

## Structural and electronic properties of superconductor MgB<sub>2</sub> under high pressure

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

2002 J. Phys.: Condens. Matter 14 10623

(<http://iopscience.iop.org/0953-8984/14/44/345>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 144.213.253.16

The article was downloaded on 03/06/2010 at 02:51

Please note that [terms and conditions apply](#).

# Structural and electronic properties of superconductor MgB<sub>2</sub> under high pressure

J Tang<sup>1</sup>, L-C Qin<sup>2</sup>, H-W Gu<sup>1</sup>, A Matsushita<sup>1</sup>, Y Takano<sup>1</sup>, K Togano<sup>1</sup>,  
H Kito<sup>3</sup> and H Ihara<sup>3</sup>

<sup>1</sup> National Institute for Materials Science, 1-2-1 Sengen, Tsukuba 305-0047, Japan

<sup>2</sup> Department of Physics and Astronomy, University of North Carolina at Chapel Hill, Chapel Hill, NC 27599, USA

<sup>3</sup> National Institute of Advanced Industrial Science and Technology, 1-1-4 Umezono, Tsukuba 305-8568, Japan

Received 1 June 2002

Published 25 October 2002

Online at [stacks.iop.org/JPhysCM/14/10623](http://stacks.iop.org/JPhysCM/14/10623)

## Abstract

The superconductivity and the lattice properties of a sintered MgB<sub>2</sub> material have been investigated under high pressure up to 10 GPa. The transition temperature was found to decrease linearly with increasing hydrostatic pressure at a rate of 1.03 K GPa<sup>-1</sup>, which can be explained with the classical Bardeen–Cooper–Shrieffer theory based on an electron–phonon coupling mechanism. The crystal lattice exhibits an anisotropic compressibility characterized by a larger compressibility along the *c*-direction than the *a/b*-directions. The anisotropy is attributed to a weaker inter-plane bonding along the *c*-axis in comparison with a stronger intra-plane bonding perpendicular to the *c*-axis. The bulk modulus of the measured material was deduced to be 172 GPa.

(Some figures in this article are in colour only in the electronic version)

## 1. Introduction

The simple MgB<sub>2</sub> crystal structure with the space group of *P6/mmm* ( $a = 3.086 \text{ \AA}$  and  $c = 3.524 \text{ \AA}$ ) consists of a layered stacking with alternating Mg and B layers on top of each other. The surprising discovery of superconductivity in magnesium diboride (MgB<sub>2</sub>) at 39 K by Nagamatsu *et al* [1] has stimulated great interest in this material. This represents the highest  $T_c$  discovered so far in a binary system, much higher than that for the Nb<sub>3</sub>Ge alloy ( $T_c = 23.2 \text{ K}$ ). A few theoretical analyses have been presented to consider the fundamental mechanism responsible for the superconductivity in this material. The conduction bands of the sp<sup>2</sup> bonded boron sheets have been suggested to contribute to the superconductivity, which results from the strong electron–phonon interaction and the high phonon frequency associated with the honeycomb-like boron structure [2].

Since the announcement of the discovery, several reports have been released reporting measurements of pressure effects on MgB<sub>2</sub> materials prepared under various conditions. Vogt *et al* [3] characterized the bulk modulus of commercially available high-purity MgB<sub>2</sub> powders using high pressure and obtained  $B_0 \approx 151$  GPa based on the first-order Murnaghan equation of state

$$V = V_0 \left( 1 + P \frac{B'_0}{B_0} \right)^{-1/B'_0},$$

where  $V$  is the unit-cell volume at pressure  $P$ ,  $B'_0 = 4$ , and  $V_0$  and  $B_0$  are the unit-cell volume and the bulk modulus at ambient conditions, respectively. This measurement gives rise to a value for the volume compressibility, defined as

$$\kappa = \frac{1}{B_0} = -\frac{1}{V_0} \frac{dV}{dP},$$

of about  $6.7 \times 10^{-3}$  GPa<sup>-1</sup> to a good approximation. Prassides *et al* [4] measured the compressibility of the material used by Nagamatsu *et al* [1] and obtained a volume compressibility of  $8.3 \times 10^{-3}$  GPa<sup>-1</sup>. Lorenz *et al* [5] prepared their MgB<sub>2</sub> material by a solid-state reaction method and measured the dependence of  $T_c$  on hydrostatic pressure up to 1.84 GPa; they obtained  $dT_c/dP \approx -1.6$  GPa<sup>-1</sup>. Loa and Syassen [6] gave a theoretical analysis and suggested a rate of decrease of 1.6 K GPa<sup>-1</sup> in response to pressure. Jorgensen *et al* [7] reported their results on the crystal lattice properties of MgB<sub>2</sub> versus both temperature (11–297 K) and pressure (0–0.62 GPa) using neutron diffraction.

