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EXPERIMENTAL DETERMINATION OF ANOMALOUS SCATTERING LENGTHS OF SAMARIUM FOR THERMAL NEUTRONS

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ABSTRACT

Anomalous scattering lengths of natural Sm for thermal neutrons with wavelengths between 0.827 and 1.300 Å have been determined using a single crystal of a Sm-complex of known structure. 140 selected reflections were measured at each wavelength and b_o+b' and b" refined in each case. The values obtained are in good agreement with theoretical values obtained from a Breit-Wigner calculation using tabulated resonance parameters for ^{149}Sm. A value of b_o = 4.3 ± 0.2 fm is deduced from the diffraction experiment.

INTRODUCTION

Anomalous scattering of thermal neutrons by resonant nuclei has been exploited for crystal structure determination[1-5]. For successful application of phase determination techniques the anomalous scattering lengths must be known at all the wavelengths used. We report here the determination of the scattering lengths of natural Sm in a diffraction experiment. Anomalous scattering lengths have previously been determined by diffraction[2, 6-9] for Cd, Li, B and Sm.

BREIT WIGNER CALCULATION OF b

The scattering length of a nucleus is $b = b_o+b'+ib"$ where b' and b" are dispersion terms due to a resonance near the primary neutron energy. The real and imaginary parts can be written as

$$b_{re} = b_o + b' = b_o + \frac{A(E-E_o)}{(E-E_o)^2+B^2} \qquad (1)$$

$$b" = \frac{A\,B}{(E-E_o)^2+B^2} \qquad (2)$$

where $A = g\omega\lambda_o\Gamma_n/4\pi$ and $B = \Gamma/2$. g is a spin weighting factor $\frac{1}{2}(2J+1)/(2I+1)$ where I and J are the spins of the nucleus and compound nucleus respectively, ω is the abundance of the relevant isotope, λ_o the resonance wavelength, E_o the resonance energy, E the primary neutron energy, Γ_n the resonance width for re-emission of the neutron, Γ_a that for absorption of the neutron and $\Gamma = \Gamma_n+\Gamma_a$ the total width.

The wavelength-independent term is given

$$b_o = R + \Sigma g\omega\lambda_o\Gamma_n/(-4\pi E_o) \qquad (3)$$

where the sum is taken over all higher energy resonances of all isotopes present. R is the scattering length for potential scattering (nuclear radius).

Values of A, B, E_o and b_o were calculated for natural Sm from tables of absorption data[10] and are shown in Table 1.

EXPERIMENTAL

A single crystal of a sodium samarium edta complex, $Na^+[Sm(C_{10}H_{12}N_2O_8).3H_2O]^-.5H_2O$ was used for the diffraction experiment. The crystal was mounted in a helium atmosphere at 37 K on an automated four-circle diffractometer at the Brookhaven High Flux Beam Reactor. The neutron beam was monochromated using the 002 face of a Be crystal. 1800 independent reflections were measured at a wavelength of 1,300 Å and the crystal structure refined to a final R-value of 0.058. 450 parameters including the real and imaginary Sm scattering lengths were varied in the final refinement.

140 reflections with strong Sm-contribution to the structure factor were now selected and measured at a number of different wavelengths. Using the structural parameters obtained in the full refinement at 1.300 Å the real and imaginary scattering lengths of Sm were refined together with the scale factor for each limited data set.

DISCUSSION

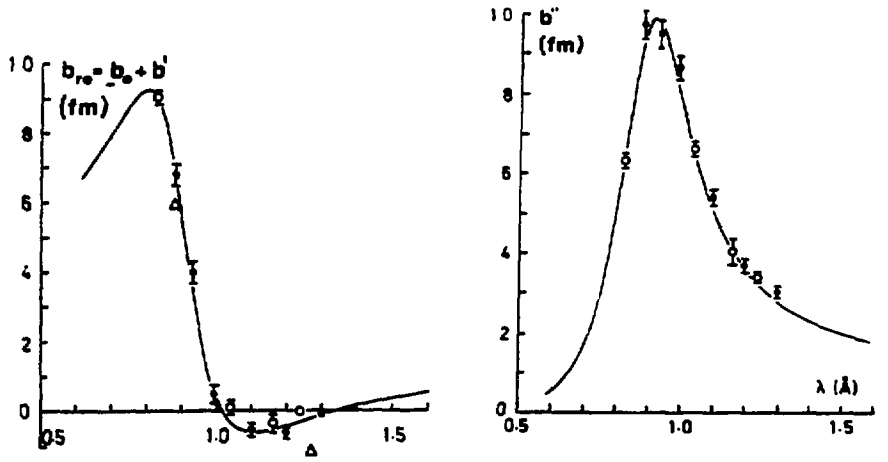
In Figure 1 the refined scattering lengths of natural Sm (points) can be compared with the curves calculated from the absorption data. (The curve of b_{re} was drawn using b_o = 4.3 fm to provide a slightly better fit.) The parameters A, B E_o and b_o were also calculated by a least squares fit of the values of b_{re} and b" from the diffraction experiment to equations 1 and 2. The refined values are compared to those deduced from absorption data in Table 1.

Table 1 Parameters for scattering lengths of natural Sm in equations 1 and 2. Comparison of values deduced from tables of absorption data and from the diffraction experiment.

		Absorption	Diffraction	
			from b_{re}	from b"
A	(fm.eV)	0.302(6)	0.299(32)	0.310(23)
B	(eV)	0.0305(3)	0.0310(24)	0.0310(12)
E_o	(eV)	0.0976(3)	0.0966(11)	0.0972(8)
b_o	(fm)	≲4.02	4.32(21)	-
Γ_n	(meV)	0.533(8)	0.526(60)	0.546(41)
Γ	(eV)	0.0611(6)	0.0619(49)	0.0620(24)

The agreement is good. The e.s.d.'s of A, B and E_o deduced from absorption data are lower than those obtained in the diffraction experiment. However, the value of b_o from equation 3 may be in error due to omission from the sum of resonances not tabulated and due to uncertainty in the value of R, taken here as 7.98 fm for natural Sm. The diffraction value of $b_o = 4.3 \pm 0.2$ fm is thus probably the more reliable one.

Fig. 1 Scattering lengths of natural Sm plotted against neutron wavelength. Full curve: Breit-Wigner calculation from tables of absorption resonance data. Experimental points are values refined from diffraction data. Triangles are values from Sikka[8].



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