

## **Evaluation of Silicon Neutron Resonance Parameters in the Energy Range Thermal to 1800 keV**

H. Derrien, L. C. Leal, K. H. Guber, and N. M. Larson  
Oak Ridge National Laboratory  
P.O. Box 2008, MS 6171  
Oak Ridge TN 37831-6171  
E-mail: [derrienh@ornl.gov](mailto:derrienh@ornl.gov)

### **ABSTRACT**

Because silicon is a major constituent of concrete and soil, neutron and gamma-ray information on silicon is important for reactor shielding and criticality safety calculations. Therefore, much effort was put into the ENDF/B-VI evaluation for the three stable isotopes of silicon. The neutron capture cross section of natural silicon was recently measured at the Oak Ridge Electron Linear Accelerator (ORELA) in the energy range 1 to 700 keV. Using the ENDF/B-VI evaluation for initial values, a new evaluation of the resonance parameters was performed by adding the results of the ORELA capture measurements to the experimental data base. The computer code SAMMY was used for the analysis of the experimental data; the new version of SAMMY allows accurate calculations of the self-shielding and multiple scattering effects in the capture measurements. The accuracy of the radiative capture widths of the resonances was improved by this analysis. Accurate values of the s-, p-, and d-wave neutron strength functions were also obtained. Although the resonance capture component of the present evaluation is 2 to 3 times smaller than that in ENDF/B-VI, the total capture cross section is much larger, at least in the energy range above 250 keV, because the direct capture component contributes values of the same order of magnitude as the resonance component. The direct component was not taken into account in the ENDF/B-VI evaluation and was calculated for the first time in the present evaluation.

# **Evaluation of Silicon Neutron Resonance Parameters in the Energy Range Thermal to 1800 keV**

H. Derrien, L. C. Leal, K. H. Guber, and N. M. Larson  
Oak Ridge National Laboratory  
P.O. Box 2008, MS 6171  
Oak Ridge TN 37831-6171  
E-mail: [derrienh@ornl.gov](mailto:derrienh@ornl.gov)

## **INTRODUCTION**

The neutron resonance parameters of the silicon isotopes have been obtained from a SAMMY<sup>(1)</sup> analysis of high-resolution neutron transmission and neutron capture cross-section measurements in the energy range 0 to 1850 keV. This evaluation continues the work performed by Hetrick et al.<sup>(2)</sup> for the ENDF/B-VI Evaluated Neutron Data File by adding to the experimental data base the results of a recent neutron capture measurement performed at the Oak Ridge Electron Linear Accelerator (ORELA) by Guber et al.<sup>(3)</sup> In the present paper, the experimental data base is described. The results of the new SAMMY evaluation are given, and the cross sections calculated with the resonance parameters are compared with the experimental data and with ENDF/B-VI cross sections. Some properties of the resonance parameters are also presented.

## **EXPERIMENTAL DATA BASE**

The experimental data base consisted mainly of results of neutron transmission and neutron capture measurements performed by using ORELA as a neutron pulsed source. Transmission measurement of a sample of thickness 0.666 at/b of natural silicon was performed by Perey et al.<sup>(4)</sup> in 1972 at the ORELA 47-m flight path in the neutron energy range 200 to 1800 keV. Transmission measurements of a sample of 0.0376 at/b of natural silicon were performed by

Larson et al.<sup>(5)</sup> in 1976 at the ORELA 200-m flight path in the neutron energy range 5 eV to 700 keV. Transmission measurements of a sample of thickness 0.3472 at/b of natural silicon were performed by Harvey et al.<sup>(6)</sup> in 1993 at the ORELA 200-m flight path in the energy range 300 eV to 1800 keV. In order to identify the <sup>29</sup>Si and <sup>30</sup>Si resonances in the natural sample data, neutron transmission measurements of enriched <sup>29</sup>Si and <sup>30</sup>Si oxide samples were performed by Harvey et al.<sup>(7)</sup> in 1983 at the ORELA 80 m-flight path in the energy range 10 keV to 1 MeV. Neutron capture cross sections were measured by Guber et al.<sup>(8)</sup> in 2000 at the 40-m ORELA flight path in the energy range 1 to 700 keV.

