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The equation of state of Bi and cross-checking of Au and Pt scales to megabar pressure

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Abstract

By means of x-ray diffraction experiments using a synchrotron radiation source, the equation of state (EOS) of body-centred cubic Bi has been investigated over a range of multimegabar pressure up to 222 GPa on the basis of the Pt pressure scale and it is proposed as an internal pressure standard over a range of megabar pressures. Pressure scales of the EOS of Au and Pt were cross-checked and the accuracy of the scales is discussed.

1. Introduction

Recently, the arrival of third-generation synchrotron radiation (SR) sources and development of the diamond anvil cell (DAC) technique have extended the pressure range of materials research by means of x-ray diffraction experiments to 300 GPa. However, there are only a limited number of equations of state (EOS) for elemental materials available as a pressure scale for this extremely high-pressure range.

Bismuth (Bi) is a prototype group Vb element and shows a structural sequence of pressure-induced phase transitions, A7–(distorted sc)–distorted bcc–bcc [1, 2]. These transitions have been used as pressure fixed points at room temperature. The bcc phase, which occurs at 7.7 GPa, has a larger compressibility than Au and Pt and is stable up to 90 GPa [3]. Therefore, the EOS of the bcc phase is considered a candidate for providing the internal pressure standard for *in situ* high-pressure x-ray diffraction studies in the megabar pressure region.

The stability of the bcc phase is examined to multimegabar pressures and the EOS of the bcc phase has been determined on the basis of the Pt pressure scale. This report also includes cross-checking between Pt and Au pressure scales up to 150 GPa.

2. Experimental details

A DAC was used for the high-pressure generation. Powder x-ray diffraction experiments were carried out at 300 K by an angle-dispersive method with an image plate (IP) detector

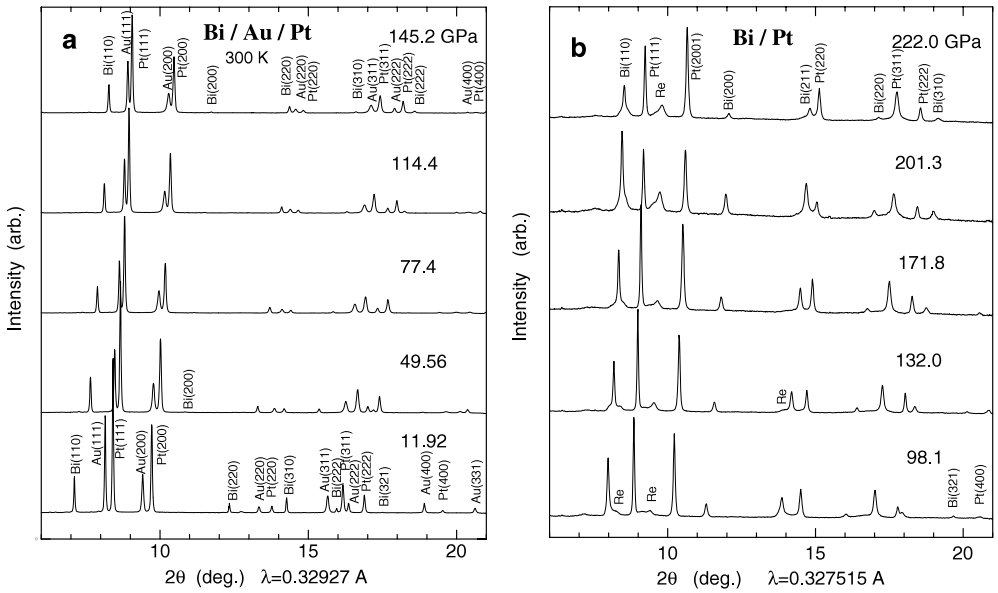

Figure 1. Typical x-ray diffraction patterns: (a) the patterns of the first run to 145 GPa; (b) those of the second run to 222 GPa.

and a high-energy SR source of $\lambda = 0.3292$ or 0.3275 Å on BL04B2 at SPring-8. The x-ray wavelength, the pixel size of the IP detector and the sample-to-detector distance were calibrated using a powder CeO_2 standard sample. In the first run, foil samples of Bi (99.9999% purity), Pt (99.98% purity) and Au (99.98% purity) were put into a hole in a Re gasket together with a ruby chip and compressed to 145 GPa with anvils of culet diameter 150 μm. The relation between the Au and Pt scales was also calibrated. In the second run, the Bi and the Pt foil samples were compressed to 222 GPa with anvils of 50 μm culet diameter. Pressure was determined from the EOS of Pt proposed by Holmes *et al* [4]. No pressure-transmitting medium was used.

