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The Axial Expansions of BeO Between Room Temperature and 1700°C*

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The temperature dependencies of the lattice constants of BeO have been determined to provide the necessary intermediate data for assigning sample temperatures to high-temperature X-ray powder diffraction experiments. An accuracy of 10 °C at temperatures up to at least 1700 °C can be attained if precise diffraction measurements are made. The lattice-constant values, used to precalculate diffraction maxima locations at various temperatures, are given by $a_{t_2}=a_{t_1}+\Delta a_{t_2}\pm X_a$ and $c_{t_2}=c_{t_1}+\Delta c_{t_2}\pm X_c$ where t_1 is the room temperature, t_2 is the test temperature, Δa_{t_2} and Δc_{t_2} are defined by

$$\Delta a_{t_2}=-5\cdot30_3\times10^{-4}+1\cdot87_1\times10^{-5}(t_2)+8\cdot06_4\times10^{-9}(t_2)^2\ \text{Å}$$
$$\Delta c_{t_2}=-7\cdot27_4\times10^{-4}+2\cdot56_2\times10^{-5}(t_2)+1\cdot26_5\times10^{-8}(t_2)^2\ \text{Å}$$

and X_a and X_c are the corrections, calculated from the delta-equations, for the difference between the 28 °C room temperature of these experiments and the room temperature at which the lattice constants, a_{t_1} and c_{t_1}, are determined for the user's BeO material.

Introduction

The poorest known and, perhaps, the most important experimental parameter in high-temperature X-ray diffractometry is the sample temperature. If the sample has any appreciable thickness, if it is of low thermal conductivity, and if it is of relatively low bulk density such as a powder, it is very difficult to measure accurately the temperature within the diffracting volume.

However, an indirect sample temperature assignment can be made if the thermal expansion values of an admixed internal standard are accurately known. The temperature dependency data for any suitable material, over a large temperature range, were not known to any reasonable precision or accuracy until Campbell (1962) reported such data for platinum at temperatures up to about 1100°C. This paper reports the axial expansion data for beryllium oxide, another suitable reference material, in the range from 28° to 1700°C with respect to the platinum data.

Although the BeO lattice-constant values are used to precalculate the temperature calibration data, the absolute values of the constants are not of particular importance; only the differences in values from one temperature to another were used to obtain the axial expansion characteristics. Systematic and random diffractometry error corrections need not be applied to the experimental data (to obtain accurate lattice-constant values) if the same errors, and their magnitudes, are present throughout the temperature range of the experiments. Because the Debye temperature correction is small, its use does not significantly affect the temperature measurement accuracy (10°C) for the reported data. Perhaps that correction should be considered when the basic reference data (the Campbell platinum expansion data) are more accurately known.

Therefore, the present data are given in terms of the changes in the lattice-constant values with respect to temperature so that the experimentalist can adjust the observed and/or calculated data, if desired, to account for applicable corrections related to the instrumentation and procedures being used. After the room temperature lattice-constant values have been determined for the BeO reference material, the locations of the diffraction maxima are calculated at the temperatures of interest with respect to the radiation and with or without the correction factors.

Literature

There are considerable room-temperature diffraction and expansion data available for platinum, cubic, *Fm*3*m* (O_h^5). Swanson & Tatge (1953) and Campbell (1962) provide rather complete summaries. Campbell reported a polynomial equation describing the expansion of platinum from 25°C:

$$\%\ \text{Expansion}=[8\cdot91+1\cdot28\times10^{-3}\,(t-25)+0\cdot04\times10^{-6}\,(t-25)^2]\,(t-25)/100$$

where t is in degrees Celsius. The equation was derived from data having reported accuracies of 2°C from 25° to 700°C, 5°C from 700° to 1100°C, and 25°C above 1100°C.

The temperature calibration data for the platinum sample were obtained by using the platinum expansion equation, the value of the uncorrected platinum lattice constant at 28°C ($3\cdot923_3$ Å), and 1·5405 Å for the wavelength of Cu $K\alpha_1$ radiation. The °2θ locations of the nine platinum diffraction maxima reported by

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Swanson & Tatge (1953) were precalculated at 5 °C intervals in the range from 100° to 1700 °C.

