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STRUCTURE ANALYSIS OF NEW SUPERCONDUCTOR MgB_2

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The superconductivity of a sintered pellet of the newly discovered MgB_2 superconductor has been studied with magnetic measurements and its crystal structure was analysed using the Rietveld method of powder X-ray patterns. It has hexagonal symmetry (S.G. $P6/mmm$) with unit cell lattice parameters a=0.308136(14)nm and c=0.351782(17)nm.

Keywords: structure, superconductor, MgB_2
PACC: 7470, 7870C

I. INTRODUCTION

The discovery of superconductivity with $T_c > 39$ K in magnesium diboride MgB_2 was announced in January 2001 by Akimitsu and co-workers.[1] This has caused excitement in the world's physics community, because it is a new binary alloy superconductor with a new record of superconducting transition temperature for non copper–oxygen and non rare-earth based alloy compounds. In early studies of the B isotope effect, Bud'ko and co-workers[2] found the superconducting transition temperature T_c increased from 39.2 K for $Mg^{11}B_2$ to 40.2 K for $Mg^{10}B_2$ giving a partial isotope exponent α_B=0.26 for the isotope relation $T_c \sim M^{-\alpha^B}$ where M is the isotope mass. This is a clear indication that phonons play an important role in the superconducting interaction. The band structure calculations[3] show a rather isotropic electrical transport in spite of the obviously layered appearance of honeycombed boron and hexagonal magnesium networks in the material.

A X-ray powder structure analysis of MgB_2 is reported in this paper, which shows that it has hexagonal symmetry (S.G. $P6/mmm$) with refined unit cell parameters a=0.308136(14)nm and c=0.351782(17)nm.

II. EXPERIMENT

Bulk-sintered samples of MgB_2 were prepared by the standard ceramic process. A stoichiometric amount of Mg (99.5% purity in powder form) and boron (98% purity in powder form) were mixed in a sealed Ta tube. The Ta tube was then sealed in a quartz ampoule, placed in a 950°C box furnace for two hours, then removed and allowed to cool to room temperature. The sintering process might be repeated until the sintered sample crystallized in single phase exactly. The samples were monitored by X-ray diffraction (XRD), and the crystal structures of the samples were refined from step-scanning (0.02°/step) XRD data using the Rietveld method. The temperature-dependent magnetizations of the samples were measured by a Quantum Design MPMS SQUID magnetometer in an applied field of 2×10^{-3}T.

III. RESULTS AND DISCUSSION

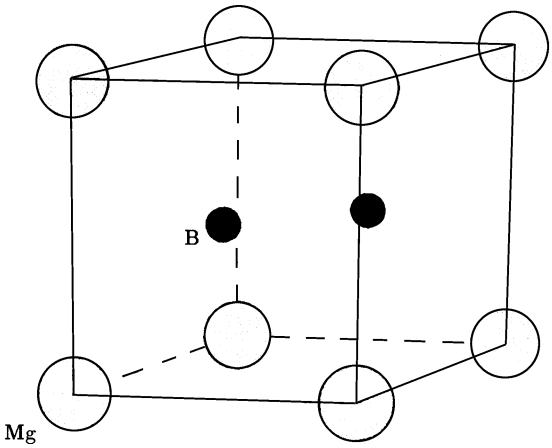


Fig.1. Unit cell of MgB_2.

