

X-ray diffraction study of Be to megabar pressure

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

2002 J. Phys.: Condens. Matter 14 10569

(<http://iopscience.iop.org/0953-8984/14/44/334>)

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

Download details:

IP Address: 171.66.16.96

The article was downloaded on 18/05/2010 at 15:22

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

X-ray diffraction study of Be to megabar pressure

Kazutaka Nakano, Yuichi Akahama and Haruki Kawamura

Faculty of Science, Himeji Institute of Technology, Koto, Kamigohri, Hyogo 678-1297, Japan

E-mail: knakano@sci.himeji-tech.ac.jp

Received 21 June 2002

Published 25 October 2002

Online at stacks.iop.org/JPhysCM/14/10569

Abstract

Powder x-ray diffraction experiments on a low- Z element, Be, were performed at pressures up to 171 GPa using the synchrotron radiation source at SPring-8. All profiles were assigned to the hcp structure of the ambient phase, and the theoretically predicted hcp–bcc phase transition was not observed. The previously proposed hcp–hexagonal phase transition around 14.5 GPa was also not confirmed. The equation of state of hcp-Be was determined by a least mean squares fitting to the Birch–Murnaghan equation from these diffraction data. Calculated values of K_0 and K'_0 were 97.2 ± 2.5 GPa and 3.61 ± 0.07 , respectively.

1. Introduction

Beryllium (Be) has an hcp structure at ambient conditions. At ambient pressure and 1534 K, just before melting at 1560 K, the ambient hcp phase transforms to a bcc structure. The hcp–bcc transition is accompanied by a volume reduction of about 6% [1, 2]. The hcp–bcc phase boundary has a negative slope ($-60^\circ\text{C GPa}^{-1}$), and the transition temperature decreases with increasing pressure [3, 4]. Therefore, the hcp–bcc phase transition is expected under high pressure at room temperature. Theoretical calculations have predicted that the hcp–bcc (or fcc) phase transition occurs below 200 GPa at 0 K [5, 6]. A few static high-pressure experiments on the structure and the compressibility have been reported up to now [6, 8]. The x-ray study by Ming and Manghnani [8] has reported the structure transition from the hcp to *hexagonal* phase at pressure between 8.6 and 14.5 GPa [7] and the structure of the high-pressure phase has been reanalysed [9]. However, the hcp–bcc transition has not been confirmed yet.

In this paper, we report the results of powder x-ray diffraction experiments of Be at pressures up to 171 GPa at room temperature.

2. Experimental procedure

High-pressure x-ray diffraction experiments on Be were carried out by using a synchrotron radiation source of wavelength $\lambda = 0.4959$ Å on beam line BL10XU at the SPring-8 (Super

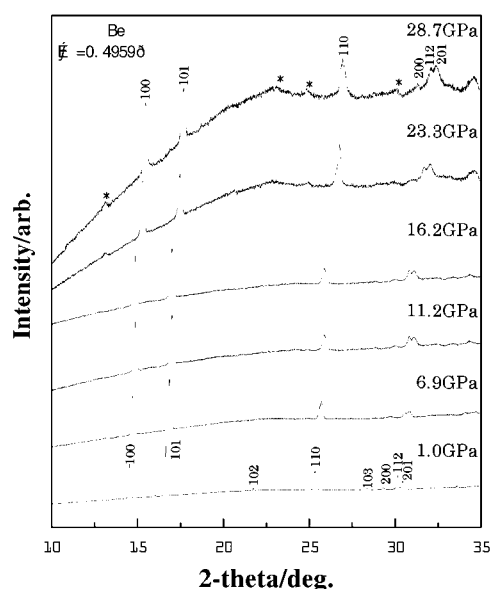


Figure 1. X-ray diffraction profiles of Be at lower pressure to 28.7 GPa. Peaks marked by asterisks come from the Kössel line.

Table 1. Diffraction data of hcp-Be at 28.7 GPa. hcp-Be: $a = 2.1284$ (2) Å, $c = 3.3564$ (20) Å.

| d_{obs} (Å) | (hkl) | d_{cal} (Å) | Error (%) |
|---------------|-----------|---------------|-----------|
| 1.8440 | 110 | 1.8436 | -0.020 |
| 1.6146 | 101 | 1.6150 | -0.023 |
| 1.0641 | 110 | 1.0644 | -0.030 |
| 0.9214 | 200 | 0.9218 | -0.046 |
| 0.8987 | 112 | 0.8982 | 0.053 |
| 0.8890 | 201 | 0.8888 | 0.028 |

Photon ring 8 GeV, Nishi-Harima, Japan, $E = 8$ GeV). Powder x-ray patterns were obtained by the angle dispersive method with an image plate detector and a diamond anvil cell. Three experimental runs were carried out using different culet sizes of diamond anvils, 600, 300 and 100 μm diameters, and powder patterns were collected at pressure up to 171 GPa. Beryllium sheet sample with a purity of 99.8% was put into a hole of a Re gasket together with a ruby chip and loaded by diamond anvils. No pressure transmitting medium was used. Pressure up to 80 GPa was determined by the ruby fluorescence method, and pressure higher than 80 GPa was estimated from the equation of state of a Re gasket [9].