The data and bibliographies reported by Swanson & Tatge (1953), by Bellamy, Baker & Livey (1962), and by Grain & Campbell (1962) summarize most of the known information for beryllium oxide, hexagonal, $P6_3mc$ (C_{6v}^4). Table 1 gives some of these data. At 28 °C, the uncorrected lattice-constant values for the BeO sample were determined from the observed data to be: $a = 2{\cdot}698_8$, $c = 4{\cdot}379_2$ Å with standard deviations of $0{\cdot}001_1$ and $0{\cdot}002_0$ Å, respectively; these values were not corrected for any random or systematic diffractometry errors.

Table 1. *Data for* BeO

	Lattice constants (Å)	
	a	*b*
Zachariasen, 1925, 1926	2·699	4·401
Aminoff, 1925	2·69	4·37
Brakken & Jore, 1935 (18 °C)	2·6929	4·3972
Swanson & Tatge, 1953 (26 °C)	2·698	4·380
Elston & Caillet, 1958	2·6981	4·3767
Bellamy, Baker & Livey, 1962 (21 °C)	2·6978	4·3772

Spectrochemical analyses of the BeO and platinum showed that each was free of appreciable contamination. The major impurities occurring in the platinum were 500 ppm of gold and 200 ppm of palladium of the total 730 ppm impurity detected. The major impurities occuring in the BeO were 600 ppm of aluminum, 350 ppm of calcium, and 300 ppm of silicon of the total 1500 ppm impurity detected.

Procedures

BeO plus 10 wt.% Pt mixtures were thoroughly mixed and dry-pressed at 8000 psi into 60Pt/40Rh sample holders; both as-mixed and presintered (1750 °C) samples were used. It had been shown that no reactions occur between these materials at any of the test temperatures.

All of the high-temperature X-ray diffraction data were obtained in a normal air atmosphere in an inductively heated diffractometer apparatus developed in this laboratory. In all instances, the test temperatures were controlled within 1 °C. The actual temperatures were assigned by comparing the locations of the experimental platinum diffraction maxima with those precalculated for four reflections: 111, 200, 220, and 311. None of the temperature conversion values varied by more than 5 °C from each of the reported test temperatures.

All diffraction data were obtained in the range from 90° to 29° 2θ at both $\frac{1}{4}$° and $\frac{1}{8}$° 2θ/min. scanning speeds. Although no major differences were noted for these results, only the slow-scan data were used to derive the axial expansion characteristics of BeO. At each temperature, the sample was aligned at the zero position of the diffractometer with an accuracy of 0·005° 2θ or less at a precision between 0·0017° and 0·002° 2θ. The procedure developed in this laboratory is not concerned with the diffraction from any component of the sample; the alignment is made with respect to the sample surface and the central ray of the X-ray beam. The procedure and the mechanical components of the apparatus permit detection of, and correction for, misalignments of 0·0001 inch or more. This precision is equivalent to a theoretical angular misalignment error of 0·0017° 2θ at the diffractometer zero; the value goes to zero at 180° 2θ. At each temperature, the alignment was rechecked after the diffraction data were obtained. If the sample had changed position because of an unexpected expansion, warping or tilting of the sample holder assembly or of the sample itself, mechanical movements in the system, *etc*, the results were discarded, the alignment was reestablished, and the diffraction scan was remade. This occurred infrequently and only at the highest test temperatures.

Many of the data obtained at temperatures between 1625° and 1750 °C were not included in any of the computational analyses because of deterioration of the platinum diffraction maxima (but not the BeO maxima). This was attributed to a reaction of the platinum standard with the volatile rhodium of the alloy sample holder. Eight BeO maxima, 100, 002, 101, 102, 110, 103, 112, and 201, were measured at each of the test temperatures. The 200 maximum was used whenever it could be clearly defined.

Two methods were used to obtain the uncorrected BeO lattice-constant values from the observed data: (1) a least-squares solution without subsequent refinement, and (2) a purely algebraic solution. In the latter method, *a* and *c* were evaluated by simultaneous solutions of algebraically derived equations relating the constants to the *d*-spacings of two indexed diffraction maxima. The values reported are the averages of the solutions for all possible combinations of two maxima; the standard deviations ($n-1$ method) of the mean values were calculated.

