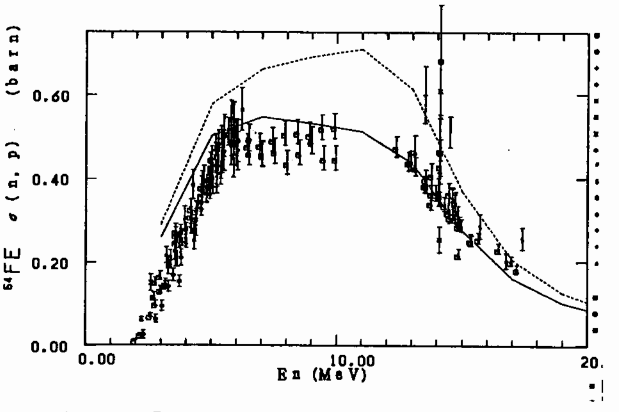

Figure 5 Comparisons of calculated and experimental ^{54}Fe(n,p) cross sections. Dashed and solid lines indicate the cross sections calculated using prior and posterior parameters, respectively.

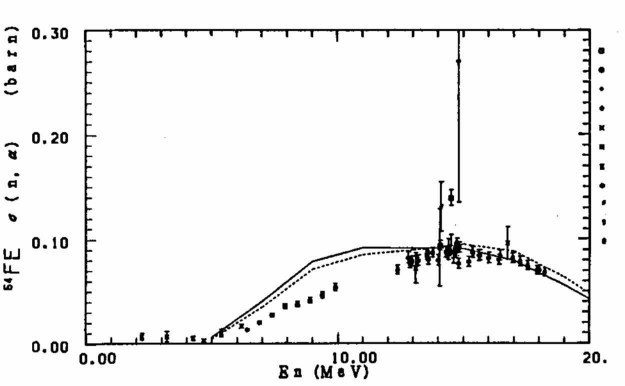

Figure 6 Comparisons of calculated and experimental ^{54}Fe(n, α) cross sections. Dashed and solid lines indicate the cross sections calculated using prior and posterior parameters, respectively.

more weak than that to ^{54}Mn. Consequently, the a of ^{53}Fe increased and that of ^{50}Cr, which is a residual nucleus of (n,nα), decreased to obtain larger (n,2n) cross sections. The ^{50}Cr is a residual nucleus of ^{50}Cr(n,n') reaction. The decrease of a for ^{50}Cr caused the weak neutron emission. Therefore, its decrease gave the larger ^{50}Cr(n,2n)^{49}Cr and the smaller ^{50}Cr(n,α)^{47}Ti cross sections. The (n,2n) and (n,α) prior cross sections agree with the experimental data as shown in Figures 8, and 9. The a of ^{49}Cr increased and that of ^{47}Ti decreased.

Conclusion

In the present work, the optical model parameters and level density parameters for Sc to Ni were estimated systematically by applying Bayesian method. The optical model parameters were estimated within the several percent of prior ones. The overestimations were observed in the estimated level density parameters for Mn, Fe, Co, and Ni. The underestimations were done in the level density parameters for Sc, Ti, V, Cr. The estimated parameters improved the calculations of cross sections and energy spectra. It was verified that Bayesian method can be applied to estimate nuclear reaction model parameters.

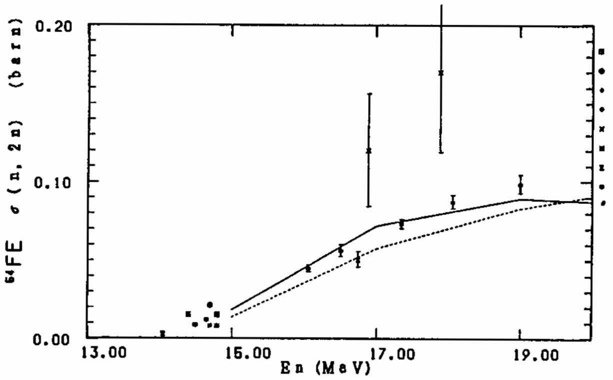

Figure 7 Comparisons of calculated and experimental ^{54}Fe(n,2n) cross sections. Dashed and solid lines indicate the cross sections calculated using prior and posterior parameters, respectively.

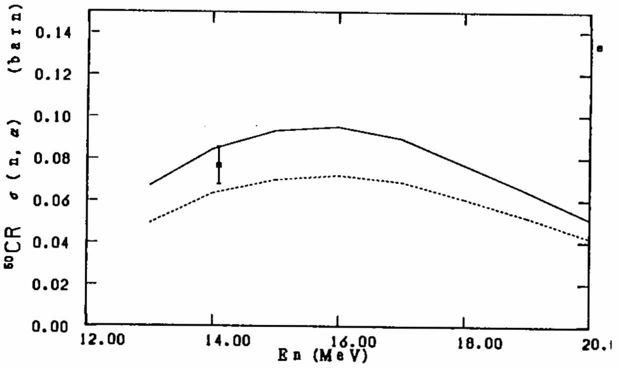

Figure 8 Comparisons of calculated and experimental ^{50}Cr(n,α) cross sections. Dashed and solid lines indicate the cross sections calculated using prior and posterior parameters, respectively.

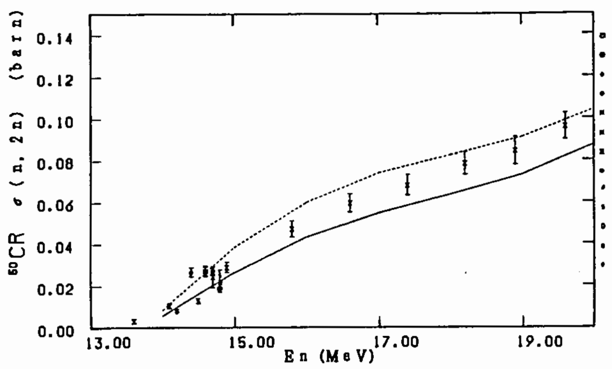

Figure 9 Comparisons of calculated and experimental ^{50}Cr(n,2n) cross sections. Dashed and solid lines indicate the cross sections calculated using prior and posterior parameters, respectively.

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