Slow-Neutron Scattering Cross Sections of Terbium, Ytterbium, and Lutetium*

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The coherent neutron scattering cross sections of terbium, ytterbium, and lutetium as determined from the neutron diffraction measurements on TbC_2, YbC_2, Yb, and Lu metals are found to be 7.2±0.4, 20.0±0.4, and 6.70±0.37 barns, respectively, all with amplitude of positive phase. The total scattering cross sections of Tb, Yb, and Lu and the magnetic scattering cross sections of Tb^{+3} and Yb^{+3} are evaluated for thermal neutron energies. The neutron diffraction data also show the Debye temperatures of Yb and Lu metals to be 109±5°K and 161±7°K, respectively.

SLOW-NEUTRON scattering cross sections for most of the rare-earth nuclides have been evaluated by Koehler and Wollan[1] and Koehler *et al.*[2] However, those for terbium, ytterbium, and lutetium have not been reported. The coherent neutron scattering cross sections of Tb, Yb, and Lu reported here were obtained from the neutron diffraction analyses on TbC_2, YbC_2, and Yb and Lu metals. The total scattering cross sections were evaluated from the transmission measurements corrected for capture, or from the diffuse scattering analyses. The transmission data of Yb_2O_3, Lu_2O_3, and Tb metal were also used in processing the values listed in Table I. However, their diffraction data were not used for determining the coherent scattering cross sections, because of uncertainties in the structural parameters (Yb_2O_3 and Lu_2O_3) and in the magnetic ordering scattering (Tb metal).

TABLE I. Nuclear scattering properties of Tb, Yb, and Lu.[a]

Nucleus	Coherent scattering amplitude (10^{-12} cm)	Coherent scattering cross section (barns)	Total nucleus scattering cross section (barns)
$_{65}Tb^{159}$	+0.756±0.020	7.2±0.4	20±2
$_{70}Yb$	+1.262±0.012	20.0±0.4	30±3
$_{71}Lu$	+0.730±0.020	6.70±0.37	13±2

[a] Potential scattering cross sections of $_{65}Tb^{159}$, $_{70}Yb$, and $_{71}Lu$ are 8.64, 9.13, and 9.20 barns, respectively.

Neutron powder diffraction intensities were obtained using the neutron diffractometer at the Oak Ridge National Laboratory. All data were obtained with the neutron wavelength of 1.055±0.002 A (0.0735 ev) and were standardized against the nickel powder intensities. The optimum experimental conditions were so chosen that the recorded peak shape of the Bragg reflection can be approximated by the Gaussian error function. Therefore, if $C(\theta)$ and I_j represent, respectively, the background counts and the integrated intensity of the jth Bragg reflection with the Bragg angle of θ_j, the total diffracted neutrons $I(\theta)$ at the given angle θ is expressed by

$$I(\theta)=C(\theta)+\sum_j I_j\frac{h(\theta)}{\sqrt{\pi}}\exp\left[-h(\theta)(\theta-\theta_j)\right]^2,$$

where peak-width function $h(\theta)$ can be determined empirically[3] and the x-ray lattice constants give the precision θ_j values. The least-squares method based on the above expression was extensively utilized for deducing the individual I_j values from the overlapped peaks and for determining the background intensities.

Complete spectroscopic, chemical, and x-ray analyses for impurities in the neutron samples gave the following results in weight percent with the maximum detectable limits of 0.05% and 0.1%, respectively, for metallic and nonmetallic impurities: no impurities detectable in Yb and Tb metals, TbC_2, Yb_2O_3, and Lu_2O_3; 2±0.2% Ta metal in Lu metal; 4.04±0.03% crystalline graphite in YbC_2. Special efforts were made for detecting the high-capturing rare-earth impurities, but none of them were detectable within 0.05 to 0.02% limits in these samples. The impurity peaks were substracted from the diffraction patterns using the least-squares method described above and the neutron diffraction data of Ta metal and graphite. The preferred-orientation effect of crystallites in the sample holder was kept negligible by choosing the appropriate packing technique.