Results

All of the data were obtained from the °2θ locations, the half-width at two-thirds height of the clearly resolved α_1 maxima; nickel-filtered Cu *K* radiation was used. Only the experimental data for test temperatures up to about 1200 °C were used for the computations. This is the temperature range in which the greatest confidence (2° to 5 °C accuracy) can be placed upon the reported platinum expansion data (Campbell, 1962). When the derived BeO data were extrapolated to higher temperatures, they agreed (within 5 °C) with the higher temperature experimental data that were not used in the analyses. Table 2 gives the uncorrected lattice-constant values obtained from the two computational methods; there were no significant differences. The standard deviations of the mean values (from the algebraic solutions) at all test temperatures were averaged;

these were $0{\cdot}001_1$ Å for a and $0{\cdot}002_0$ Å for c. Table 3 gives an example of the observed and the calculated d-values at one test temperature. Because the standard deviations of the mean values of the uncorrected lattice constants were relatively small, because there was good agreement between the calculated and the observed diffraction maxima locations (the effect of diffraction measurement precision will be noted later), and because the uncorrected lattice-constant values calculated from each of the platinum diffraction maxima were within an average of 0·0005 Å of the mean value at each temperature, it seemed reasonable to assume that the systematic and random errors were essentially the same at each of the precisely controlled (1 °C) test temperatures and that their magnitudes were quite small. Then, the differences in the uncorrected axial lengths at different temperatures should reflect, accurately, their expansion characteristics. Therefore, only the uncorrected a and c mean values, obtained by the algebraic method, were used in the polynomial curve-fitting analyses of the temperature-expansion relations.

Table 2. *Uncorrected* BeO *lattice constants at various test temperatures*

	Algebraic solution*		Least-squares solution	
Temp. (°C)	a (Å)	c (Å)	a (Å)	c (Å)
28	$2{\cdot}698_8$	$4{\cdot}379_2$	$2{\cdot}698_3$	$4{\cdot}379_6$
245	$2{\cdot}703_3$	$4{\cdot}385_3$	$2{\cdot}703_1$	$4{\cdot}385_0$
580	$2{\cdot}711_8$	$4{\cdot}396_5$	$2{\cdot}711_7$	$4{\cdot}396_5$
782	$2{\cdot}717_9$	$4{\cdot}407_2$	$2{\cdot}717_8$	$4{\cdot}406_4$
1005	$2{\cdot}725_0$	$4{\cdot}416_7$	$2{\cdot}724_5$	$4{\cdot}416_5$
1192	$2{\cdot}732_0$	$4{\cdot}426_7$	$2{\cdot}731_9$	$4{\cdot}426_4$
1289	$2{\cdot}735_5$	$4{\cdot}432_8$	$2{\cdot}735_1$	$4{\cdot}432_1$
1383	$2{\cdot}739_3$	$4{\cdot}438_4$	$2{\cdot}738_6$	$4{\cdot}438_1$
1492	$2{\cdot}743_4$	$4{\cdot}444_3$	$2{\cdot}742_3$	$4{\cdot}444_2$
1570	$2{\cdot}747_1$	$4{\cdot}450_2$	$2{\cdot}746_9$	$4{\cdot}450_0$

* The standard deviations of the mean values obtained for all test temperatures were averaged. These average values are $\sigma(a)=0{\cdot}001_1$ Å and $\sigma(c)=0{\cdot}002_0$ Å.

