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CALCULATED POWDER X-RAY DIFFRACTION
DATA FOR BORON

C. E. Holcombe, Jr
A. L. Coffey, Jr

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ABSTRACT

A literature review has been made of the crystallographic data, and a study has been made of computer-simulated powder X-ray diffraction data and of the solid solution formation for boron polymorphs.

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SUMMARY

Pertinent literature involving boron and its solid solutions was reviewed. The powder X-ray diffraction patterns were computed for the three forms of boron for which refined crystal parameters are available: α -rhombohedral, β -rhombohedral, and α -tetragonal. The data include reflections for both $\text{CuK}\alpha_{1-2}$ and $\text{CrK}\alpha_{1-2}$ up to 145 degrees 2θ , and both integrated and peak-height intensities are listed. The solid solutions which can occur with these forms of boron are discussed in terms of the interstitial and substitutional types which can occur.

INTRODUCTION

An understanding of the crystallography of boron and an improved understanding of its associated powder diffraction data should be a beneficial aid to predicting the behavior of its compounds and solid solutions.

Although much effort has been devoted in the literature to the preparation and characterization of compounds of boron, the element itself has not been studied in depth. Relationships of the various forms of boron and their solid solutions with other elements have been discussed in many separate papers, and the appropriate powder X-ray diffraction data are scattered throughout the literature and contain many deficiencies although the crystal structures have been studied in detail. It is the purpose of this study: (1) to combine all the pertinent crystallographic data necessary for studying boron and its solid solutions; (2) to present computer-simulated (from reported single-crystal data) X-ray powder diffraction patterns for the forms of boron; (3) to illustrate the utility of obtaining computer-simulated patterns, and (4) to discuss possible solid solutions with boron.

X-RAY DIFFRACTION DATA FOR BORON

LITERATURE REVIEW

Boron

Boron has been shown^(1 - 3) to exist in three distinct polymorphic forms: α -rhombohedral, β -rhombohedral, and α -tetragonal. Of the several other polymorphic forms proposed, another tetragonal form⁽⁴⁾ may eventually be shown to be a true form of boron. Thus, the known tetragonal form is properly designated as " α -tetragonal". The α -rhombohedral form occurs from the decomposition of boron iodide or hydrides in the temperature range from 800 to 1,200° C on various substrates. The β -rhombohedral form appears to be the thermodynamically stable polymorph and is consistently produced at 1,500° C or above. A study of the α -to- β transformation in boron has recently been published.⁽⁵⁾ The α -tetragonal form is produced from the reduction of boron bromide with hydrogen on a hot filament (tungsten or tantalum) at 1,100 to 1,300° C. Each of these three forms (α -rhombohedral, β -rhombohedral, and α -tetragonal) is dependent on icosahedral packing and has its own respective structural designation: B₁₂; (B₈₄)(B₁₀)₂B; and (B₁₂)₄B₂. The B₈₄ unit consists of a central icosahedron with 12 half-icosahedra (or pentagonal pyramids) surrounding it in icosahedral symmetry.

The powder diffraction pattern, using CuK α radiation, published for α -rhombohedral boron⁽¹⁾ was not calculated from single-crystal data, and the reported d-spacings are consistently shifted when compared to those calculated from the refined lattice parameters.

The previous patterns for β -rhombohedral and α -tetragonal boron⁽⁶⁾ included only the data for the CrK α radiation. Many weak peaks were not included; and, thus, comparison with solid solutions containing dramatic intensity differences could be difficult using only the reported data. Also, their β -rhombohedral pattern was presumably based on the best refinement of that structure in 1960. Later data^(2, 7) used in the present calculations included the least-squares refined positional coordinates and the partial occupancy factors. Several intensity differences occurred, compared with data reported by Hoard and Newkirk.⁽⁶⁾

Solid Solutions with Boron

When the basic framework of the parent material, boron, is unaltered upon injection of interstitial or substitutional atoms into the structure, the resultant material should properly be called a solid solution. Solid solutions with α -rhombohedral boron,^(8 - 11) β -rhombohedral boron,^(12 - 14) and α -tetragonal boron⁽¹⁵⁾ have been reported to exist with, in many cases, minimal changes in the lattice parameters and significant changes in intensities of the diffracting planes.

