Nuclear Instruments and Methods 189 (1981) 555–559
North-Holland Publishing Company

ON THE THERMAL NEUTRON SCATTERING FROM POLYCRYSTALLINE VANADIUM

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Received 17 March 1981

The total cross section of polycrystalline vanadium is evaluated for neutron energies in the range 10^{-3}–20 eV, showing excellent agreement with the more recent experimental data. On the hypothesis of isotropy in the process, the scattering cross section is evaluated as a function of neutron energy. A variation of several percent is observed for this quantity over the energy range under consideration and the implications of this are briefly discussed for time-of-flight experiments.

1. Introduction

With the advent in recent years of intense neutron sources, such as the High Flux Reactor at ILL (Grenoble), the new Harwell LINAC and the imminent appearance of a new generation of pulsed ("spallation") sources, new horizons are being opened up for the investigation of condensed matter by neutron techniques [1–3].

The increase in neutron fluxes and the corresponding improvement in the accessible statistics, simultaneously require higher accuracy and reliability in the different stages of data analysis to capitalise on the effort in both design and building of these facilities.

In neutron scattering experiments, obtaining an absolute differential cross section always requires some kind of normalization by the incident spectrum, whether a steady state or a pulsed source is being used. This normalization procedure is crucial for the latter case because, regardless of the absolute scale, a non-trivial spectrum shape is usually involved.

Polycrystalline vanadium has been widely used as a standard in diffraction work, because it does approach the ideal conditions of an isotropic incoherent elastic scatterer. The first two properties are well satisfied for real vanadium and furthermore, very precise values of the *nuclear constants* σ_c, σ_i and σ_a are now available [4,5]. However, it seems adequate to discuss in more detail the degree of validity of the elastic scatterer assumption for vanadium so far accepted.

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2. The total cross section

The total neutron cross section σ_T of polycrystalline vanadium in the thermal energy range has been measured many times, as reviewed in ref. 5. On the other hand, $\sigma_T(E)$ for any polycrystalline solid at a given temperature can be calculated [6] if the values of the constants σ_c and σ_i are known, together with the absorption component $\sigma_{abs}(E)$ and the structure of its crystalline cell; our computer program CRIPO [7] was developed to evaluate $\sigma_T(E)$ and its components

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

under the assumptions of a Debye frequency spectrum, incoherent approximation for σ_{coh}^{inel} and a $1/v$ behaviour for $\sigma_{abs}(E)$. CRIPO has proved to be very reliable and indeed most useful in allowing us to obtain consistent sets of nuclear parameters from measured $\sigma_T(E)$ curves at thermal neutron energies.

Fig. 1 shows some of the more recent total cross section measurements of vanadium together with a calculation by CRIPO. The input data for the latter were [5,14,15]:

σ_c^{atomic} = 0.014 b,

σ_i = 4.97 b,

σ_{abs}(2200 m/s) = 5.08 b,

M = 50.942 amu,

a = 3.028 Å,

θ_D = 390 K,

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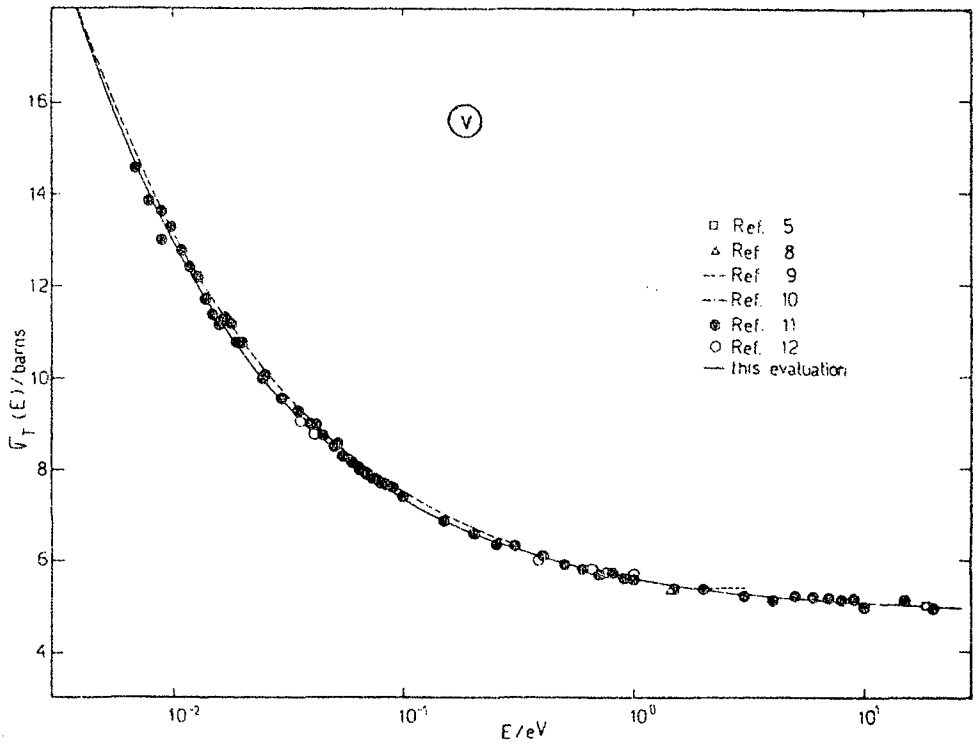