These relations were obtained in terms of the changes of the lattice-constant values (rather than in terms of the absolute values) because such data are more readily applicable. The changes at various temperatures are precalculated. They are added to the room-temperature lattice constant determined for the user's BeO sample according to

$$a_{t_2}=a_{t_1}+\Delta a_{t_2}\pm X_a \quad \text{and}$$
$$c_{t_2}=c_{t_1}+\Delta c_{t_2}\pm X_c$$

where t_1 is the user's room temperature, t_2 is the test temperature, Δa_{t_2} and Δc_{t_2} are defined by

$$\Delta a_{t_2}=-5{\cdot}30_3\times10^{-4}+1{\cdot}87_1\times10^{-5}(t_2)+8{\cdot}06_4\times10^{-9}(t_2)^2\ \text{Å}$$

$$\Delta c_{t_2}=-7{\cdot}27_4\times10^{-4}+2{\cdot}56_2\times10^{-5}(t_2)+1{\cdot}26_5\times10^{-8}(t_2)^2\ \text{Å}$$

and X_a and X_c are the corrections, obtained from the Δ equations, for the difference between the 28 °C room temperature of these experiments and the room temperature condition used for the determination of the BeO lattice constants, a_{t_1} and c_{t_2}. The Δ equations were obtained with unbiased standard errors of estimate* of $1{\cdot}1\times10^{-4}$ and $8{\cdot}6\times10^{-4}$, coefficients of determination of 0·9999 and 0·9986, and multiple regression coefficients of 0·9999 and 0·9993, respectively. Table 4 gives the calculated values for the room-temperature correction factor in the range from 16° to 35 °C; the applicability of the significance of the correction can be evaluated only by the user with respect to the precision and accuracy of his instrumentation and procedures.

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* The unbiased standard error of estimate (in units of the dependent variable of the equation – the lattice-constant values) is the standard deviation of the fit of the regression analysis (*i.e.*, the deviation about a line of regression) at the mean value of the dependent variable; it cannot be precisely evaluated at either end of the line of regression.

Table 3. *Observed and calculated d-values for* BeO *at* 1005 °C

Experimental data				Uncorrected lattice constants by algebraic solution	Uncorrected lattice constants by least-squares solution
hkl	I/I_0 (%)	Location (°2θ)	d obs.* (Å)	d calc.† (Å)	d calc.‡ (Å)
100	91	38·080	2·3611	2·3599	2·3595
002	61	40·805	2·2095	2·2083	2·2082
101	100	43·418	2·0824	2·0813	2·0811
102	22	57·068	1·6125	1·6124	1·6123
110	29	68·865	1·3622	1·3625	1·3622
103	24	76·160	1·2489	1·2491	1·2490
200§	~4	(81·5)	—	—	—
112	16	83·275	1·1593	1·1595	1·1594
201	5	85·035	1·1397	1·1399	1·1398

* Computed with $\lambda=1{\cdot}54050$ Å.
† Computed with $a=2{\cdot}72503$, $c=4{\cdot}41670$ Å; see Table 2.
‡ Computed with $a=2{\cdot}72446$, $c=4{\cdot}41647$ Å; see Table 2.
§ Not clearly resolved at this temperature.

Table 4. *Room-temperature correction factors*

These values are added to, or subtracted from, the room temperature lattice-constant values.

Temp.	X_a	X_c
16 °C	+0·00022 Å	+0·00031 Å
17	+0·00020	+0·00028
18	+0·00019	+0·00026
19	+0·00017	+0·00023
20	+0·00015	+0·00020
21	+0·00013	+0·00018
22	+0·00011	+0·00015
23	+0·00009	+0·00013
24	+0·00007	+0·00010
25	+0·00005	+0·00007
26	+0·00003	+0·00005
27	+0·00001	+0·00002
28	0·00000	0·00000
29	−0·00001	−0·00002
30	−0·00003	−0·00005
31	−0·00005	−0·00007
32	−0·00007	−0·00010
33	−0·00009	−0·00013
34	−0·00011	−0·00015
35	−0·00013	−0·00018

For the direct temperature conversion of the user's experimental diffraction data, the user should precalculate the locations of the diffraction maxima of his BeO material at the temperatures of interest with respect to the X-radiation used and with or without systematic, or other, correction factors. These are the observer's reference data. They provide the means to assign high-temperature X-ray diffraction test temperatures to within 10°C for his particular BeO with other data generated within his own laboratory or in another laboratory and to compute and to compare experimentally derived reflection locations, corrected or uncorrected lattice-constant values, expansion values, *etc.*