Interstitial derivatives of α -rhombohedral boron are formed when Positions 1b or 2c of Space Group $R\bar{3}m$ are filled with atoms such as boron, carbon, oxygen, aluminum, silicon, phosphorus, sulfur, or arsenic. These sites may be either partially or completely filled. Silicon has been shown⁽¹¹⁾ to substitute for boron atoms in the icosahedra as well as in the interstitial sites. Alpha tetragonal boron has interstitial sites at Positions 2a, 4a, and 4c

which can easily accommodate foreign atoms. Smaller atoms (beryllium, carbon, and aluminum), according to Matkovich, et al.,⁽¹⁵⁾ can fill either the 4a or 4c sites. Larger atoms (such as tantalum or tungsten) can be inserted into the 2a sites up to a limit of 3.8 atom percent of the impurity atom, according to Hoard and Newkirk.⁽⁶⁾

In β -rhombohedral boron, Sullenger⁽⁷⁾ listed the various holes in the structure suitable for interstitial atoms. The radius of the largest atoms which could be inserted was 1.18 Å (two available sites), and eight other sites occurred which would accommodate atoms with radii greater than 1.0 Å. These sites could be occupied by such atoms as aluminum, silicon, arsenic, and phosphorus, as well as smaller atoms. A substitutional solid solution⁽¹²⁾ of smaller atoms for some of the 21 boron atoms which are not included in the B₈₄ polyhedral units is also possible. This situation apparently occurs with silicon and aluminum atoms. Also, larger transition elements may substitute in the 2c sites for the two B₁₀ units. Other substitutional variants have been discussed by Anderson and Lundstrom.⁽¹⁴⁾ These variants would explain the solid solutions with boron described by Carlsson and Lundstrom⁽¹³⁾ for many transition elements (Sc, Ti, V, Cr, Mn, Fe, Co, Ni, and Cu) up to 4.8 atom percent. Also, a similar solid solution occurred with zinc up to 4.2 atom percent dissolved in boron⁽¹⁶⁾ under gas pressure autoclaving. These transition elements caused small or no changes in the lattice parameters, but caused substantial intensity variations. These changes in the diffraction pattern combined with possible superlattice lines from ordered solid solutions may be responsible for the many reported polymorphs of boron.

COMPUTER SIMULATION

Calculation of a complete set of integrated intensity values for a random powder sample of a crystalline material can be readily accomplished with a computer program developed by Smith.^(17, 18) If the input structure data are of high quality, the integrated intensities match very closely with the experimentally observed data. This degree of fit justifies the use of such calculated patterns as standards for quantitative phase analysis as well as identification.

The fundamental equation used by Smith's program in the calculation of the set of integrated intensity values from a specific atomic arrangement and unit cell size is:

$$I = ap \cdot LPAT |F|^2,$$

where "a" represents a scale factor used to place the data on a relative scale with a maximum of 100, "p" the multiplicity factor, "LP" the Lorentz-polarization factor, "A" the absorption factor, "T" the Debye temperature factor, and "F" the structure factor.

The necessary input data include the unit cell parameters, the space group, the atom position parameters and their scattering and temperature factors, the mass absorption coefficient and crystal density, and the X-ray wavelength used. Other useful data include the extinction conditions and the Miller indices of the strongest reflection. Using the space group and the unit cell constants, the full set of nonredundant indices and d-spacings is generated. Reflections not allowed by space-group extinction are eliminated to minimize calculations. Integrated intensities for each HKL are then generated by calculating the temperature-modified structure factor using the appropriate multiplicity factor and