Fig. 1. Experimental and calculated total cross section of vanadium.

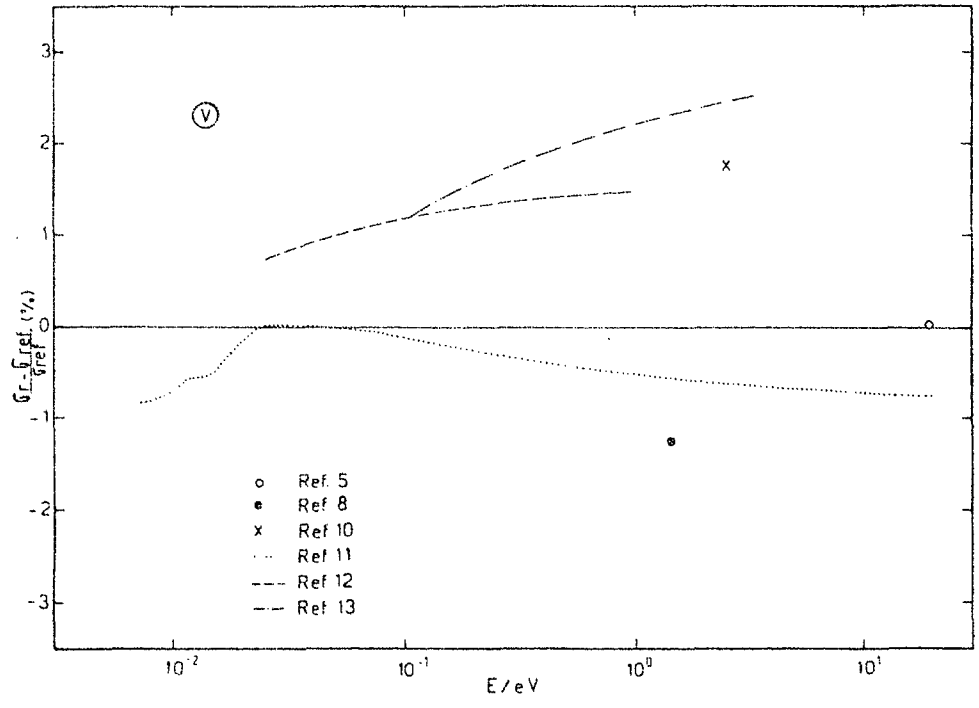

Fig. 2. Relative difference between experimental and calculated total cross section curves (see text for details).