Comparison of the average neutron effective total cross sections obtained from the transmission data shows that the Harvey and Larson data agree within 1%; the cross sections obtained from the Perey natural sample transmission are on average about 2.5% smaller. The discrepancies, which are compatible with the experimental errors, are corrected in the SAMMY analysis by normalization and background adjustments.

## SAMMY ANALYSIS OF THE EXPERIMENTAL DATA

The computer code SAMMY allows a sequential analysis of the experimental data by using Bayes' method, in which the parameters covariance matrix calculated in one sequence is used as input in the next sequence. Consistency among the several experiments being analyzed is obtained by properly treating experimental uncertainties (the systematic errors for each data set). This approach allows all experimental data to be described by a single set of resonance parameters.

The spin and parity  $I^\pi$  of the nuclei  $^{28}\text{Si}$ ,  $^{29}\text{Si}$ , and  $^{30}\text{Si}$  are  $0^+$ ,  $\frac{1}{2}^+$ , and  $0^+$ , respectively. The spin and parity of the resonances excited in the silicon compound nuclei by the neutron of angular momentum  $l = 0, 1, 2,$  and  $3$  are given in Table 1. In running SAMMY, resonances are assigned to a particular spin group, each of which is characterized by spin and parity; the spin group contains the interfering resonances of the R-matrix formalism. There is one channel spin ( $s = 1/2$ ) for  $^{28}\text{Si}$  and  $^{30}\text{Si}$  and two channel spins ( $s = 0$  and  $1$ ) for  $^{29}\text{Si}$ . For a physically sound calculation of the cross sections of  $^{29}\text{Si}$ , one should use two neutron entrance channels for the  $l > 0$  resonances. However, to conform to the old ENDF/B-VI format, only one neutron entrance channel was used for all the resonances, the groups of resonances being defined according to the same value of  $l, s,$  and  $J^\pi$ . [It should be noted that the new ENDF/B-VII R-matrix limited (LRF = 7) format would permit proper treatment of the two entrance channels. However, that format was not yet available when this work was undertaken.]

The prior values of the resonance parameters were those obtained in the previous evaluation by Hetrick et al. for ENDF/B-VI. The radiative capture widths were obtained primarily from the Brookhaven National Laboratory (BNL) recommended data.<sup>(8)</sup> In the present evaluation, the Guber et al. experimental capture data were analyzed in the energy range 1 to 700 keV. Self-shielding and multiple scattering effects were included in the SAMMY calculations. At the beginning of the analysis, the fit of the capture data was performed separately for each individual resonance appearing in the experimental data. Some resonances with very small neutron width values were not seen in the transmission data; these resonances are at the energies 16.672, 31.751, 70.840, 86.993, 147.681, 298.800, 369.79 and 399.621 keV. All the resonances were assigned to  $^{28}\text{Si}$ , except for that at 369.79 keV, which was assigned to  $^{29}\text{Si}$ .

Examples of SAMMY fits of the experimental data are given in Figs. 1 to 3. Figure 1 shows the result of the fit of the transmission data in the energy range 400 to 700 keV; the upper, middle, and lower curves represent the data of Larson et al., Harvey et al., and Perey et al., respectively. Figure 2 shows the results of the fit of the transmission data in the energy range 700 to 1100 keV; the upper and lower curves represent the data of Harvey et al., and Perey et al., respectively. Figure 3 shows the results of the SAMMY fits of the experimental capture cross section of Guber et al. in the energy range 360 to 700 keV. In each figure the solid lines represent the cross section calculated by SAMMY from the final values for the resonance parameters.

## RESONANCE PARAMETERS

A table of the resonance parameters is given in Ref. 9; the parameters are also available in the ENDF/B-VI nuclear data file. There are 50  $^{28}\text{Si}$  resonances in the energy range 0 to 1850 keV. The corresponding neutron strength functions are  $S_0 = (0.79 \pm 0.45) \times 10^{-4}$ ,  $S_1 = (1.03 \pm 0.40) \times 10^{-4}$ , and  $S_2 = (1.37 \pm 0.40) \times 10^{-4}$  for the angular momenta  $l = 0$ ,  $l = 1$ , and  $l = 2$ , respectively. The values of  $S_1$  and  $S_2$  could be questioned, because the spin assignment of the resonances was made in order to obtain the best fit to the experimental transmission data and is probably not the unique solution. However, they do not contradict the values that are found for other nuclei in the same mass region.