Table 1
CRYSTAL DATA USED FOR BORON

α -Rhombohedral Boron	β -Rhombohedral Boron	α -Tetragonal Boron
Reference: Decker and Kasper (1959)	References: Hoard, Sullenger, Kennard, and Hughes (1970), and Sullenger (1969)	Reference: Hoard, Hughes, and Sands (1958)
Space Group: $R\bar{3}m$ (166)	Space Group: $R\bar{3}m$ (166)	Space Group: $P4_2/nm$ (134)
Crystal System: Rhombohedral	Crystal System: Rhombohedral	Crystal System: Tetragonal
Rhombohedral Lattice Parameters: $a_0 = 5.057 \pm 0.003$ A; $a = 58.06 \pm 0.05^\circ$	Rhombohedral Lattice Parameters: $a_0 = 10.145 \pm 0.015$ A; $a = 65.28 \pm 0.13^\circ$	Lattice Parameters: $a_0 = 8.74 \pm 0.015$ A; $c_0 = 5.068 \pm 0.010$ A
Hexagonal Lattice Parameters: $a_0 = 4.908 \pm 0.003$ A; $c_0 = 12.567 \pm 0.007$ A	Hexagonal Lattice Parameters: $a_0 = 10.944 \pm 0.015$ A; $c_0 = 23.81 \pm 0.03$ A	
Crystal Density: 2.46 gms/cc	Crystal Density: 2.29 gms/cc	Crystal Density: 2.33 gms/cc
Structural Designation: B_{12}	Structural Designation: $(B_{84}) (B_{10})_2B$	Structural Designation: $(B_{12})_4B_2$
Number Atoms in Unit Cell: 12	Number Atoms in Unit Cell: 105	Number Atoms in Unit Cell: 50

applying the Lorentz polarization and absorption factors. Finally, a scale factor is introduced to reduce the calculated intensities to values with a usual maximum of 100. The numbers obtained are relative integrated intensities and are directly comparable with the total area under a diffractometer profile.

POWDER DIFFRACTION DATA

The most refined data available on the three forms of boron were used as input for the computer code. The data are listed in Table 1. The references given also contain the atomic positional parameters. For the rhombohedral boron polymorphs, hexagonal parameters were used to generate the diffraction patterns.

The calculated powder diffraction data for α -rhombohedral, β -rhombohedral, and α -tetragonal boron are reported in Tables 2 through 4, respectively.

Table 2
SIMULATED POWDER DIFFRACTION DATA FOR α -RHOMBOHEDRAL BORON

d-Spacings (Å)	HKL	CuK α 1-2 Relative Intensities Flat Absorption		CrK α 1-2 Relative Intensities Flat Absorption		d-Spacings (Å)	HKL	CuK α 1-2 Relative Intensities Flat Absorption	
		Integrated	Peak Height	Integrated	Peak Height			Integrated	Peak Height
4.189	003	55	52	55	56	1.048	{ 042 0012 }	2 < 1	1
4.026	101	100	100	100	100	1.007	{ 404 2011 }	2 ≪ 1	1
3.521	012	4	4	4	4	0.9945	039	5	3
2.526	104	65	57	61	52	0.9854	137	1	< 1
2.454	110	11	10	10	8	0.9426	{ 318 1013 }	2 2	2
2.163	015	4	3	3	3	0.9313	{ 324 1211 }	18 4	10
2.117	113	4	4	4	3	0.9217	229	< 1	≪ 1
2.095	021	54	44	50	38	0.9144	407	≪ 1	≪ 1
2.013	202	< 1	< 1	< 1	< 1	0.9091	235	2	1
1.654	107	6	5	7	4	0.9056	{ 413 143 }	2 < 1	1
1.623	205	12	9	13	8	0.8800	{ 048 0213 }	2 3	2
1.594	{ 211 116 }	11 ≪ 1	9	12 < 1	8	0.8598	1310	2	< 1
1.473	018	10	7	14	8	0.8569	327	8	3
1.430	214	24	17	36	19	0.8481	{ 051 146 416 }	7 ≪ 1 1	3
1.417	300	11	8	18	9	0.8422	{ 502 0312 3012 }	≪ 1 9 17	10
1.396	009	6	4	10	5	0.8378	0015	4	2
1.371	027	13	9	24	11	0.8285	{ 238 2113 }	13 2	5
1.353	125	16	11	32	15	0.8269	2014	≪ 1	≪ 1
1.342	{ 303 033 }	9 16	17	18 33	24	0.8206	{ 054 3111 }	15 3	6
1.263	208	19	13	59	24	0.8180	330	13	4
1.227	220	5	3	19	7	0.8114	4010	< 1	≪ 1
1.197	217	< 1	< 1						
1.177	223	4	2						
1.174	{ 131 306 036 }	4 ≪ 1 ≪ 1	3						
1.159	312	1	< 1						
1.123	128	1	< 1						
1.103	{ 134 0111 }	< 1 2	1						
1.082	0210	≪ 1	< 1						
1.059	{ 401 226 }	≪ 1 < 1	< 1						