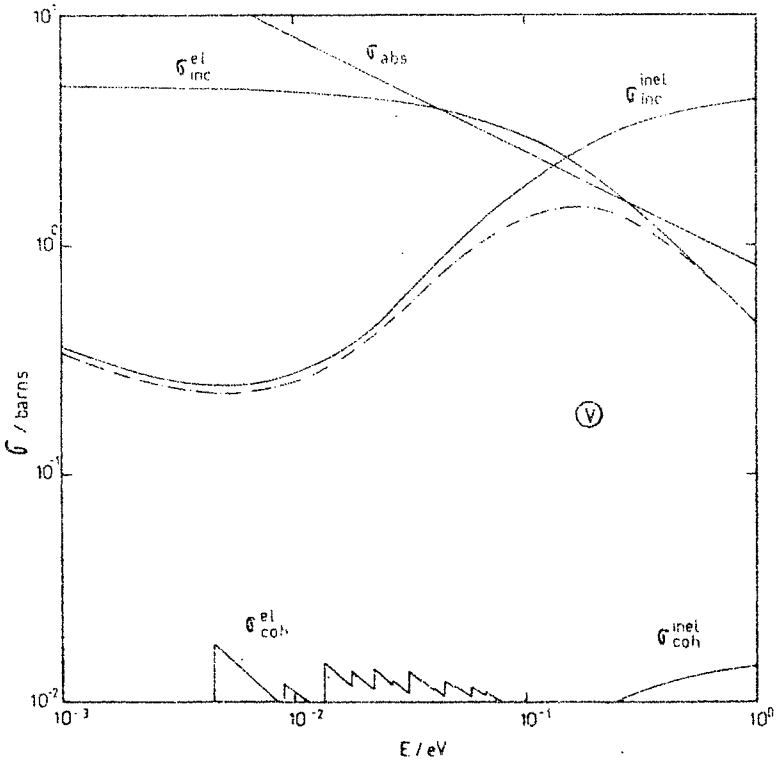

Fig. 3. The calculated components of the total cross section of vanadium from 10^{-3} to 1 eV.

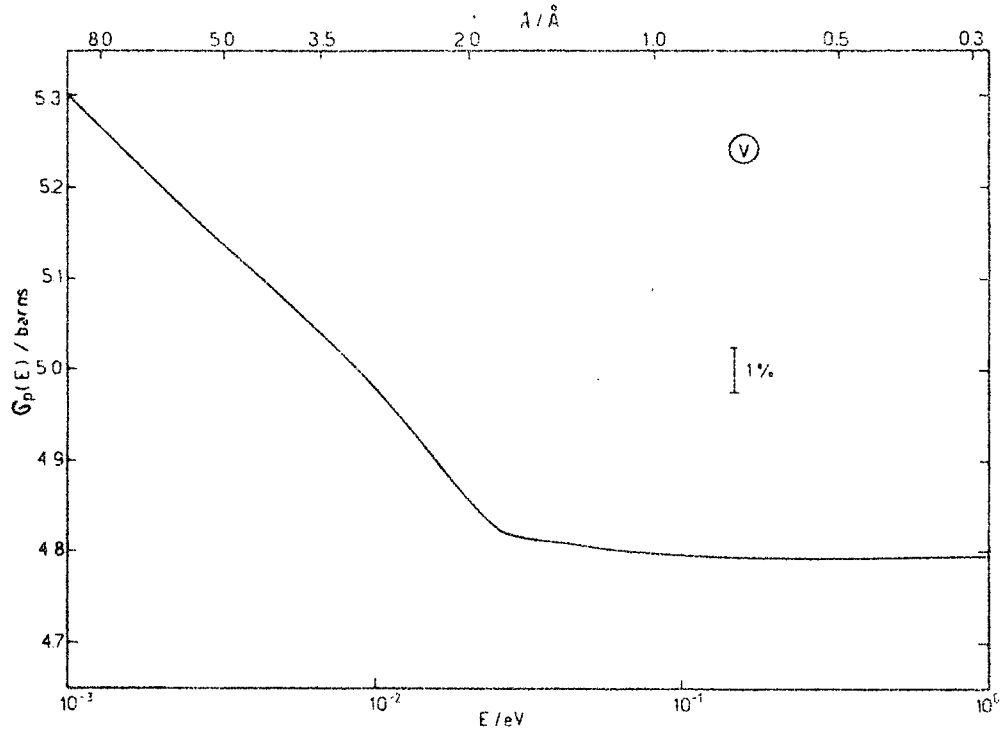

Fig. 4. The calculated "pedestal" σ_p for vanadium from 10^{-3} to 1 eV (see text for details).

where a is the cell parameter of the vanadium bcc lattice and θ_D its Debye temperature. The calculation was performed for a sample temperature $T = 293$ K. A discrepancy between the smoothed curve of ref. 9 and the present evaluation can be observed; there is however, a gratifying agreement with both Dilg's [5] precise $\sigma_T(18.8\ \text{eV})$ value and the total cross section more recently reported [11].

It has been a common practice in the past to fit the experimental data by the expression:

$$\sigma_T(E) = \sigma_s + \sigma_a(0.0253/E)^{1/2}, \quad E \text{ in eV}. \tag{2}$$

Although this may satisfactorily reproduce the total cross section in the thermal energy region, the parameters σ_s and σ_a above do not represent, respectively, the actual scattering and absorption (at 2200 m/s) contributions to σ_T. In fact, binding effects are responsible for the much more complex decomposition of eq. (1) (see fig. 3).

The differences of some total cross section measurements, parameterized according to eq. (2) by their authors, relative to our computed curve are given in fig. 2; also shown are those corresponding to the single energy measurements at 1.44 eV [8], 2.5 eV [10] and 18.8 eV [5].

The calculated components of σ_T for vanadium in the range 10^{-3}–1 eV are shown in fig. 3; for comparison purposes the one-phonon contribution to the incoherent inelastic component is also shown.