One important result of the analysis is the improvement of the accuracy of the neutron capture widths of the resonances in the energy range up to 700 keV. The  $^{28}\text{Si}$  average capture widths obtained in the present work are 1.634 eV for the s-wave resonances, 1.409 eV for the

p-wave resonances, and 0.550 eV for the d-wave resonances. Each of these average capture widths is much smaller than the average value of 3.6 eV for the combined s-, p-, and d-wave resonances recommended by Mughabghab<sup>(8)</sup>, mainly from the experimental data of Boldeman et al.<sup>(10)</sup> The average value of the resonant component of the capture cross section in the energy range 700 to 1800 keV is 0.484 mb when calculated using the Mughabghab capture widths and only 0.171 mb using the Mughabghab values normalized to values consistent with the present evaluation.

It was expected that the analysis of the two SiO<sub>2</sub> transmission data with samples enriched to 95.3% of <sup>29</sup>Si and 95.6% of <sup>30</sup>Si, respectively, could give the resonance parameters of the corresponding isotopes. Unfortunately, the experimental data were not sufficiently accurate (poor resolution and poor statistical accuracy) to allow identification of all the resonances and a good evaluation of the neutron widths. Moreover, the strong resonances of oxygen at 434 and 1000 keV impeded the analysis of a large part of the data. However, the analysis of the Guber et al. capture data allowed the accurate evaluation of the capture area of five p-wave resonances of <sup>29</sup>Si at the energies 15.29, 38.83, 159.88, 184.59, and 389.16 keV and of three p-waves resonances of <sup>30</sup>Si at the energies 49.81, 15.14, and 190.23 keV. The average values of the capture widths of these resonances are 2.93 and 0.37 eV, respectively, for <sup>29</sup>Si and <sup>30</sup>Si. These results were used in another publication<sup>(11)</sup> in stellar models to predict the abundance of elements in the solar system.

## RESONANT CAPTURE AND DIRECT CAPTURE

The direct capture component was recently calculated by Rauscher et al.<sup>(12)</sup> The results of this calculation have shown that the direct capture cross section could be the same order of magnitude as the resonant component. The average capture cross section of natural silicon calculated from the resonance parameters is compared with the direct capture component and with the ENDF/B-VI values in Table 2. Taking into account the direct capture component, the evaluated total capture cross section will be much larger than in the current evaluated data files. Although the resonant component of the present evaluation is 2 to 3 times smaller than in ENDF/B-VI, the total capture is much larger, at least in the energy ranges above 250 keV.

## CONCLUSION

The neutron resonance parameters of silicon isotopes were evaluated in the neutron energy range up to the neutron inelastic scattering threshold. Compared with the previous ENDF/B-VI evaluation, better accuracy was achieved by adding to the experimental data base the results of the neutron capture measurement performed recently at ORELA. Accurate values of the capture widths were obtained from the SAMMY analysis of the data in the energy range 1 to 700 keV, allowing the determination of reliable values of the average capture widths of the s-, p- and d-waves resonances, at least for  $^{28}\text{Si}$ , suitable for the normalization of the calculated resonance capture cross section in the resolved resonance region above 700 keV. Since the average capture cross section of natural silicon between the resonances is small (less than 1 mb) and could not be measured with good accuracy due to the uncertainties in the experimental background and in other experimental effects, it is important to know the extent of the direct capture component compared with that of the average resonant component. Actually the direct average component

is larger than the average resonant component in the energy ranges above 250 keV, and the resulting average total capture cross sections are significantly larger than those in ENDF/B-VI. The results of the present evaluation were adopted in a new release of ENDF/B-VI; the direct component was added to file 3 in ENDF/B-VI format.