The X-ray diffraction study reveals that the prepared samples are of single phase with an AlB_2-type hexagonal structure ($P6/mmm$), which consists alternatively of hexagonal layers of Mg atoms and graphite-

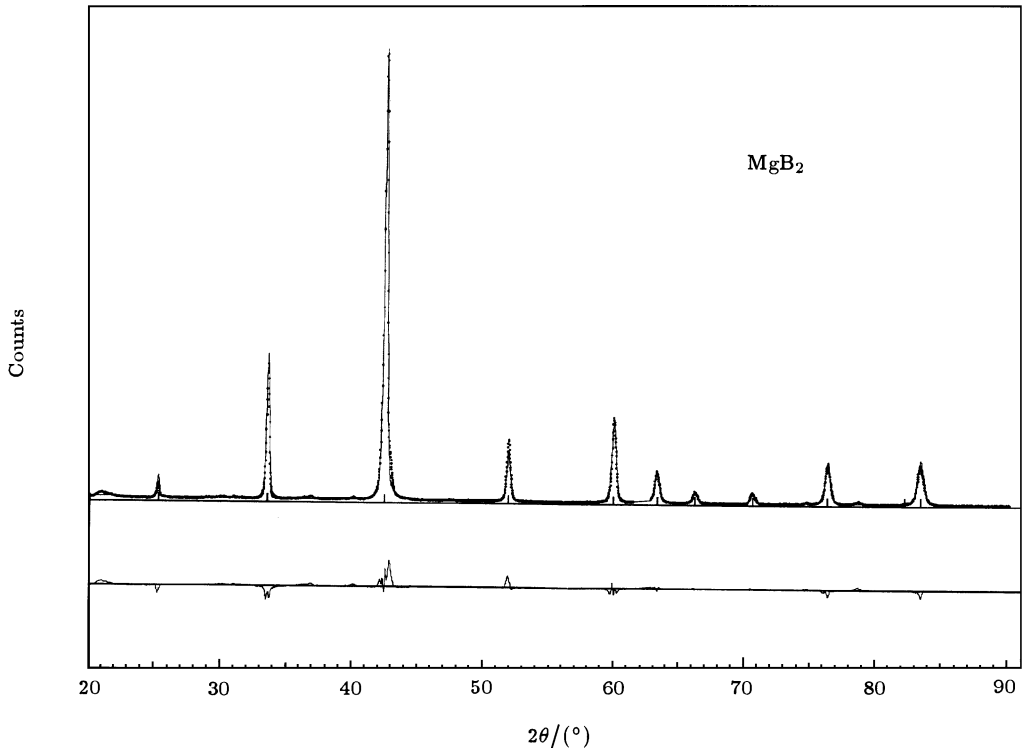


Fig.2. Observed and calculated diffraction patterns of MgB_2 at room temperature.

like honeycomb layers of B atoms (Fig.1). A Rietveld structure analysing program 'FULLPROF' was used and the results of crystal structure refinement are shown in Fig.2. The refined unit cell lattice parameters are $a = 0.308136\text{nm}\pm0.000014\text{nm}$ and $c = 0.351782\text{nm}\pm0.000017\text{nm}$. The bond lengths of Mg−B and B−B are 0.25017 ± 0.00001 and 0.17790 ± 0.00001nm, respectively.

The temperature-dependent magnetization of MgB_2 is shown in Fig.3. An onset criterion of 2% of the full, low-temperature diamagnetic signal was used to determine T_c from the zero-field cooled $M(T)$ data that were taken on warming. The superconducting transition temperature is 38.0K for our samples. The purity of boron might have much effect on the superconducting transition temperature.

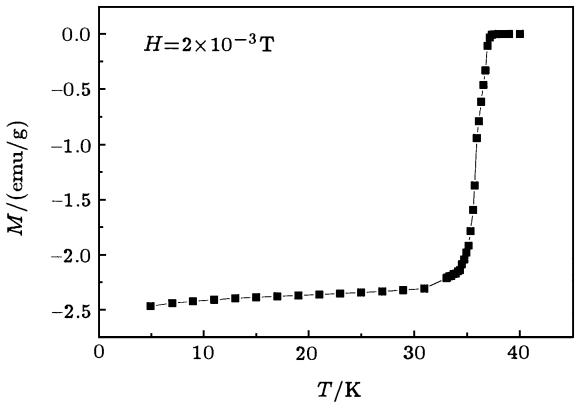


Fig.3. Temperature T dependent magnetization M curve.

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