Table 3
SIMULATED POWDER DIFFRACTION DATA FOR β -RHOMBOHEDRAL BORON

CuK α 1-2						CrK α 1-2					
Relative Intensities						Relative Intensities					
Flat Absorption						Flat Absorption					
Peak						Peak					
d-Spacings	HKL	Integrated	Height	Integrated	Height	d-Spacings	HKL	Integrated	Height	Integrated	Height
(A)						(A)					
8.806	101	10	10	10	11	1.777	333	< 1	< 1	< 1	< 1
7.937	003	48	49	49	54	1.771	422	< 1	< 1	< 1	< 1
7.415	012	5	6	5	6	1.763	{1310 505}	{1 7}	6	1	1
5.472	110	16	16	16	16	1.756	238	8	6	8	5
5.041	104	100	100	100	100	1.708	0213	4	4	4	3
4.648	021	37	38	37	38	1.607	511	< 1	< 1	1	< 1
4.505	113	20	21	20	21	1.680	{3012 4010}	{2 2}	3	2	2
4.403	202	14	14	14	14	1.674	0114	1	1	1	1
4.255	015	15	15	15	15	1.671	3111	1	1	1	< 1
3.988	008	11	11	11	10	1.656	{336 057}	{1 2}	2	2	2
3.708	024	13	14	13	13	1.637	514	< 1	< 1	< 1	< 1
3.542	211	20	20	20	19	1.629	{419 149}	< 1	1	1	1
3.430	122	10	10	10	10	1.606	2212	< 1	< 1	< 1	< 1
3.359	205	3	3	3	3	1.601	2014	< 1	< 1	< 1	< 1
3.213	116	< 1	< 1	< 1	< 1	1.549	063	12	9	14	8
3.202	107	< 1	< 1	< 1	< 1	1.518	520	< 1	< 1	1	< 1
3.159	300	< 1	< 1	< 1	< 1	1.502	339	< 1	< 1	< 1	< 1
3.069	214	4	4	4	4	1.477	158	< 1	< 1	1	< 1
2.935	{303 033}	{6 < 1}	7	{6 < 1}	6	1.470	1016	< 1	< 1	< 1	< 1
2.863	125	16	16	15	13	1.468	{606 066}	{4 < 1}	4	{6 < 1}	4
2.840	018	3	4	3	3	1.449	4013	9	7	14	7
2.763	027	4	4	4	3	1.443	161	2	2	3	2
2.736	220	8	7	8	7	1.435	612	1	1	2	1
2.646	009	8	8	8	7	1.432	{4112 1412 2410}	{2 1 13}	12	{4 2 20}	13
2.613	131	12	11	11	9	1.428	{3114 5011}	{3 < 1}	3	4	3
2.587	223	7	7	7	6	1.420	0216	5	5	7	4
2.567	312	5	5	5	4		{3015 0315}	< 1		< 1	
2.520	208	6	6	6	5	1.418	526	1	5	2	5
2.470	{306 036 217}	{6 7 10}	13	{5 6 10}	11		256	1		2	
2.405	134	10	10	10	8		437	1		2	2
2.382	119	5	4	4	4	1.405	164	2	2	4	2
2.350	401	12	10	11	9	1.386	0117	2	2	3	2
2.324	042	7	6	7	6	1.383	{6115 0414}	{9 1}	7	15	8
2.309	1010	1	1	< 1	< 1	1.380	{348 4211}	{7 < 1}	6	{12 2}	7
2.301	315	2	2	2	1	1.373	{2116 2215}	< 1	1	1	1
2.289	128	2	2	2	2	1.368	440	3	2	6	3
2.253	226	4	4	4	3	1.356	{609 069}	{3 < 1}	3	7	4
2.201	404	6	5	5	4						
2.165	321	2	1	2	1						
2.139	232	< 1	< 1	< 1	< 1						
2.121	045	< 1	< 1	< 1	< 1						
2.110	0111	< 1	< 1	< 1	< 1						
2.080	137	4	3	3	2						
2.042	324	7	6	7	5						
2.028	039	2	2	2	2						
1.834	146	< 1	< 1	< 1	< 1						
1.824	330	2	2	2	1						
1.798	1013	1	1	1	< 1						
1.786	241	1	1	1	< 1						