## REFERENCES

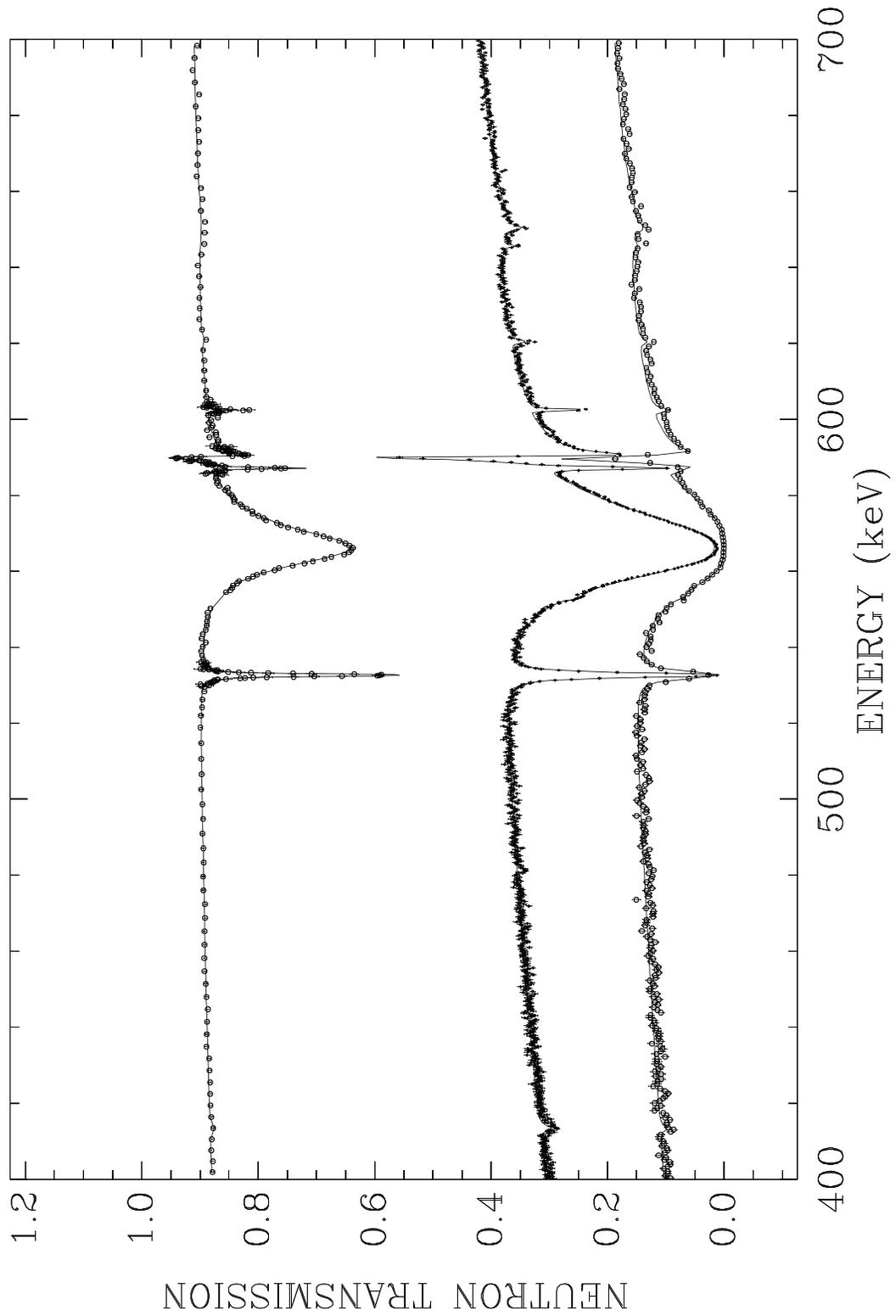
1. Larson, N. M., *Updated user's guide for SAMMY: Multilevel R-matrix fits to neutron data using Bayes' equations*, ORNL/TM-9179/R6 (July 2003).
2. Hetrick, D. M., Larson, D. C., Larson, N. M., Leal, L. C., and Epperson, S. J., *Evaluation of <sup>28, 29, 30</sup>Si Neutron Induced Cross Sections for ENDF/B-VI*, ORNL/TM-11825 (1997).
3. Guber, K. H., Leal, L. C., Sayer, R. O., Spencer, R. R., Koehler, P. E., Valentine, T. E., Derrien, H., and Harvey, J. H., *Neutron Cross Section Measurements for Light Elements at ORELA and their Application in Nuclear Criticality*, Nuclear Data for Science and Technology, Tsukuda (Japan), Oct. 7–12, 2001.
4. Perey, F. G., Love, T. A., and Kinney, W. E., *A Test of Neutron Total Cross Section Evaluations from 0.2 to 20 MeV for C, O, Al, Si, Ca, Fe and SiO<sub>2</sub>*, ORNL-4823, ENDF-178 (1972).
5. Larson, D. C., Johnson, C. H., Harvey, J. A., and Hill, N. W., *Measurements of the Neutron Total Cross Section of Silicon from 5 eV to 730 keV*, ORNL/TM-5618 (1976).