3. Results

Figures 1(a) and (b) show typical diffraction patterns for both runs. The pressure was based on the Pt scale of Holmes *et al*. The bcc Bi did not show any structural transition and was stable up to 222 GPa. In the first run, the lattice constants of bcc Bi were determined with an accuracy of about ± 0.0005 Å. Since, in the present experiments, no pressure-transmitting medium was used, non-hydrostatic effects such as uniaxial stress are expected. Due to the uniaxial stress, the lattice strain results in scatter of the lattice constant estimated from each reflection [5]. However, the scatters for Bi, Au and Pt at 145 GPa are estimated to be 0.08, 0.15 and 0.08%, respectively, and smaller than the value (0.2%) for Au at 61 GPa with He as the pressure medium [6]. No remarkable sign of uniaxial stress effects is observed in the $h^2+k^2+l^2$ dependence of the lattice constants obtained from each reflection shown in figure 2. The pressure dependences of the full width at half-maximum (FWHM) of the diffraction peaks for Bi, Au and Pt are shown in figure 3. The FWHM for each sample increases slightly with pressure, reflecting the effect of the pressure gradient and the microscopic stress. Lattice constants (a), their estimated standard deviations (esd), d-values and calculated errors in the second run are summarized in table 1 for Bi and Pt samples, respectively. The lattice constants

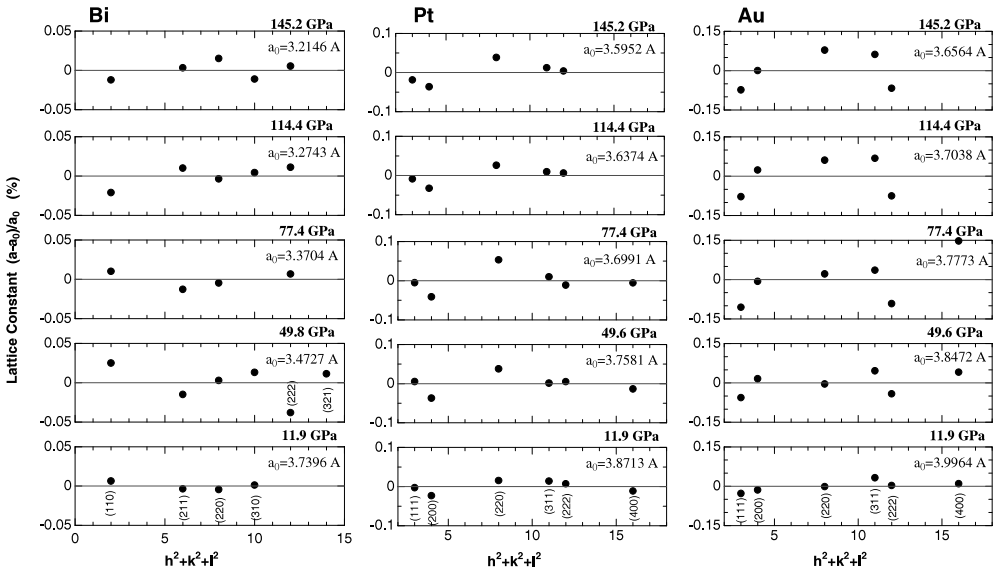

Figure 2. Lattice constants based on d-spacing at various pressures for Bi, Pt and Au.

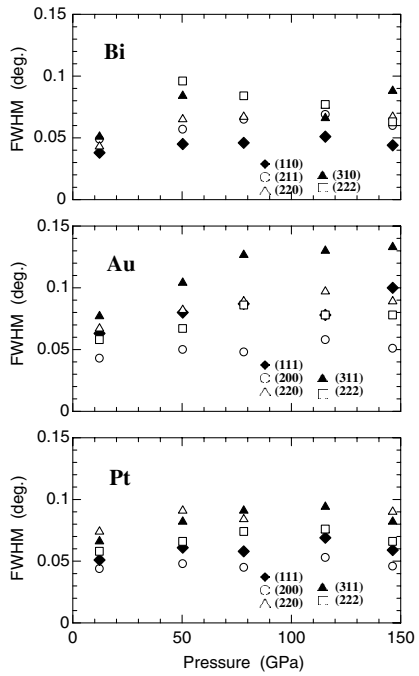

Figure 3. Changes of the FWHM for the reflection lines for Bi, Au and Pt.

of bcc Bi and fcc Pt up to 201 GPa were also determined precisely within the esd of about ± 0.0010 Å and the scatters were about 0.07%.