It is believed that the 2 °C accuracy reported for the platinum data (Campbell, 1962) cannot be achieved with mechanical diffractometers even at test temperatures less than 700 °C. Using Cu $K\alpha_1$ radiation, for example, requires significance in angular measurements of platinum diffraction maxima for a 2 °C accuracy at 500 °C of less than 0·001° 2θ for the 111 reflection (at ~39°), of about 0·002° 2θ for the 311 reflection (at ~81°), about 0·004° 2θ for the 331 reflection (at ~117°), and 0·008° 2θ for the 422 reflection (at ~147°). In order to achieve reasonable confidence in the temperature assignments made from observed data, it is recommended that at least four reflections be used to obtain the average value for each test temperature. It should be noted that the Lorentz polarization and the X-ray slit axial divergence corrections increase as the measurement angle increases and that the extent of these may nullify the tacitly assumed advantage of back-reflection region diffraction experimentation. Therefore, the conservative 10 °C accuracy claimed for the uncorrected BeO data was based upon measuring as many of the Pt and BeO α_1 maxima as could be

Table 5. *Comparison of* BeO *expansion values at* 100° C *intervals to* 2000 °C

	This report			U.S. Bur. Mines*			
Temp. °C	*a* axis %	*c* axis %	Avg.‡ %	*a* axis %	*c* axis %	Avg.‡ %	N.B.S.† Dilat. %
28	$0{\cdot}00_0$	$0{\cdot}00_0$	$0{\cdot}00_0$	0·00§	0·00§	0·00§	0·00(0·00)
100	$0{\cdot}05_1$	$0{\cdot}04_2$	$0{\cdot}04_8$	0·05	0·04	0·05	—
200	$0{\cdot}12_9$	$0{\cdot}10_9$	$0{\cdot}12_3$	0·12	0·10	0·11	0·12(0·10)
300	$0{\cdot}21_3$	$0{\cdot}18_2$	$0{\cdot}20_3$	0·20	0·17	0·19	—
400	$0{\cdot}30_3$	$0{\cdot}26_0$	$0{\cdot}28_9$	0·28	0·25	0·27	0·28(0·26)
500	$0{\cdot}40_0$	$0{\cdot}34_5$	$0{\cdot}38_1$	0·37	0·33	0·36	—
600	$0{\cdot}50_2$	$0{\cdot}43_5$	$0{\cdot}47_9$	0·47	0·42	0·45	0·48(0·45)
700	$0{\cdot}61_0$	$0{\cdot}53_1$	$0{\cdot}58_3$	0·57	0·51	0·55	—
800	$0{\cdot}72_4$	$0{\cdot}63_2$	$0{\cdot}69_3$	0·68	0·61	0·66	0·69(0·65)
900	$0{\cdot}84_4$	$0{\cdot}74_0$	$0{\cdot}80_9$	0·80	0·71	0·77	—
1000	$0{\cdot}97_0$	$0{\cdot}85_3$	$0{\cdot}93_1$	0·92	0·83	0·89	0·92
1100	$1{\cdot}10_2$	$0{\cdot}97_2$	$1{\cdot}05_9$	1·05	0·94	1·01	—
1200	$1{\cdot}24_0$	$1{\cdot}09_7$	$1{\cdot}19_2$	1·19	1·07	1·15	1·16
1300	$1{\cdot}38_4$	$1{\cdot}22_8$	$1{\cdot}33_2$	1·33	1·20	1·28	—
1400	$1{\cdot}53_4$	$1{\cdot}36_4$	$1{\cdot}47_7$	1·48	1·33	1·43	1·40
1500	$1{\cdot}69_0$	$1{\cdot}50_7$	$1{\cdot}62_9$	1·63	1·48	1·58	—
1600	$1{\cdot}85_2$	$1{\cdot}65_5$	$1{\cdot}78_6$	1·79	1·62	1·74	1·66
1700	$2{\cdot}02_0$	$1{\cdot}80_9$	$1{\cdot}95_0$	1·96	1·78	1·90	1·78
1800	$2{\cdot}19_4$	$1{\cdot}96_8$	$2{\cdot}11_9$	2·13	1·94	2·07	—
1900	$2{\cdot}37_4$	$2{\cdot}13_4$	$2{\cdot}29_4$	2·31	2·11	2·24	—
2000	$2{\cdot}56_0$	$2{\cdot}30_6$	$2{\cdot}47_6$	2·50	2·28	2·43	—

* Grain & Campbell, 1962. The values listed were computed from the reported data; those at 1200 °C and above were extrapolated from the lower temperature data.

