ELSEVIER

Journal of Nuclear Materials 277 (2000) 346–350

journal of nuclear materials

www.elsevier.nl/locate/jnucmat

Slow neutron total cross-section of Al6061 at low temperatures

J.R. Granada*,[1]

Comisíon Nacional de Energía Atómica, Neutron Physics Division, Centro Atomico Bariloche, 8400 S.C. de Barlioche (RN), Argentina

Received 18 September 1998; accepted 21 June 1999

Abstract

This work presents evaluations of the total cross-section and its components, corresponding to the aluminum based alloy Al6061 at a few temperatures of interest, over the neutron energy range from 10^{-5} to 10 eV. A practical procedure for subtraction of the cold source's vessel contribution to the measured emerging spectra is discussed, and data given for the specific cases where Al6061 is used as the vessel material. © 2000 Published by Elsevier Science B.V. All rights reserved.

PACS: 28.20.Cz; 28.41.Qb; 81.05.Bx

1. Introduction

The Aluminum alloy Al6061 is extensively used in many applications, where its properties of strength, weldability, corrosion resistance, etc., are needed. This alloy is of particular importance in the nuclear industry, due to its capacity to withstand intense radiation fields without a significant degradation of its mechanical properties. Besides, the relatively small thermal neutron absorption cross-section of its main components makes the Al6061 a convenient material for different structural elements of neutron sources.

Most existing and projected cold neutron sources therefore use Al alloys as the cell material, and this demands a proper description of its neutronic properties as part of the required information in their design stages [1]. Some of that information is given in the present report, where the evaluation of the total cross-section of Al6061 is presented over the full thermal and subthermal neutron energy ranges and for a few temperatures of interest. Data on a related alloy, AlMg3, have been produced some time ago [2].

2. Calculations

The behaviour of the total cross-section as a function of the sample characteristics and the incident neutron energy is a basic magnitude which can be predicted with a high degree of accuracy for polycrystalline solids. The present calculation was performed using the CRIPO computer code [3], which is based on a third-order mass expansion and the Debye model to represent the frequency spectrum of the solid. All components of the total cross-section are evaluated by the program according to

$$\sigma_T = \sigma_{abs} + \sigma_{el,coh} + \sigma_{el,inc} + \sigma_{inel,coh} + \sigma_{inel,inc}, \quad (1)$$

where the absorption cross-section is assumed to follow a '$1/v$' behaviour at thermal neutron energies. The incoherent approximation is used for the evaluation of the inelastic coherent component, $\sigma_{inel,coh}$, bearing in mind that the multiphonon terms which dominate the cross-section at high energies do not contribute significantly to the interference effects [4]. The situation at low energies is a more subtle matter, but nonetheless this approximation is still a good one in most cases. On the other hand, the elastic components, coherent ($\sigma_{el,coh}$) and incoherent ($\sigma_{el,inc}$), are evaluated using their exact expressions and therefore no approximation is made on them. A complete description of the equations related to each component in (1) can be found in Ref. [5]. The neutron–

* Fax: +54-2944 445 299.

E-mail address: granada@cab.cnea.gov.ar (J.R. Granada).

[1] Also at CONICET, Argentina.

PII: S0022-3115(99)00156-7

electron interaction [6] is also taken into account within CRIPO to determine the value of the energy-dependent coherent scattering length b_c [7].

The input data set required for the evaluation includes:

1. the 'nuclear' constants σ_c, σ_i, and σ_{abs}(2200 m/s);
2. crystal structure and lattice parameters;
3. sample temperature;
4. Debye temperature;
5. (effective) mass of the (average) constituents atoms.

