Short Communications

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Crystal structure of Nb_3Be_2.*

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X-ray powder diffraction studies of the Nb–Be system indicated additional phases in the composition range between Nb and $NbBe_2$.

A sample of composition of $NbBe_{1\cdot10}$ was prepared from the elemental powders contained in a BeO crucible by heating to 1550 °C. with an inductively heated molybdenum susceptor under argon. This material was repeatedly crushed, blended and reheated in vacuum at 1600–1750 °C. Weight losses, attributed to vaporization of Be, indicated a final composition of $NbBe_{0\cdot7}$; the powder pattern showed the presence of some $NbBe_2$ and the new phases. Further heating to $NbBe_{0\cdot4}$ resulted in the disappearance of the $NbBe_2$ pattern.

A single crystal in the shape of a parallelepiped, $0\cdot03 \times 0\cdot04 \times 0\cdot15$ mm. in size, was selected from the crushed product, $NbBe_{0\cdot7}$, and examined by the Weissenberg method. The cell is tetragonal with

$$a = 6\cdot49 \pm 0\cdot01,\ c = 3\cdot35 \pm 0\cdot01\ \text{Å},\ c/a = 0\cdot517\ .$$

Assuming the atomic volumes of the elements to be additive, the volume of the unit cell is consistent with a stoichiometry of Nb_3Be_2.

The structure is isomorphous with U_3Si_2 (Zachariasen, 1949). The space group is $P4/mbm$ with two formula units per unit cell. The calculated X-ray density for Nb_3Be_2 is 6·99 g.cm.$^{-3}$.

Thirty-one $hk0$ intensities were measured with Mo $K\alpha$ radiation ($\lambda = 0\cdot7107$ Å) on a Ge XRD-5 diffractometer equipped with a single-crystal orienter.

Refinement of the proposed structure by the least-squares method yielded a reliability factor of 2·93%.

The atomic positions are:

2 Nb_I $(0, 0, 0);\ (\frac{1}{2}, \frac{1}{2}, 0)$.
4 Nb_{II} $\pm(U, U+\frac{1}{2}, \frac{1}{2});\ (\frac{1}{2}-U, U, \frac{1}{2})$.
$U = 0\cdot1794 \pm 0\cdot0003$.
4 Be $\pm(V, V+\frac{1}{2}, 0);\ (\frac{1}{2}-V, V, 0)$.
$V = 0\cdot383 \pm 0\cdot005$.

The standard deviations were calculated by the method of Cruickshank (1949). The temperature factors used for the results shown in Table 1, are 0·68, 0·56 and 0·51 for Nb_I, Nb_{II} and Be, respectively. James and Brindley scattering factors for Nb (Klug & Alexander, 1954), and the Berghuis *et al.* (1955) scattering factors for Be were used.

Table 1. *Observed and calculated $hk0$ structure factors for* Nb_3Be_2

h	k	F_o	F_c
1	1	97	99
2	0	45	42
2	1	214	216
2	2	269	267
3	1	264	266
3	2	68	63
4	0	67	58
4	1	221	220
3	3	120	114
4	2	147	144
4	3	46	48
5	1	45	41
5	2	90	87
4	4	124	116
5	3	218	234
6	0	253	251
6	1	81	84
6	2	14	13
5	4	107	105
6	3	15	10
7	1	76	78
5	5	37	34
6	4	55	52
7	2	132	133
7	3	70	71
6	5	44	46
8	0	56	54
8	1	57	53
7	4	133	136
8	2	146	146
6	6	171	168

The interatomic distances are as follows:

Be–1 Be	$2\cdot14 \pm 0\cdot08$ Å	Nb_I –8 Nb_{II}	$2\cdot91 \pm 0\cdot01$ Å
–2 Nb_I	$2\cdot60 \pm 0\cdot04$	–4 Be	$2\cdot60 \pm 0\cdot04$
–4 Nb_{II}	$2\cdot58 \pm 0\cdot04$	Nb_{II}–4 Nb_I	$2\cdot91 \pm 0\cdot01$
–2 Nb_{II}	$2\cdot52 \pm 0\cdot04$	–4 Be	$2\cdot58 \pm 0\cdot04$
		–2 Be	$2\cdot52 \pm 0\cdot04$

These distances are in good agreement with those found in the other intermetallics of this system, namely $NbBe_2$, $NbBe_3$ (Sands, Zalkin & Krikorian, 1959), Nb_2Be_{17} (Zalkin, Sands & Krikorian, 1959), and $NbBe_{12}$ (Batchelder & Raeuchle, 1957). In Nb_3Be_2 the Be atoms occur in pairs rather than in continuous 3-dimensional networks as in the other niobium beryllides.

In addition to the Nb_3Be_2 phase, the powder patterns showed the presence of a face-centered cubic phase with $a = 10\cdot94$ Å. This phase has not been identified and may be an impurity or an additional Nb–Be phase.

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