† Geller & Yavorsky, 1954. The values in parentheses were determined interferometrically; the others were determined using a sapphire-rod dilatometer.

‡ Hidnert & Souder, 1950. A computational method for calculating the bulk (average) linear expansion.

§ These data were reported to begin at 25 °C.

clearly resolved. For a 10 °C accuracy (that is, no values exceeding 5 °C from the mean value) at temperatures up to at least 1700 °C, the required diffraction maxima location measurement accuracies for Cu $K\alpha_1$ radiation are 0·004° to 0·006°, 0·010° to 0·012°, 0·020° to 0·024°, and 0·040° to 0·044° 2θ for the 111, 311, 331, and 422 platinum maxima and 0·004° to 0·006°, 0·006° to 0·008°, 0·008 to 0·012°, 0·010° to 0·014°, and 0·036 to 0·040° 2θ for the 100, 101, 110, 112, and 105 BeO maxima in similar angular regions.

Because expansion data frequently are desired in other forms, the calculated BeO lattice-constant values at 100 °C intervals were used to compute the percentage expansions of the two axes: *i.e.*,

$$a\text{-axis} = \frac{(a_t - a_{28^\circ})}{a_{28^\circ}}\,100\%\ ,$$

and the average linear (bulk) expansions, *i.e.*, $(2a+c)/3$, according to Hidnert & Souder (1950). These data are given in Table 5; the data at other temperature intervals may be calculated from the following equations:

$$a\text{-axis} = -0{\cdot}020_9 + 6{\cdot}91\times10^{-4}t + 3{\cdot}00\times10^{-7}t^2\%;$$

$$c\text{-axis} = -0{\cdot}018_6 + 5{\cdot}82\times10^{-4}t + 2{\cdot}90\times10^{-7}t^2\%;$$

and

$$\text{average linear (bulk)} = -0{\cdot}020_2 + 6{\cdot}54\times10^{-4}t + 2{\cdot}97\times10^{-7}t^2\%$$

where t is in °C and where the equations allow the user to calculate the corrections from the 28 °C room temperature of these experiments to any other room temperature condition .The unbiased standard errors of estimate of these equations are $6{\cdot}8\times10^{-4}$, $1{\cdot}1\times10^{-3}$, and $8{\cdot}0\times10^{-4}$, respectively; the coefficients of determination and the multiple regression coefficient values are 0·9999 in all instances.

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AB Compounds with Sc, Y and Rare Earth Metals.
I. Scandium and Yttrium Compounds with CrB and CsCl Structure*

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The crystal structures of seven new compounds have been determined. ScSi, ScGe, ScGa, YGe and YGa crystallize with the TlI ($B33$) type (also known as CrB or B_f type) and ScMg, ScAl with the CsCl ($B2$) structure type. A survey of all known equiatomic compounds and their structures, having Sc, Y or rare earth metals as one component, is given and an effort is being made to find some general rules which govern the formation of these compounds and their structures.

Introduction

Only a few years ago, the alloy chemistry of Sc, Y and rare earth metals was a nearly unexplored area. Except for some isolated efforts, for example by Iandelli, no extensive research was conducted on these lines. However, the development of ion-exchangers for the separation of rare earth elements, a by-product of reactor fuel research, and the ready availability of the Sc, Y and rare earth metals on the market brought about an extremely rapid change. A rather intensive interest in the crystal chemistry of rare earth alloys developed about five years ago which resulted in an increased number of publications on Sc, Y and rare earth metals and their compounds. With many compounds and structures known today, it is already possible to make general conclusions concerning the compound formation in these alloys.

The compounds of interest in this study were the equiatomic compounds having Sc, Y or rare earth metals as one component, the other being another metal or nonmetal from other groups. It was found that

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* Part II, D. Hohnke & E. Parthé, submitted to *Acta Cryst.*