In the case of an alloy, formed by several elements, each in concentration c_k and characterized by scattering length $b_c^k[\sigma_c^k = 4\pi(b_c^k)^2]$ and incoherent cross-section ${\sigma_i}^k$, the values of the nuclear constants are calculated as

$$b_c = \sum c_k b_c^k, \tag{2a}$$

$$\sigma_c = 4\pi\Big(\sum c_k b_c^k\Big)^2, \tag{2b}$$

$$\sigma_i = \sum c_k(\sigma_i^k + \sigma_c^k) - \sigma_c, \tag{2c}$$

$$\sigma_{abs} = \sum c_k \sigma_{abs}^k. \tag{2d}$$

Also, if the constituents atoms have masses M_k, the effective mass (from the *neutronic* point of view) M of the alloy is determined by the free-atom condition:

$$(\sigma_c + \sigma_i)/(1 + 1/M)^2 = \sum c_k[(\sigma_i^k + \sigma_c^k)/(1 + 1/M_k)^2]. \tag{3}$$

Table 1 summarizes all the required quantities corresponding to the Al6061 alloy [8], with the following composition:

$$1.0\ \text{Mg},\quad 0.6\ \text{Si},\quad 0.3\ \text{Cu},\quad 0.2\ \text{Cr}. \tag{4}$$

The nuclear constants ${b_c}^k$, ${\sigma_c}^k$, ${\sigma_i}^k$ and σ_{abs}^k were taken from Refs. [9–11], whereas the values of the M_k's were taken from [12]. According to the formulas (2) and (3), the following set of effective quantities were obtained for the Al6061 alloy:

$$\begin{aligned} b_c &= 3.4855\ \text{fm},\\ \sigma_c &= 1.527\ \text{b},\\ \sigma_i &= 0.028\ \text{b},\\ \sigma_{abs} &= 0.246\ \text{b},\\ M &= 27.07\ \text{amu}. \end{aligned} \tag{5}$$

The phase diagram of Al–Mg alloys [13] indicates that the elements listed above, (4), are in solid solution in the Al matrix with a crystal structure *fcc*. As far as the lattice parameter a is concerned, its value was calculated from the density of the material at a given temperature. For example, in the case of pure Al, the value $\rho = 2.6989$ g/cm^3 (at 20°C) from [8] was used together with the atomic weight 26.981538 amu from [12], to obtain $a = 0.40494$ nm, in very good agreement with the values 0.40495 nm quoted in [12] and 0.404958 nm for a at 25°C given in [8].

The density of Al6061 at 20°C is $\rho = 2.70$ g/cm^3, according to [8]. However, the values given in [13] were used for the density change (%) in pure Al per addition of 0.10 wt% of the elements in the alloy, to get

$$\rho(\text{Al6061}) = 2.7047\text{g/cm}^3 \quad (\text{at } 20^\circ\text{C}) \tag{6}$$

and from this,

$$a(\text{Al6061}) = 0.40535\ \text{nm} \quad (\text{at } 20^\circ\text{C}). \tag{7}$$

To evaluate the change in the lattice parameter as a function of temperature, the thermal expansion coefficient must be known. This magnitude is itself temperature dependent. Values of the linear expansion coefficient α for pure Al taken from [8] are represented in Fig. 1, together with a polynomial fit on them. Each point on this curve should be taken as the average value of the coefficient between 20°C and the temperature that defines the range such that its centre is at the temperature corresponding to the selected point. For example, the value $\alpha = 21\times10^{-6}$ C^{-1} at $T = -40$°C is the average coefficient in the range between −100°C and 20°C.

With that information, the following results were obtained for the low temperatures of interest:

$$\begin{aligned} &\underline{100\ \text{K}:} \quad a = 0.40385\ \text{nm},\quad \rho = 2.7207\ \text{g/cm}^3,\\ &\underline{20\ \text{K}:} \quad a = 0.40377\ \text{nm},\quad \rho = 2.7224\ \text{g/cm}^3. \end{aligned} \tag{8}$$

Table 1
Values of the magnitudes required for the cross-section calculations

Element	c_k (%)	${b_c}^k$ (fm)	${\sigma_c}^k$ (b)	${\sigma_i}^k$ (b)	σ_{abs}^k (b)	M_k (au)
Al	97.9	3.449	1.495	0.011	0.231	26.982
Mg	1.0	5.375	3.631	0.049	0.063	24.312
Si	0.6	4.149	2.163	0.010	0.171	28.086
Cu	0.3	7.689	7.429	0.30	3.79	63.546
Cr	0.2	3.635	1.660	1.83	3.25	51.996
Alloy	100	3.486	1.527	0.028	0.246	27.070