Table 3 (Continued)

CuK α 1-2						CrK α 1-2					
		Relative Intensities		Relative Intensities				Relative Intensities		Relative Intensities	
		Flat Absorption		Flat Absorption				Flat Absorption		Flat Absorption	
d-Spacings			Peak		Peak	d-Spacings			Peak		Peak
(A)	HKL	Integrated	Height	Integrated	Height	(A)	HKL	Integrated	Height	Integrated	Height
1.351	351	5	4	10	5						
1.348	443	9	7	19	9						
1.345	072	≤ 1	≤ 1	< 1		0.9430	{ 835	1			
1.345	532	5	5	10	6		{ 918	< 1	1		
1.343	3312	3	3	7	4		{ 568	1			
1.340	2314	≤ 1	≤ 1	< 1	1	0.9405	5416	< 1	≤ 1		
1.338	1511	5	4	11	5	0.9360	1004	< 1	≤ 1		
1.320	704	2	2	4	2	0.9349	{ 4613	< 1	< 1		
1.317	0513	≤ 1	≤ 1	< 1	2		{ 2323	< 1	< 1		
1.316	259	4	3	9	4	0.9296	0105	< 1	≤ 1		
1.312	621	≤ 1	≤ 1	< 1	< 1	0.9269	0816	< 1	< 1		
	{ 1217	4		10		0.9260	387	1	< 1		
1.303	{ 4310	1	4	4	5	0.9213	749	< 1	< 1		
	{ 535	1		3		0.9170	{ 2812	< 1	< 1		
1.300	{ 075	1		2	3		{ 295	< 1	< 1		
1.295	618	3	2	7	3	0.9120	660	4	2		
1.293	1316	1	< 1	3	1	0.9083	2521	< 1	< 1		
1.286	446	≤ 1	≤ 1	< 1	< 1	0.8963	4223	< 1	< 1		
1.283	1118	4	2	9	4	0.8941	{ 841	< 1	< 1		
1.283	624	≤ 1	≤ 1	< 1	< 1		{ 0720	< 1	< 1		
1.281	2413	4	3	12	5	0.8924	{ 482	< 1	< 1		
1.267	265	≤ 1	≤ 1	< 1	< 1		{ 7217	1	< 1		
1.266	5014	≤ 1	≤ 1	1	< 1	0.8889	4322	1	< 1		
1.265	3411	≤ 1	≤ 1	2	< 1	0.8837	4025	1	< 1		
	{ 4016	1		4	2	0.8806	10010	3	1		
1.259	{ 4115	2	2	5	3	0.8779	4616	5	2		
	{ 707	< 1		2		0.8730	4421	< 1	≤ 1		
1.258	357	≤ 1	≤ 1	< 1	1	0.8709	393	< 1	≤ 1		
1.255	710	≤ 1	≤ 1	1	< 1	0.8683	758	2	< 1		
1.247	5113	< 1	< 1	3	1	0.8660	847	< 1	≤ 1		
1.242	1019	≤ 1	≤ 1	< 1	≤ 1	0.8579	5614	3	1		
1.240	173	< 1	< 1	3	1	0.8542	0426	2	< 1		
1.236	{ 3117	≤ 1	≤ 1	< 1	1	0.8517	{ 3813	< 1	1		
	{ 1610	≤ 1		2			{ 1019	2			
1.228	3216	≤ 1		< 1	≤ 1	0.8510	0525	2	1		
1.226	627	≤ 1	≤ 1	< 1	≤ 1	0.8494	{ 0327	2	1		
1.215	449	≤ 1	≤ 1	1	≤ 1		{ 1022	< 1			
1.206	0417	≤ 1	≤ 1	< 1	≤ 1	0.8484	3717	2	1		
1.203	1514	≤ 1	≤ 1	2	< 1	0.8454	7022	< 1	≤ 1		
1.202	268	≤ 1	≤ 1	< 1	≤ 1	0.8440	2326	1	< 1		
1.197	176	1	< 1			0.8432	5518	2	1		
1.183	081	< 1	< 1			0.8416	{ 10013	1	2		
1.143	{ 636	1	1				{ 6123	2			
	{ 547	< 1					{ 7121	2			
1.120	0615	< 1	≤ 1			0.8402	6024	< 1	≤ 1		
1.094	550	< 1	≤ 1			0.8382	8410	< 1	≤ 1		
0.9972	5218	< 1	≤ 1			0.8345	850	< 1	≤ 1		
0.9943	4121	< 1	≤ 1			0.8328	764	1	< 1		
0.9540	{ 3615	1	1			0.8318	939	< 1	≤ 1		
	{ 476	< 1				0.8299	583	1	< 1		
0.9487	0423	1	< 1			0.8279	01014	< 1	≤ 1		
0.9466	{ 0324	< 1	< 1			0.8222	6321	< 1	≤ 1		
	{ 3420	< 1				0.8164	767	< 1	≤ 1		