Table 1. Diffraction data for Bi and Pt at various pressures in the second experimental run.

		98.1 GPa			132.0 GPa			171.8 GPa			201.3 GPa			222.0 GPa	
Bi	*a*	3.315 46		*a*	3.240 83		*a*	3.172 43		*a*	3.130 41		*a*	3.104 6	
	esd	0.000 82		esd	0.000 31		esd	0.000 42		esd	0.001 04		esd	0.002 02	
	d-value	*a*	Error (%)	*d*-value	*a*	Error (%)	*d*-value	*a*	Error (%)	*d*-value	*a*	Error (%)	*d*-value	*a*	Error (%)
110	2.344 3	3.315 34	−0.003 52	2.291 8	3.241 1	0.008 13	2.243 11	3.172 23	−0.006 35	2.212 71	3.129 25	−0.037 05	2.194 32	3.103 23	−0.043 99
200	1.657 98	3.315 96	0.015 24	1.620 54	3.241 08	0.007 5	1.586 29	3.172 58	0.004 73	1.565 53	3.131 05	0.020 53	1.553 94	3.107 89	0.105 97
211	1.353 3	3.314 88	−0.017 25	1.323 15	3.241 04	0.006 37	1.295 1	3.172 32	−0.003 47	1.278 12	3.130 75	0.010 88	1.267 24	3.104 09	−0.016 36
220	1.171 86	3.314 53	−0.027 93	1.145 79	3.240 77	−0.001 87	1.121 5	3.172 08	−0.011 12	1.106 4	3.129 38	−0.032 68	1.097 01	3.102 8	−0.057 89
310	1.048 79	3.316 57	0.033 45	1.024 66	3.240 27	−0.017 22	1.003 13	3.172 17	−0.008 18	0.990 3	3.131 61	0.038 4	0.981 88	3.104 98	0.012 32
222				0.935 52	3.240 74	−0.002 86	0.916 03	3.173 21	0.024 36						
Pt	*a*	3.662 76		*a*	3.612 35		*a*	3.563 47		*a*	3.532 24		*a*	3.512 21	
	esd	0.000 88		esd	0.000 63		esd	0.001 53		esd	0.000 92		esd	0.000 97	
	d-value	*a*	Error (%)	*d*-value	*a*	Error (%)	*d*-value	*a*	Error (%)	*d*-value	*a*	Error (%)	*d*-value	*a*	Error (%)
111	2.114 05	3.661 63	−0.030 82	2.085 46	3.612 12	−0.006 31	2.057 57	3.563 82	0.009 98	2.038 88	3.531 45	−0.022 34	2.026 99	3.510 85	−0.038 6
200	1.831 96	3.663 92	0.031 51	1.805 79	3.611 58	−0.021 42	1.780 72	3.561 43	−0.057 05	1.766 73	3.533 47	0.034 74	1.756 75	3.513 49	0.036 55
220	1.295	3.662 8	0.001 02	1.277 42	3.613 1	0.020 8	1.260 25	3.564 53	0.029 74	1.248 47	3.531 2	−0.029 44	1.241 68	3.512	−0.006 07
311	1.104 51	3.663 23	0.012 71	1.089 21	3.612 49	0.003 86	1.074 1	3.562 4	−0.029 96	1.065 1	3.532 54	0.008 42	1.059 1	3.512 63	0.011 94
222	1.057 2	3.662 23	−0.014 42	1.042 99	3.613 01	0.018 22	1.029 71	3.565 15	0.047 25	1.019 76	3.532 54	0.008 58	1.013 85	3.512 07	−0.003 84
400				0.902 95	3.611 8	−0.015 11									