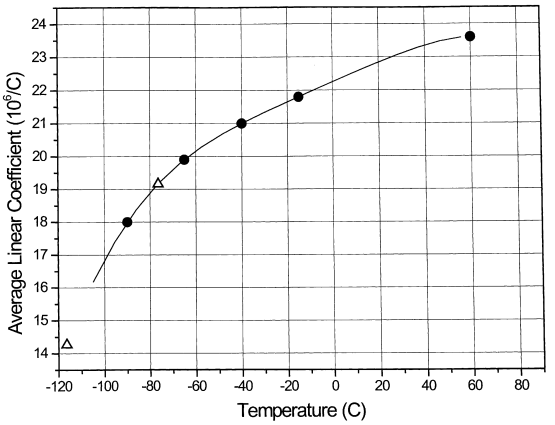

Fig. 1. Average thermal expansion coefficient for pure Al.

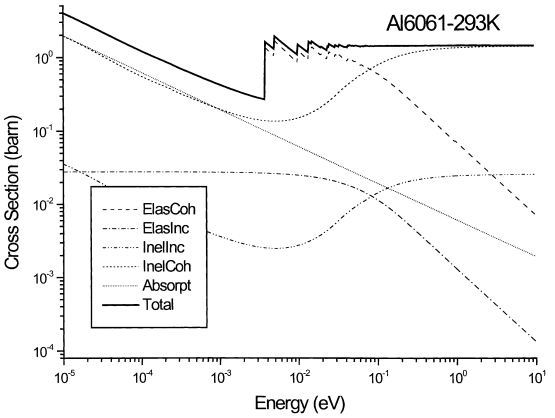

Fig. 2. Evaluated total cross-section of Al6061 at 293 K.

Finally, the values adopted for the Debye temperature were

$$\theta_D\ (297\ \mathrm{K}) = 391\quad \mathrm{K}\ \text{and}$$
$$\theta_D(\text{'low temp'}) = 423\ \mathrm{K}. \tag{9}$$

from [14]. Using the values indicated in (5)–(9), the total cross-section of Al6061 at 293, 100 and 20 K was calculated over the neutron energy range from 10^{-5} to 10 eV, and the results are shown in Figs. 2–4.[2] The ratios between the low temperature cross-sections and the room temperature one are shown in Fig. 5, illustrating the strong dependence with temperature of the inelastic components which dominate the total cross-sections below the Bragg cut-off region.

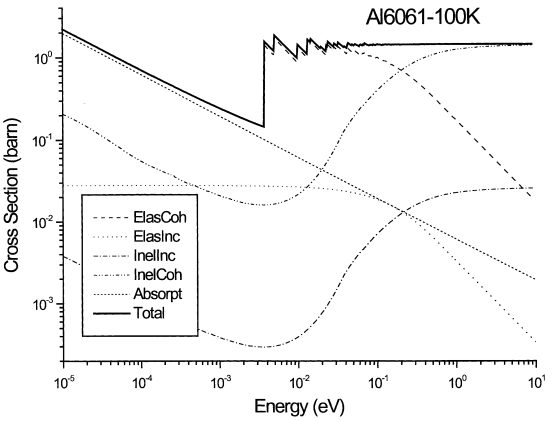

Fig. 3. Evaluated total cross-section of Al6061 at 100 K.

3. Discussion

It is a common situation that determinations of the neutron flux emerging from a cold source require the subtraction of the metallic cell contribution to the measured spectrum. The information given here is aimed at providing the data needed to perform that subtraction, as long as the (Al6061) cell material is in a polycrystalline form.

However, a large degree of texture or preferred orientations might be expected in actual cells, very much dependent on the particular fabrication process of both the original material and the vessel, its thermal history, etc. In those cases, the 'practical' solution is to measure the transmission of the empty cell at room temperature, and then project its contribution at the working, low temperature, in a proper way. Under the plausible

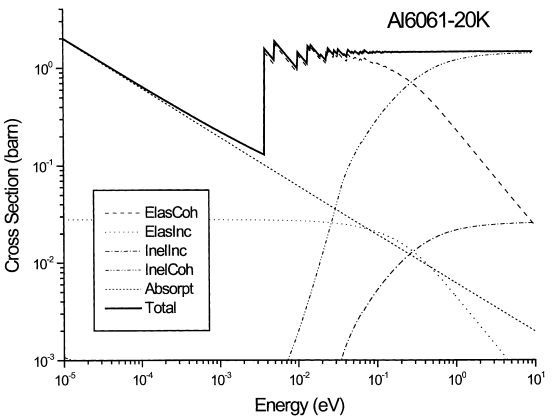

Fig. 4. Evaluated total cross-section of Al6061 at 20 K.