3. Results and discussion

Figure 1 shows x-ray diffraction profiles of Be at lower pressures from 1.0 to 28.7 GPa. Six diffraction lines of (100), (101), (110), (200), (112) and (201) for hcp-Be are detected up to 28.7 GPa. The peaks marked by asterisks come from the Kössel line and become strong with increasing pressure. All profiles are assigned to the hcp structure of the ambient phase. The d -values of the pattern at 28.7 GPa are well explained as the hcp structure with the lattice parameters of $a = 2.1284$ (2) and $c = 3.3564$ (20) Å shown in table 1. In this study,

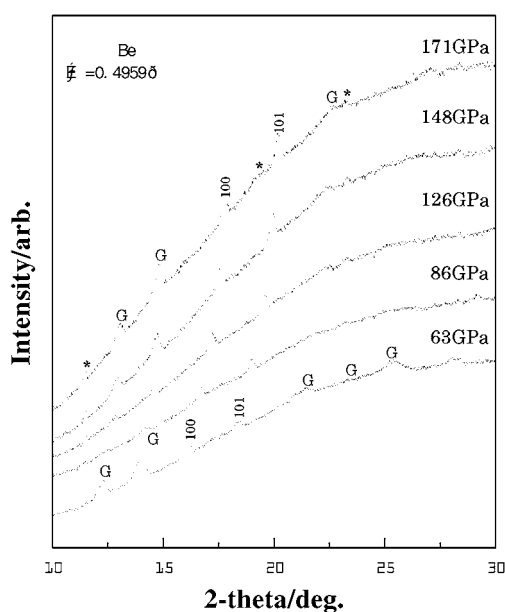


Figure 2. X-ray diffraction profiles of Be at higher pressures from 63 to 171 GPa. The peaks marked by asterisks come from the Kössel line and the diffraction lines marked by 'G' are from a Re gasket.

the hcp–hexagonal phase transition previously reported by Ming and Manghnani [8] was not observed.

Figure 2 shows x-ray diffraction profiles of Be at higher pressures from 63 to 171 GPa. Two diffraction lines of (100) and (101) from hcp-Be are clearly observed at the maximum pressure of 171 GPa. The previously reported hcp–hexagonal and the theoretically predicted hcp–bcc (or fcc) phase transitions were not observed up to 171 GPa. Actually, in several shock-compression experiments, no structural transition has been observed either [11–14]. The pressure dependences of the d -values of the two lines were consistent with present data in the lower-pressure region.

Figure 3 shows pressure dependences of lattice parameters, a and c , and their ratio, c/a , for hcp-Be. The lattice parameters decrease continuously with increasing pressure up to 171 GPa. The a axis is slightly more compressible than the c axis. The c/a ratio consequently increases with pressure and closes to the ideal value of 1.633. The value of c/a reaches 1.609 at 171 GPa.

Figure 4 shows the pressure dependence of the relative volume, V/V_0 , for hcp-Be together with previous data [8, 14]. The value of V/V_0 decreases monotonically with increasing pressure. From these data, the equation of state of hcp-Be was determined by a least mean squares fitting to the following Birch–Murnaghan equation [16]:

$$P(\text{GPa}) = \frac{3}{2}K_0 \left[\left(\frac{V_0}{V} \right)^{\frac{7}{3}} - \left(\frac{V_0}{V} \right)^{\frac{5}{3}} \right] \left\{ 1 - \frac{3}{4}(4 - K'_0) \left[\left(\frac{V_0}{V} \right)^{\frac{2}{3}} - 1 \right] \right\}.$$

Calculated values of K_0 and K'_0 are 97.2 ± 2.5 GPa and 3.61 ± 0.07 , respectively. These values are summarized in table 2 compared with previous data. Our value of K_0 is in good agreement with the previous data by the static compression [7, 8, 17] while the values of K_0 by the shock wave method [12, 14, 17, 18] are larger by 20 GPa than the present result. The value of K'_0 in this study agrees with the results in shock wave experiments.