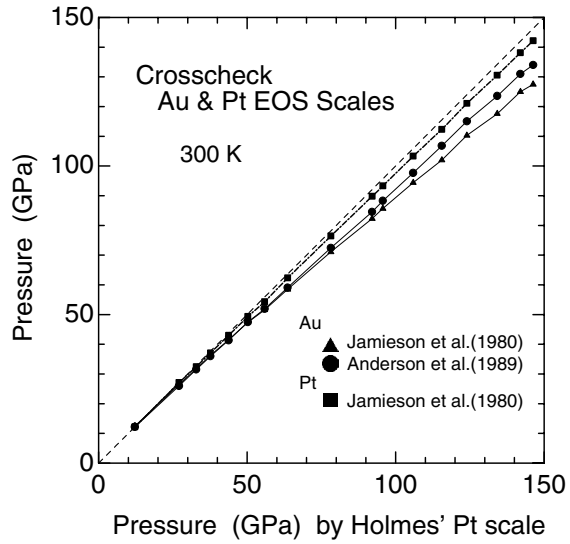

Figure 4. The relation between the Holmes Pt scale and the others.

4. Cross-checking of the Pt and Au pressure scales

The EOS of Pt has been proposed as a pressure scale by Holmes *et al* on the basis of Hugoniot data up to 660 GPa [4] while Jamieson's scales of Au and Pt were limited to about 100 GPa [7]. In order to compare with our previous compression data on Bi [3], which were scaled with the EOS of Au by Jamieson *et al*, the Pt and Au scales were cross-checked. Figure 4 shows the relation between these scales based on the Holmes Pt scale. It is found that there is the remarkable difference between Holmes' Pt and Jamieson's Au scales, and around 150 GPa the latter scale provides pressure lower by 20 GPa than the former. The difference in the higher-pressure region between Au and Pt scales is an open question. It is crucial to verify the accuracy of these scales in the megabar pressure range.

5. The equation of state of bcc Bi

The pressure dependence of the unit-cell volume is shown in figure 5 together with previous data [3] which were measured with a laboratory source, Mo Kα, by using the Au pressure scale given by Jamieson *et al* [3]. If we replot the present P–V curve with the Au scale, the result is in good agreement with our previous data shown in this figure. The bulk modulus, B_0, its pressure derivative, B_0', and the relative atomic volume, V/V_0, of the bcc phase at atmospheric pressure are estimated to be 51.8(5), 4.91(6) and 0.862(7) GPa, respectively, from a least-squares fitting to the Birch–Murnaghan equation. B_0 and B_0' for bcc Bi are smaller than the values for Au and Pt. The bcc phase is stable up to 222 GPa and the FWHM of the diffraction peaks and the scatter of the lattice constant based on the d-spacing are also small compared with those for these elements. The EOS of bcc Bi may be proposed as a candidate for providing the pressure scale at megabar pressure.

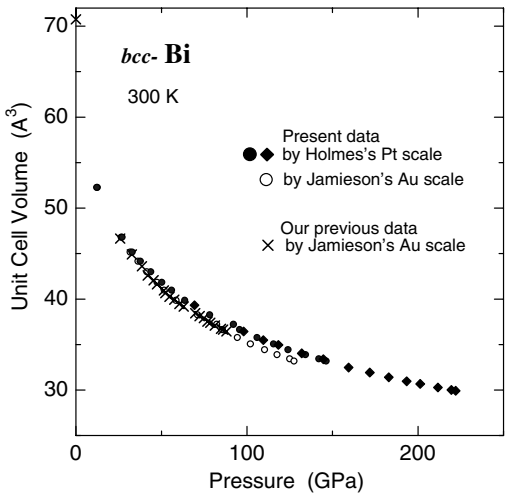

Figure 5. The pressure dependence of the unit-cell volume of bcc Bi.

Acknowledgments

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References

[1] Iwasaki H and Kikegawa T 1997 *Acta Crystallogr.* B **53** 353
[2] Aoki K, Fujiwara S and Kusakabe M 1982 *J. Phys. Soc. Japan* **51** 3826
[3] Akahama Y, Kobayashi M and Kawamura H *Proc. 31th High Pressure Conf. (Osaka 1990)* pp 392–3
[4] Holmes N C *et al* 1989 *J. Appl. Phys.* **66** 2962
[5] Singh A K 1993 *J. Appl. Phys.* **73** 4278
[6] Singh A K 1993 *J. Appl. Phys.* **74** 5920
[7] Takemura K 2001 *J. Appl. Phys.* **89** 662
[8] Jamieson J C *et al* 1980 *Adv. Earth Planet. Sci.* **12** 27
[9] Anderson O L, Isaak D G and Yamamoto S 1989 *J. Appl. Phys.* **65** 1534