[2] Data files corresponding to those calculations should be requested to the author.

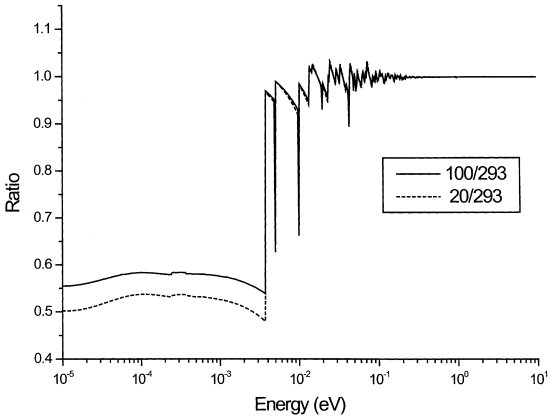

Fig. 5. Ratios of the low temperature total cross-sections to the room temperature one for Al6061.

assumption of a reasonable neutron transparency, the transmission of the empty cell is given by

$$T = \exp\{-nd\sigma_T(E)\}, \tag{10}$$

where n is the number density of scattering centres and d the effective thickness. Using the free-atom cross-section $\sigma_T(\text{Al6061}) = 1.461$ b, the quantity (nd) can be determined, as well as the actual, normalized $\sigma_T(E)$ over the full energy range.

The next step involves isolating the real – normally non-polycrystalline – elastic coherent component of the total cross-section:

$$\sigma_{el,coh}(E) = \sigma_T(E) - \sigma_r(E) \tag{11}$$

with

$$\sigma_r = \sigma_{abs}(E) + \sigma_{el,inc}(E) + \sigma_{inel,coh}(E) + \sigma_{inel,inc}(E). \tag{12}$$

The different terms in (12) do not depend on the crystallinity state of the cell material, but on its atomic mass, Debye temperature and physical temperature. In order to get a good description of the elastic coherent contribution at a different (say lower) temperature, one can take the values (11) 'measured' at room temperature and then shrink the neutron wavelength scale of this measurement to that corresponding to the temperature of interest by using the factors relating the lattice parameters in (7) and (8):

$$E^*/E = (\lambda/\lambda^*)^2 = (a/a^*)^2 = f^{-2}. \tag{13}$$

[3]Of course, those factors f can be generated for any temperature $T(C)$ as $\{1 + \alpha[T(C) - 20]\}$, using the α values given in Fig. 1 corresponding to the abscissa $(T/2 + 10)$.

Not only there is a change in the Bragg cut-off energies in going from one temperature to another, accounted for through Eq. (13), but also in the behaviour of the pedestal on which the interference contribution is superimposed. It is therefore proposed to build the 'real' elastic coherent contribution at the temperature of interest as

$$\sigma^*_{el,coh}(E) = \sigma_{el,coh}(E^*)\sigma^*_{el,inc}(E)/\sigma_{el,inc}(E), \tag{14}$$

where E^* is evaluated according to (13). The actual total cross-section at the temperature of interest is then given – in a good approximation – by

$$\sigma^*_T(E) = \sigma^*_{el,coh}(E) + \sigma^*_r(E). \tag{15}$$

Finally, under the assumption of symmetric wall thickness of the vessel, the effective transmission of the moderator cell on the viewing side is

$$T^* = \exp\{-0.5(\rho^*/\rho)(\text{nd})\sigma^*_T(E)\}, \tag{16}$$

where the change in the number density has been also accounted for.

As a test of the procedure outlined above, the total cross-section of Al6061 at 100 K has been 'regenerated' by obtaining $\sigma^*_{el,coh}$ [100 K] from $\sigma_{el,coh}$ [293 K] with the use of Eqs. (13) and (14). The ratio of the total cross-section at 100 K thus obtained to the exact one at the same temperature is shown in Fig. 6. It is seen that the discrepancies between the approximated and the exact total cross-sections are in the range of a few percent, except for the sharp peaks due to the residual differences in the actual Bragg-cut-off positions, which may be expected to be largely smooth-out in a real case by instrument resolution effects.