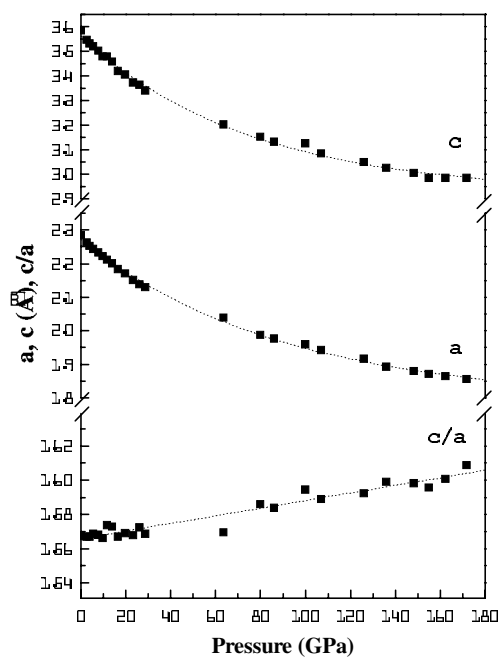


Figure 3. Pressure dependences of lattice parameters, a and c , and their ratio, c/a , for hcp-Be.

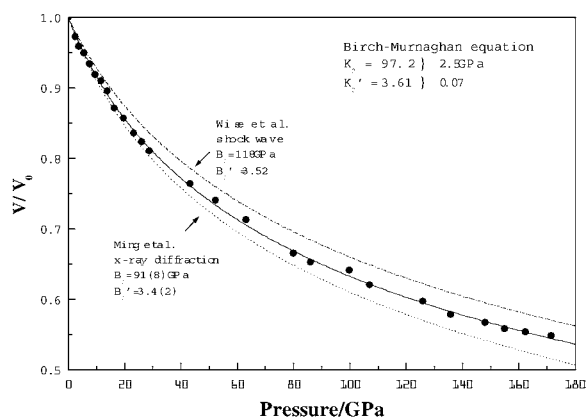


Figure 4. Pressure dependence of the relative volume, V/V_0 , for hcp-Be.

4. Conclusion

The present x-ray diffraction study on Be revealed that the hcp phase was stable at pressure up to 171 GPa at room temperature. Previously proposed hcp–bcc and hcp–hexagonal phase transitions were not observed. From the present diffraction data, the equation of state of hcp-Be was determined to 171 GPa by a least mean squares fitting to the Birch–Murnaghan equation. Estimated values of K_0 and K'_0 were 97.2 ± 2.5 GPa and 3.61 ± 0.07 , respectively.

Table 2. Values of K_0 and K'_0 for the equation of state of hcp-Be in the present study, together with previous data.

| K_0 (GPa) | K'_0 | Method | Reference |
|-------------|---------|------------|-----------|
| 118 | 3.52 | Shock wave | [14] |
| 119 | 3.48 | Shock wave | [18] |
| 118 | 3.50 | Shock wave | [12] |
| 120 | 3.5(1) | Shock wave | [17] |
| 89(13) | 21(7) | Volumetric | [7, 17] |
| 91(8) | 3.4(2) | X-ray dif. | [8, 17] |
| 97.2(2.5) | 3.61(7) | X-ray dif. | This work |

Acknowledgment

This work was performed under proposal No 1999A0092-CD-np at SPring-8.

References

- [1] Martin A J and Moore A 1959 *J. Less-Common Met.* **1** 85
- [2] Aldinger F *et al* 1979 *Beryllium Science and Technology* vol 1 p 235
- [3] Contre F M 1965 *Int. Met. Beryllium Comm.* **3** 201
- [4] Pistorius C W F T 1976 *Progress in Solid State Chemistry* vol 11 p 11
- [5] Lam P K, Chou M Y and Cohen M L 1984 *J. Phys. C: Solid State Phys.* **17** 2065
- [6] McMahan A K 1982 *AIP Conf. Proc.* **78** 304
- [7] Bridgman P W 1948 *Proc. Am. Acad. Arts Sci.* **76** 71
- [8] Ming L C and Manghnani M H 1984 *J. Phys. F: Met. Phys.* **14** L1
- [9] Vijayakumar V *et al* 1984 *J. Phys. F: Met. Phys.* **14** L65
- [10] Vohra Y K *et al* 1987 *Phys. Rev. B* **36** 9790
- [11] Rice M H, McQueen R G and Walsh J M 1962 *Solid State Phys.* **6** 1
- [12] McQueen R S *et al* 1970 *High Velocity Impact Phenomena* ed R Kinslow (New York: Academic)
- [13] Chhabildas L C, Wise J L and Assay J R 1982 *AIP Conf. Proc.* **78** 422
- [14] Wise J L 1982 *AIP Conf. Proc.* **78** 417
- [15] Kennedy G C and Keller R N 1972 *American Institute of Physics Handbook* 3rd edn (New York: McGraw-Hill) p 4
- [16] Birch F 1947 *Phys. Rev.* **71** 809
- [17] Schulte O and Holzapel W B 1996 *Phys. Rev. B* **53** 569
- [18] Neal T 1974 *High Pressure Science and Technology* vol 1, ed K D Timmerhaus *et al* (New York: Plenum) p 80