3. The scattering cross section

We need to invoke isotropy in the scattering of neutrons by vanadium to proceed further in our discussion. There is experimental evidence supporting this assumption from both reactor and pulsed source techniques [16].

Once the so called "experimental" corrections (absorption correction, multiple scattering, the effect of the container if necessary) have been applied, the quantity that one would obtain in a scattering experiment from vanadium after taking the ratio of the corrected intensity to the *true* incident spectrum shape, is

$$R = \alpha \left.\frac{d\sigma}{d\Omega}\right|_V = \alpha \frac{\sigma_p}{4\pi} + \text{Bragg peaks}, \tag{3}$$

with the "pedestal" σ_p given by [from eq. (1)]:

$$\sigma_p = \sigma_T - \sigma_{abs} - \sigma_{coh}^{el}. \tag{4}$$

The constant α in eq. (3) accounts for the strength of the neutron beam, the effective sample thickness and the geometrical factors involved in the experimental set-up. It is worth emphasizing that the incident spectrum must be recorded by the same detector (i.e. a detector with the same efficiency response) used in the scattering configuration.

σ_p is shown in fig. 4 for neutron energies in the range 10^{-3}–1 eV. A very rapid increase in the magnitude of σ_p can be observed below 0.03 eV (λ = 1.65 Å) which is due to the combined contributions of elastic (approaching a constant value) and one-phonon inelastic scattering. Even though we are using a very expanded scale in this figure, the percentual change as a function of neutron energy is by no means negligible.

In table 1 we present our calculated $\sigma_T(E)$ and $\sigma_p(E)$ for polycrystalline vanadium at $T = 293$ K.

Table 1
Calculated $\sigma_T(E)$ and $\sigma_p(E)$ for vanadium at $T = 293$ K

E (eV)	λ (Å)	σ_T(b)	σ_p(b)
1.000×10^{-3}	9.045	30.858	5.306
1.259×10^{-3}	8.061	28.042	5.269
1.585×10^{-3}	7.184	25.531	5.235
1.995×10^{-3}	6.403	23.292	5.203
2.512×10^{-3}	5.707	21.294	5.172
3.162×10^{-3}	5.086	19.511	5.143
3.981×10^{-3}	4.533	17.919	5.113
5.012×10^{-3}	4.040	16.512	5.082
6.310×10^{-3}	3.601	15.236	5.050
7.943×10^{-3}	3.209	14.093	5.016
1.000×10^{-2}	2.860	13.071	4.980
1.259×10^{-2}	2.549	12.151	4.940
1.585×10^{-2}	2.272	11.331	4.900
1.995×10^{-2}	2.025	10.594	4.861
2.512×10^{-2}	1.805	9.939	4.828
3.162×10^{-2}	1.608	9.371	4.814
3.981×10^{-2}	1.433	8.874	4.812
5.012×10^{-2}	1.278	8.428	4.807
6.310×10^{-2}	1.139	8.031	4.803
7.943×10^{-2}	1.015	7.677	4.800
1.000×10^{-1}	0.904	7.363	4.798
1.259×10^{-1}	0.806	7.083	4.797
1.585×10^{-1}	0.718	6.833	4.796
1.995×10^{-1}	0.640	6.611	4.796
2.512×10^{-1}	0.571	6.413	4.795
3.162×10^{-1}	0.509	6.236	4.795
3.981×10^{-1}	0.453	6.079	4.795
5.012×10^{-1}	0.404	5.939	4.795
6.310×10^{-1}	0.360	5.815	4.795
7.943×10^{-1}	0.321	5.704	4.795
1.000×10^{-0}	0.286	5.605	4.795

4. Discussion

The evaluation of the total cross section of vanadium in the thermal region successfully reproduces the experimental data. The incoherent approximation on which our computer program CRIPO is based is certainly more than justified in this case and departures from this condition [6] are clearly negligible.

On this basis we show in fig. 4 what we expect will be the measured pedestal σ_p ($\% 4\pi$) in a scattering experiment as a function of neutron energy. This conclusion means that the vanadium reference method has to be reanalyzed, particularly for time-of-flight experiments where a "white" beam is used and the spectrum shape is obtained directly from scattering by a vanadium sample.

Admittedly the present analysis depends on the hypothesis of isotropy in the scattering process, whereas one would expect at least the Debye–Waller factors to be angular dependent. However, as previously stated, there is no clear sign of anisotropy in the scattering pattern of vanadium at a given neutron wavelength.

Our analysis stresses the need for more clear and conclusive experimental evidence on the scattering properties of V for its use as a reference standard.

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