Here we report the results on an experimental measurement of the electrical resistivity and lattice compressibility, under hydrostatic pressure up to 10 GPa, of the MgB<sub>2</sub> superconducting material.

## 2. Experimental details

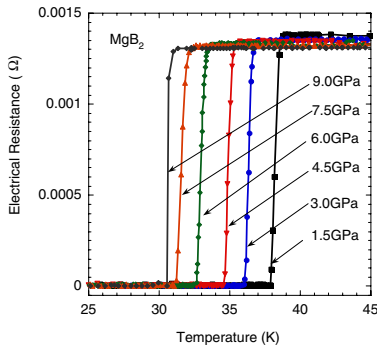
The MgB<sub>2</sub> material employed in the present investigation was prepared using a higher pressure (3.5 GPa compared with the pressure of 0.2 GPa used by Nagamatsu *et al* [1]) and higher sintering temperature (1000 °C). This material shows a substantial improvement in its superconducting performance [8]. Since it was high-pressure sintered, no porosity was observed in the material and it has a mass density of 2.66 g cm<sup>-3</sup>, close to the theoretical value of MgB<sub>2</sub> of 2.63 g cm<sup>-3</sup>.

For the *in situ* measurement of the lattice parameters under pressure, a diamond anvil cell was employed and synchrotron x-ray diffractograms were collected on imaging plates, using the Photon Factory beamline 18 C at the High Energy Accelerator Research Organization (KEK), Tsukuba, Japan.

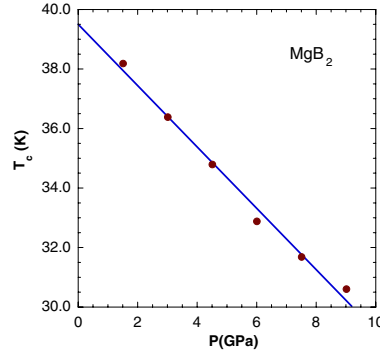
The electrical resistivity of the MgB<sub>2</sub> superconducting material was measured as a function of temperature at each fixed pressure with the DC four-probe method using a cubic anvil apparatus operated up to 10 GPa. The cubic anvil device is compressed evenly from six directions with six anvil tops, thereby producing a hydrostatic pressure on the sample material sealed in a gasket. The gasket material is a mixture of amorphous boron and epoxy resin in 4:1 weight ratio. Fluorinert liquid is used as the pressure medium to maintain the hydrostatic pressure. Low temperature down to 7 K is attained with continuous flows of liquid nitrogen and helium, successively.

## 3. Results and discussion

We measured the dependence of the superconductivity transition temperature  $T_c$  on pressure up to 10 GPa. The sharp drop of resistivity observed under ambient conditions was retained



**Figure 1.** Electrical resistivity versus temperature when the sample is subjected to various pressures up to 10 GPa. The transition from the normal state to the superconducting state takes place within a very narrow temperature range of about 0.2 K.



**Figure 2.** A plot of transition temperature  $T_c$  versus pressure  $P$ . A linear behaviour is observed and  $T_c$  decreases with increasing pressure at a rate of about  $1.03 \text{ K GPa}^{-1}$ .

even when the pressure was applied, as is shown in figure 1. A remarkable linear behaviour is observed up to the full range of 10 GPa and figure 2 shows the experimental data with a fitted linear curve that is expressed by

$$T_c = 39.6 - 1.03P.$$

The rate of decrease of  $T_c$ ,  $1.03 \text{ K GPa}^{-1}$ , is much lower than the value of  $1.6 \text{ K GPa}^{-1}$  obtained by Lorenz *et al* [5], and the negative slope of the  $T_c$ - $P$  relationship goes against the theoretical predictions by Hirsch [9]. On the other hand, the experimental observation suggests that  $T_c$  could be increased further if a chemical substitution could increase the lattice parameter while maintaining the same electronic structures, which is equivalent to producing a negative pressure.

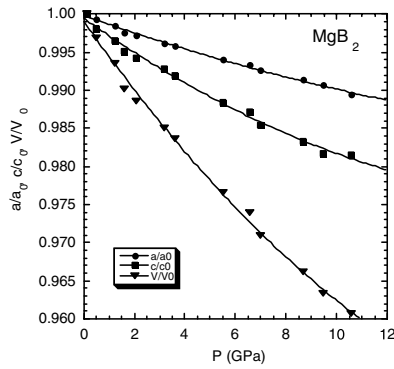
The transition range is about 0.5 K between the normal state and the superconducting state, demonstrating the superb quality of the MgB<sub>2</sub> material. Even when the material was subjected to high pressure, the transition width changed only slightly. For example, at the pressure 7.5 GPa, the transition width is measured to be 0.6 K, giving rise to an increase of the transition width at a rate less than  $0.1 \text{ K GPa}^{-1}$ . In addition, before the transition to superconducting behaviour occurred, the material showed a metallic behaviour upon cooling with a ratio of electrical resistivities

$$\frac{\rho(300 \text{ K})}{\rho(40 \text{ K})} = 1.93$$

at 1.5 GPa pressure and the ratio increased linearly with pressure, reaching 2.05 at 9.0 GPa pressure.