COHERENT SCATTERING CROSS SECTIONS

The complete-matrix least-squares treatment on the neutron diffraction intensities of the polycrystalline TbC_2 crystals with the CaC_2-type structure,[4] yielded the coherent amplitude, $b(\mathrm{Tb})=+0.762\pm0.030$ in 10^{-12} cm, the positional parameter for carbon atoms, $z=0.3960\pm0.0007$, and the temperature-factor coefficient $B=0.75\pm0.06$ A^2. The reported value[5] of $b(\mathrm{C})=+0.662\pm0.0024$ was treated as an invariable in

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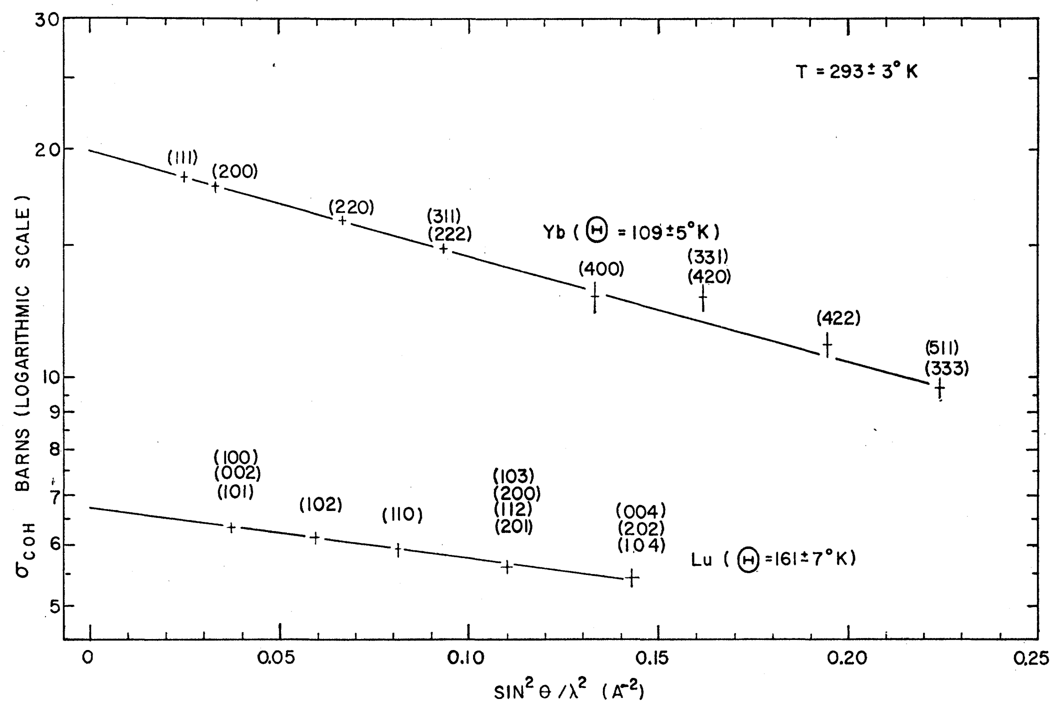

FIG. 1. Determination of the coherent scattering cross sections from Yb and Lu metals.

the least-squares calculation. The agreement factor, $R=[\sum w(I_{\text{obs}}-I_{\text{calc}})^2/\sum wI_{\text{obs}}^2]^{\frac{1}{2}}$ with the weighting factor w, is as low as 0.025 for these parameters. Recently, Koehler[6] obtained $b(\text{Tb})=+0.75\pm0.03$ from the TbN data. The weighted average of these two independent measurements yields $b(\text{Tb})=0.756\pm0.020$ and $\sigma_{\text{coh}}(\text{Tb})=7.2\pm0.4$ barns.

The results for YbC_2 also with the CaC_2 type structure[4] are: $b(\text{Yb})=+1.263\pm0.036$, $z=0.3946\pm0.0012$, $B=0.77\pm0.10$ A^2, and $R=0.016$. As shown in Fig. 1, $\sigma_{\text{coh}}=20.0\pm0.4$ barns was obtained from Yb metal. The weighted averages of these results are: $b(\text{Yb})=+1.262\pm0.012$ and $\sigma_{\text{coh}}(\text{Yb})=20.0\pm0.4$ barns.

The diffraction data of Lu metal yielded $b(\text{Lu})=+0.730\pm0.020$ and $\sigma_{\text{coh}}(\text{Lu})=6.70\pm0.37$ barns (Fig. 1). The positive sign in $b(\text{Lu})$ was determined from the Lu_2O_3 data.

The B values of Yb and Lu metals at 293±3°K are 1.65±0.15 A^2 and 0.75±0.065 A^2, respectively. These values correspond to the Debye characteristic temperatures of 109±5°K for Yb metal and 161±7°K for Lu metal. The Lu value is comparable with the calorimetric value of 166°K.[7] No comparable value is available for Yb metal.