6. Harvey, J. A., private communication (unpublished data taken in 1993).
7. Harvey, J. A., Good, W. M., Carlton, R. F., Cartel, B., MacGrory, J. B., and Mughabghab, S. F., *Phys. Rev.* **C28**, 24 (1983).
8. Mughabghab, S. F., Divadeenam, M., Holden, N. E. *Neutron Cross Sections, Vol. 1, Neutron Resonance Parameters and Thermal Cross Sections, Part. A: Z=1-60*, Academic Press, NY (1981).
9. Derrien, H., Leal, L. C., Guber, K. H., Valentine, T. E., Larson, N. M., and Rauscher, T., *Evaluation of Silicon Resonance Parameters in the energy range thermal to 1800 keV*, ORNL/TM-2001/271 (2002).
10. Boldeman, J. W., Allen, B. J., Musgrove, A. R., and Macklin, R. L., *Nucl. Phys.* **A252**, 62 (1975).
11. Guber, K. H., Derrien, H., Valentine, T. E., Leal, L. C., Sayer, R. O., Rauscher, T., Koehler, P., Gallino, E. R., *Maxwellian Average Neutron Capture Cross Sections for Silicon and their impact on the origin of Presolar Mainstream SiC Grains*, *Phys. Rev. C* **67**, 062801(R) (2003).
12. Rauscher, T., private communication to K. H. Guber.