Figure 3 shows the dependence of the lattice parameters  $a$  and  $c$  and the unit-cell volume  $V$  on the applied pressure.

There is a significant difference between the contraction rates of the intra-planar periodicity  $a$  and the inter-planar periodicity  $c$ ; the latter reduces about 1.4 times as fast as the former, signifying that the structure is more compressible in the  $c$ -direction than in the  $a/b$ -directions. A least-squares linear fitting of the experimental data yielded a value for the bulk modulus  $B_0 = 172 \text{ GPa}$  while a value of  $B_0 = 174 \text{ GPa}$  was obtained using a least-squares fitting of the Murnaghan equation. The volume compressibility  $\kappa$  was also deduced from the experimental data and showed a weak dependence on the pressure.



**Figure 3.** Dependences of the lattice parameters  $a$  and  $c$  and the unit-cell volume  $V$  on the applied pressure up to 10 GPa. The plots are given as ratios to the corresponding values at ambient conditions. The deduced bulk modulus of the  $\text{MgB}_2$  material is  $B_0 = 172$  GPa.

The boron isotope effect has indicated that the superconductivity in the  $\text{MgB}_2$  material is phonon mediated, and can be described within the framework of the BCS theory [10]. Using the McMillan formula [11], we estimated the pressure dependence of the transition temperature  $T_c$  within the framework of the BCS theory [12] and obtained

$$\frac{dT_c}{dP} \approx -1.22 \text{ K GPa}^{-1},$$

which is very close to our experimental value of  $-1.03 \text{ K GPa}^{-1}$ . However, we should note here that since the McMillan formula was deduced for isotropic structures, given the anisotropic nature of the  $\text{MgB}_2$  structure, the above analysis has limits on its validity [13].

#### 4. Conclusions

The  $\text{MgB}_2$  material synthesized under high pressure and high temperature shows an improved superconducting performance characterized by (a) a sharp transition from the normal state to the superconducting state, (b) a lower rate of decrease ( $\sim 1.03 \text{ K GPa}^{-1}$ ) of the transition temperature  $T_c$  with increasing pressure, and (c) lower ratios of electrical resistivities  $\rho(300 \text{ K})/\rho(40 \text{ K})$ . These characteristics of the transport properties are preserved under pressure at least up to 10 GPa and the pressure effect on  $T_c$  is well explained within the framework of the classical BCS theory based on the electron–phonon coupling mechanism.

#### References

- [1] Nagamatsu J, Nakagawa N, Muranaka T, Zenitani Y and Akimitsu J 2001 *Nature* **410** 63
- [2] Kortus J, Mazin I I, Belashchenko K D, Antropov V P and Boyer L L 2001 *Preprint cond-mat/0101446v2*
- [3] Vogt T, Schneider G, Hriljac J A, Yang G and Abell J S 2001 *Preprint cond-mat/0102480*
- [4] Prassides K, Iwasa Y, Ito T, Chi D H, Uehara K, Nishibori E, Takata M, Sakata S, Ohishi Y, Shimomura O, Muranaka T and Akimitsu J 2001 *Preprint cond-mat/0102507*
- [5] Lorenz B, Meng R L and Chu C W 2001 *Preprint cond-mat/0102264v2*
- [6] Loa I and Syassen K 2001 *Preprint cond-mat/0102462*
- [7] Jorgensen J D, Hinks D G and Short S 2001 *Preprint cond-mat 0103069*
- [8] Takano Y, Takeya H, Fujii H, Kumakura H, Hatano T, Togano K, Kito H and Ihara H 2001 *Appl. Phys. Lett.* **78** 2914
- [9] Hirsch J E 2001 *Preprint cond-mat/0102115*
- [10] Bud'ko S L, Lapertot G, Petrovic C, Cunningham C E, Anderson N and Canfield P C 2001 *Phys. Rev. Lett.* **86** 1877
- [11] McMillan W L 1968 *Phys. Rev.* **167** 331
- [12] Tang J, Qin L C, Matsushita A, Takano Y, Togano K, Kito H and Ihara H 2001 *Phys. Rev. B* **64** 132509
- [13] Wang Y, Plackowski T and Junod A 2001 *Preprint cond-mat/0103181*