The form of the elastic coherent component corresponding to a polycrystalline system was used in this

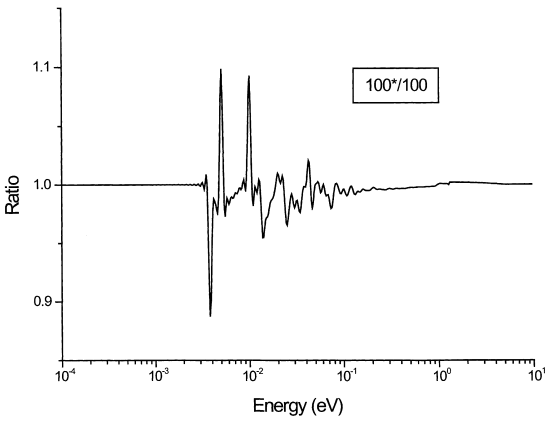

Fig. 6. Ratio of the approximate total cross-section at 100 K to the exact one at the same temperature for Al6061.

[3] The notation Q^* is being used to indicate quantities corresponding to a temperature different from the ambient one.

test, but the result is indicative of what can be expected in a real situation by using the proposed procedure. Concerning scattering kernels for the Al6061 alloy, they can be produced according to the formalism given in Ref. [15].

4. Conclusions

The different components of the total cross-section of the Al6061 alloy were evaluated over the full thermal and subthermal neutron energy range. The calculations were performed under the assumption of polycrystalline materials, at room and low temperatures; the latter were selected on account of the standard use of Al6061 as the vessel material for liquid H_2 and CH_4 cold moderator sources.

A simple procedure has been introduced to obtain a realistic estimate of the vessel contribution to the observed flux emerging from a cold neutron source, in order to properly isolate the relevant spectrum characteristics of the actual moderator. In addition to the use of the inelastic and elastic incoherent components of the total cross-section given here, the proposed procedure requires a transmission measurement of the empty can at room temperature to extract the real elastic coherent contribution, most likely affected by distortions due to texture or preferred orientations.

It is hoped that the ideas and calculations presented here could be useful for the performance analysis of existing cold neutron sources and for the design stages of new ones, through a proper account of the vessel's neutronic characteristics.

References

[1] International Workshop on Cold Moderators for Pulsed Neutron Sources, Argonne, Ill., USA, September 28–October 2, 1997.
[2] J.R. Granada, Thermal Neutron Total Cross-section of AlMg3 at 77 and 297 K, Internal Report AlMg3/JRG/NyR/CAB, 1984.
[3] F. Kropff, J.R. Granada, CRIPO: A fast computer code for the evaluation of Total Cross-sections in Polycrystalline Materials, unpublished Report CAB, 1977.
[4] G. Placzek, Phys. Rev. 86 (1952) 377.
[5] J.R. Granada, Z. Naturforsch, 39a (1984) 1160.
[6] L. Koester, in: Neutron Physics, Springer Tracts in Modern Physics, Springer, Berlin, 1977.
[7] J.R. Granada et al., Physica B 190 (1993) 259.
[8] ASM Handbook, vol. 2 (Fourth printing), 1995.
[9] V. Sears, Neutron News 3 (1992) 29.
[10] F. Kropff et al., Ann. Nucl. Energy 3 (1976) 55.
[11] F. Kropff, J.R. Granada, L.A. Remez, Atomkernen. 30 (1977) 62.
[12] M. Winter, The Periodic Table on the WWW, http://www.shef.ac.uk/chemistry.
[13] L.F. Mondolfo, Aluminum Alloys: Structure and Properties, Butterworths, London, 1979.
[14] Y.S. Touloukian, E.H. Buyco, Thermophysical Properties of Matter, vol. 4, Specific Heat, Metallic Elements and Alloys, IFI/Plenum, New York, 1977.
[15] G.J. Cuello, J.R. Granada, Ann. Nucl. Energy 24 (1997) 763.