**Table 1. Neutron channel spin  $s$  and resonance spin  $J^\pi$  for angular momentum  $l = 0, 1, 2, 3$ .**

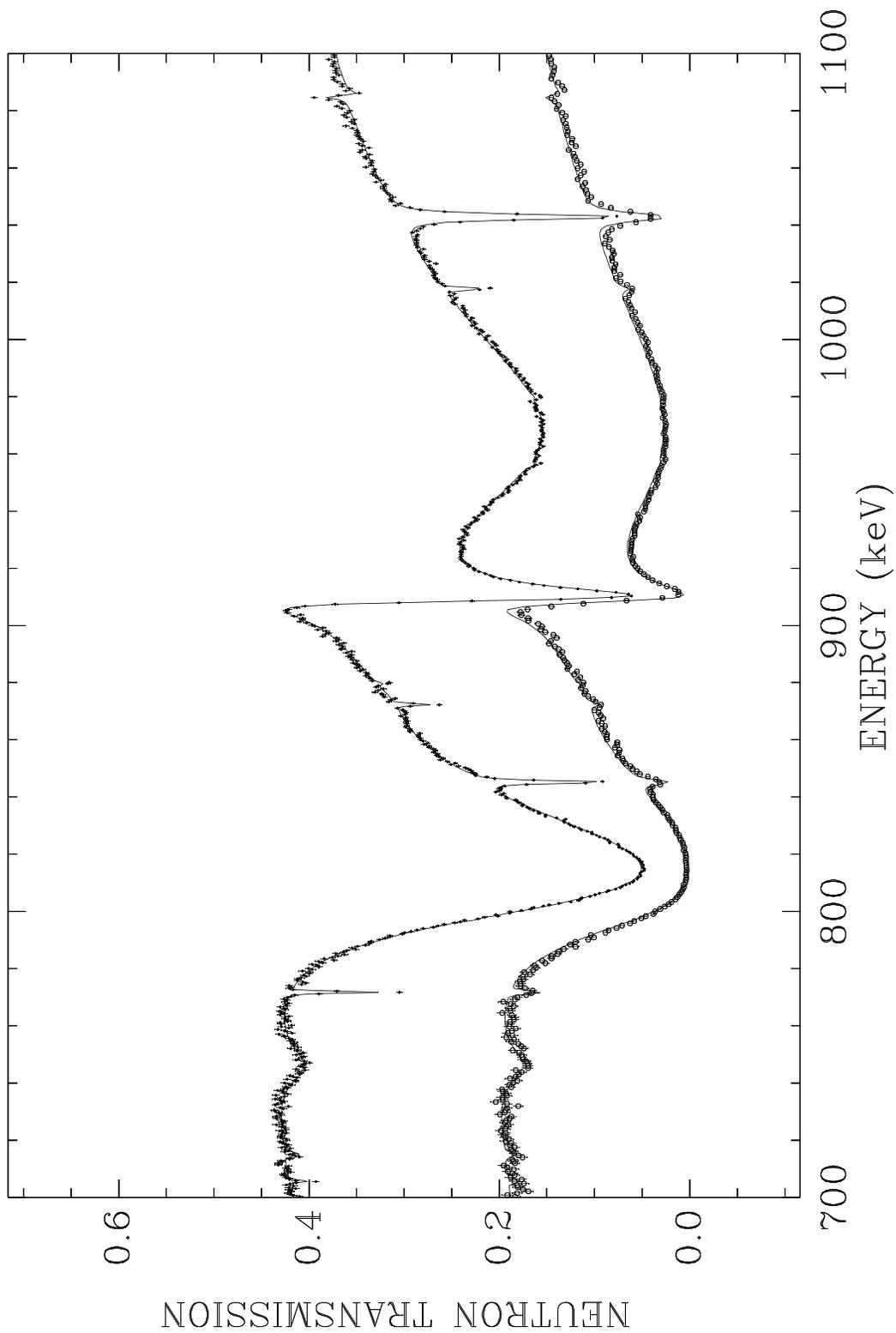
	$l$	$s = I \pm 1/2$	$J^\pi$
$^{28}\text{Si} (0^+)$ and $^{30}\text{Si} (0^+)$	0	1/2	1/2 <sup>+</sup>
	1	1/2	1/2 <sup>-</sup> 3/2 <sup>-</sup>
	2	1/2	3/2 <sup>+</sup> 5/2 <sup>+</sup>
	3	1/2	5/2 <sup>-</sup> 7/2 <sup>-</sup>
$^{29}\text{Si} (1/2^+)$	0	0	0 <sup>+</sup>
	1	0	1 <sup>-</sup>
	1	1	0 <sup>-</sup> 1 <sup>-</sup> 2 <sup>-</sup>
	2	0	2 <sup>+</sup>
	2	1	1 <sup>+</sup> 2 <sup>+</sup> 3 <sup>+</sup>
	3	0	3 <sup>-</sup>
	3	1	2 <sup>-</sup> 3 <sup>-</sup> 4 <sup>-</sup>

