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SUBMITTED TO: American Institute of Physics Conference Proceedings

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LOW-TEMPERATURE THERMAL EXPANSION OF MnB_2

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ABSTRACT

The anisotropic thermal expansion of manganese diboride has been determined with neutron diffraction over the temperature range 5-298 K. The variation of lattice parameter with temperature is defined by the equations

$$a = 3.0044 + 4.9 \times 10^{-6} T$$
$$c = 3.0358 - 2 \times 10^{-6} T + 7 \times 10^{-8} T^2.$$

The c parameter is found to contract initially, passing through a minimum at 14 K.

INTRODUCTION

The determination of the magnetic susceptibility of manganese diboride indicates that this compound is ferromagnetic with a Curie temperature of about 150 K.^{1,2} Neutron diffraction studies^{3,4} and NMR measurements⁵ suggest, however, that MnB_2 has an antiferromagnetic layer structure at room temperature. Neutron diffraction data were taken over the temperature range 5-298 K in an effort to observe a magnetic transition. While no transition was observed, the data do show the variation of the lattice parameters with change in temperature.

EXPERIMENTAL

The MnB_2 sample was prepared by arc-melting a compacted mixture of the elemental powders, and was used without further heat treatment. The boron powder was 98% - enriched boron - 11, which contained an unidentified impurity that appeared in the final sample. The hexagonal lattice parameters of MnB_2 were $a = 3.005$; $c = 3.038\text{\AA}$ at 25°C.

The neutron diffraction data were obtained at the Los Alamos Omega West Reactor. A monochromatic neutron beam, with wave-length of 1.1422\AA, was produced by reflection from a lead single crystal. The beam intensity was monitored by means of a thin fission counter. The sample was contained in a 3 in. diameter parallel-sided holder made from a null-matrix (Ti-Zr) alloy. The sample was surrounded by a helium gas atmosphere in a variable temperature cryostat (Union Carbide Corporation, Linde Division Model CD 171). The temperature was maintained to ± 0.2 K by means of an electric heater. The temperature was measured with a germanium resistance thermometer below 50 K, and with an iron-constantan thermocouple above 50 K.

The data were recorded as number of neutron counts per fixed number of monitor counts, at intervals of 0.1° in 2θ . The data were fitted to the equation⁶

$$N = B + \frac{I}{\sqrt{2\pi}} \exp(-(2\theta - b)^2/2s^2) \quad (1)$$

by the method of least squares,⁷ where N is the observed neutron count at 2θ , B is a constant background term, and I , s , and b are the intensity, standard deviation, and mean value of 2θ of the diffraction peak, respectively. The (001) and (100) peaks were scanned and fitted separately. The lattice parameters were obtained from the calculated values of b with a precision of $\pm 0.0005\text{\AA}$.

RESULTS AND DISCUSSION

The lattice parameter data were fitted by least squares to the equations

$$a = 3.0044 \text{ (1)} + 4.9 \text{ (5)} \times 10^{-6}T \quad (2)$$

$$c = 3.0358 \text{ (2)} - 2 \text{ (4)} \times 10^{-6}T + 7 \text{ (1)} \times 10^{-8}T^2 \quad (3)$$

with the standard deviations shown in parentheses. The data points and the calculated curves are plotted in Fig. 1. The anisotropic coefficients of thermal expansion are

$$\alpha_{\perp} = 1.6 \times 10^{-6}$$

$$\alpha_{\parallel} = -6 \times 10^{-7} + 2.2 \times 10^{-8} T.$$

These equations fit the total data set, but should not be expected to describe accurately the actual thermal expansion near 0 K. The data are not precise enough to describe this region, but they are consistent with $\alpha = 0$ at $T = 0$. The equation (3) for the c parameter variation shows a minimum at 14 K, but the volume function shows a monotonic increase at all temperatures, as shown in Fig. 1.

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Fig. 1. Lattice parameters and volume of MnB_2 .