TOTAL AND MAGNETIC SCATTERING CROSS SECTIONS

The total cross section of Tb evaluated from the transmission data of Tb metal and TbC_2 is 29.8±1.0 barns at 0.0735 ev. The diffuse scattering analysis on the TbC_2 data, which were measured at large angles to eliminate the magnetic contribution, yielded the total nuclear scattering cross section of 19.5±2.0 barns. The observed magnetic scattering cross section of Tb^{+3} at 0.0735 ev is 6.42 barns. Therefore, the capture cross section of 3.9±2.3 barns at 0.0735 ev is obtained, while 2.7±2.3 barns is expected from the literature value[5] with the inverse velocity law. The paramagnetic scattering cross sections of $Tb^{+3}(4f^8\,{}^7F_6)$ were plotted against neutron energies in Fig. 2, where the Trammell-Koehler-Wollan method[8,9] and the empirical effective nuclear charge of $(Z\text{-}S)=22$ for $4f$ electrons obtained from the angular dependency of the diffuse scattering of the TbC_2 were employed.[10] However, the total cross section values of ${}_{65}$Tb for the neutron energies less than 2 ev are not available except for the present value at 0.0735 ev. Hence, the Tb values in Fig. 2 are retained for future application.

The total cross sections of Yb at 0.0735 ev are 50.7±0.5 barns from Yb_2O_3, 50.8±0.5 barns from YbC_2, and 49.4±0.5 barns from Yb metal. The diffuse-scattering analyses indicated that Yb ions in Yb_2O_3 and YbC_2 are in the paramagnetic $4f^{13}\,{}^2F_{7/2}$ state,[10] while Yb metal is nonparamagnetic.[11] The observed magnetic scattering cross section of $Yb^{+3}({}^2F_{7/2})$ is 2.7 barns at 0.0735 ev. The average total nuclear cross

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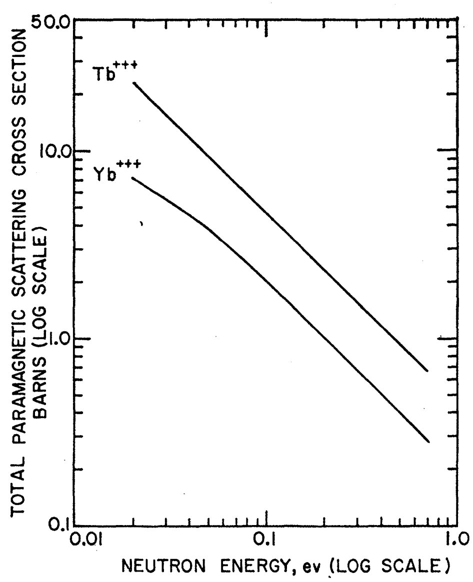

FIG. 2. Total paramagnetic scattering cross section of Tb^{+3} and Yb^{+3} as a function of neutron energy.

section corrected for the magnetic part is 48.5±0.3 barns at 0.0735 ev. Although the neutron resonance at 0.6 ev has been reported for Yb,[5,12] if the $1/v$ law is valid, the total nuclear scattering cross sections of 27±2 barns is obtained. The diffuse scattering analysis on the Yb metal data gives 32±2 barns for this value. Because of additional uncertainties involved in both cases, the average value of 30 barns with the estimated standard deviation of 3 barns is chosen for the total nuclear scattering cross section of Yb. The $_{70}Yb$ is composed of seven stable isotopes and hence the sum of the spin and isotopic incoherent scattering cross sections is about 19 barns at thermal energies. The total paramagnetic scattering cross sections of $Yb^{+3}(^2F_{7/2})$ are also calculated using the experimentally determined $(Z\text{-}S)$ value of 27 (Fig. 2). It should be noted that the Yb values in Fig. 2 are too small to explain the variation in the total cross sections for the neutron energies, 0.3 to 0.07 ev.[5]

The average total cross section of Lu obtained from the Lu metal and Lu_2O_3 data is 105±2 barns at 0.0735 ev, which is in accord with the reference value of 107 barns obtained at this energy by the chopper measurements (see curve).[5,13] The diffuse scattering value of Lu metal shows the total scattering cross section of 13±2 barns, while the $1/v$ law predicts about 40 barns.[5] The failure of the $1/v$ law is evident, since $_{71}Lu^{176}$ shows a neutron resonance at 0.142 ev.[13] The proximity of this resonance energy to the neutron energy employed in this study may imply the complex coherent scattering amplitude. However, the structure analyses of Lu_2O_3 and LuC_2 indicate that the imaginary part in b(Lu) is not significantly large. As expected from the $^1S_0$ state of Lu^{+3}, no magnetic scattering was detectable in the diffraction patterns of the Lu samples.

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