**Table 2. Average capture cross section of natural silicon**

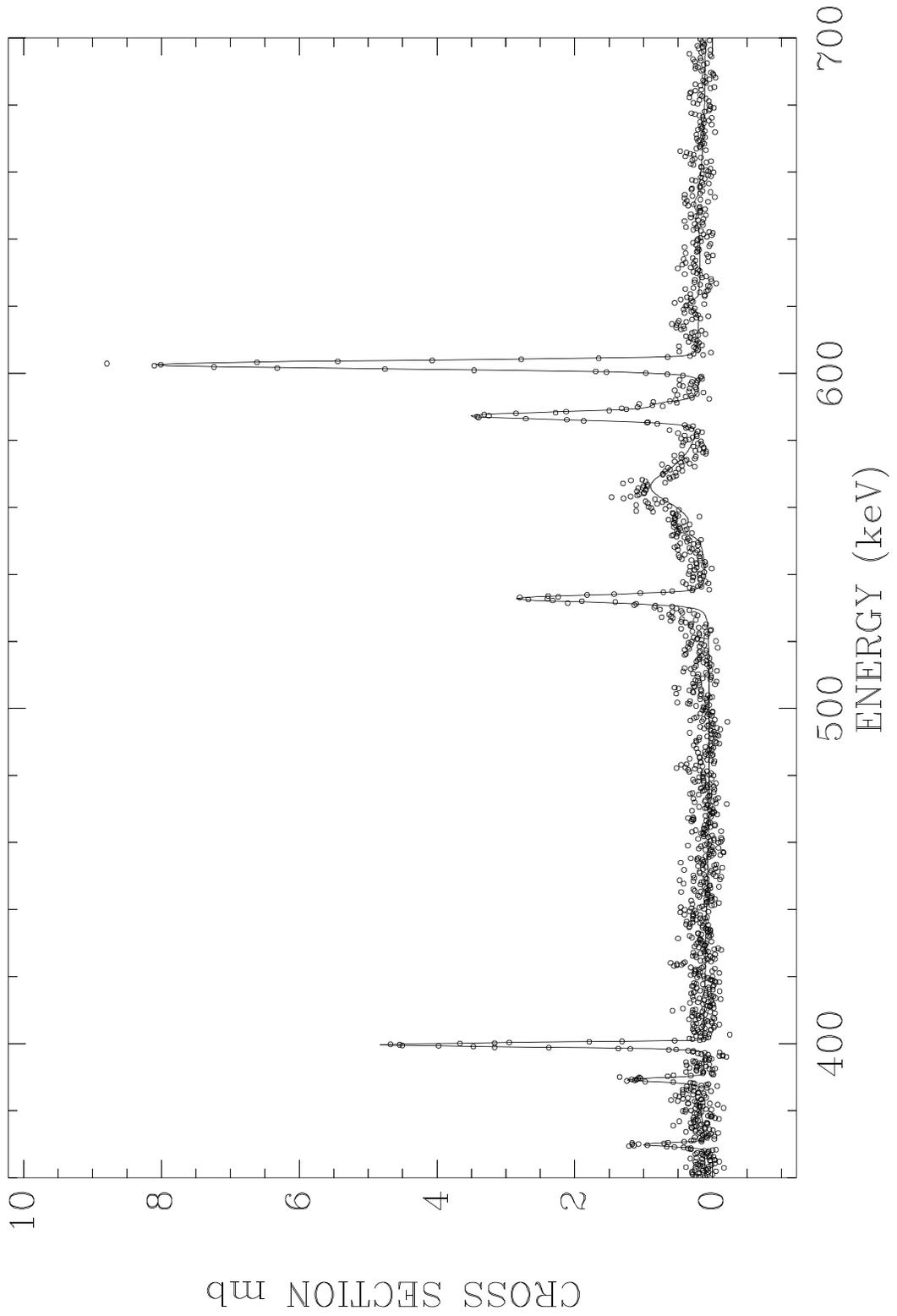
Energy Range (keV)	Direct (mb)	Resonance (mb)		Total (mb)
		Present	ENDF/B-VI	
1–250	0.31	0.978	2.172	$1.29 \pm 0.18$
250–450	0.50	0.212	0.532	$0.71 \pm 0.29$
450–700	0.64	0.326	0.875	$0.96 \pm 0.37$
700–1100	0.79	0.249	0.663	$1.04 \pm 0.47$
1100–1450	0.95	0.142	0.336	$1.09 \pm 0.55$
1450–1750	1.07	0.118	0.432	$1.18 \pm 0.62$



**Fig. 1.** Natural silicon neutron transmissions in the energy range 400 to 700 keV. The experiment data are from Larson, et al. (upper curve), Harvey et al. (middle curve), and Perey et. al (lower curve)



**Fig. 2. Natural silicon neutron transmission in the energy range 700 to 1100 keV. The experimental data are from Harvey et al. (upper curve), and from Perey et al. (lower curve)**



**Fig. 3. Natural silicon neutron capture cross section in the energy range 360 to 700 keV. The experimental data are from Guber et. al.**