Table 3 (Continued)

		CuK α 1-2		CrK α 1-2				CuK α 1-2		CrK α 1-2	
		Relative Intensities		Relative Intensities				Relative Intensities		Relative Intensities	
		Flat Absorption		Flat Absorption				Flat Absorption		Flat Absorption	
d-Spacings			Peak		Peak	d-Spacings			Peak		Peak
(A)	HKL	Integrated	Height	Integrated	Height	(A)	HKL	Integrated	Height	Integrated	Height
0.8154	4226	< 1	≪ 1								
0.8133	{5713 2623}	< 1	≪ 1								
0.8099	1115	7	2								

Table 4
SIMULATED POWDER DIFFRACTION DATA FOR α -TETRAGONAL BORON

		CuK α 1-2		CrK α 1-2				CuK α 1-2		CrK α 1-2	
		Relative Intensities		Relative Intensities				Relative Intensities		Relative Intensities	
		Flat Absorption		Flat Absorption				Flat Absorption		Flat Absorption	
d-Spacings			Peak		Peak	d-Spacings			Peak		Peak
(A)	HKL	Integrated	Height	Integrated	Height	(A)	HKL	Integrated	Height	Integrated	Height
6.180	110	12	11	12	13	1.306	333	8	5	19	9
4.370	{101 200}	9 100	100	9 100	100	1.267	004	4	2	12	5
3.919	111	72	65	72	69	1.203	002	1	1	3	2
3.095	{211 220}	9 2	9	9 2	9	1.262	631	1	< 1	3	2
2.764	310	3	2	2	2	1.250	612	5	3	17	7
2.534	002	26	23	24	20	1.236	550	< 1	$\ll$ 1	3	1
2.526	301	9	10	9	9	1.217	204	< 1	< 1	4	2
2.426	311	83	70	78	66	1.215	503	2	2	7	3
2.192	202	3	3	3	3	1.213	622	3	3	14	6
2.187	321	20	17	18	15	1.212	{701 640}	1 2	2	5 7	4
2.060	330	< 1	< 1	< 1	< 1	1.205	214	< 1	< 1	3	1
1.956	{411 420}	8 < 1	7	8 < 1	6	1.203	513	$\ll$ 1	$\ll$ 1	1	< 1
1.908	331	8	6	8	6	1.202	542	$\ll$ 1	$\ll$ 1	2	< 1
1.868	312	1	< 1	1	< 1	1.201	711	$\ll$ 1	$\ll$ 1	< 1	$\ll$ 1
1.752	322	1	< 1	1	< 1	1.172	224	< 1	$\ll$ 1	4	1
1.655	402	1	2	1	1	1.170	523	$\ll$ 1	$\ll$ 1	1	$\ll$ 1
1.653	501	5	4	6	4	1.168	721	$\ll$ 1	$\ll$ 1	3	< 1
1.630	113	4	3	4	3	1.159	632	3	2	33	6
1.626	412	4	4	5	3	1.152	314	$\ll$ 1	$\ll$ 1		
1.624	511	< 1	1	< 1	< 1	1.148	730	$\ll$ 1	$\ll$ 1		
1.551	213	< 1	< 1	1	< 1	1.096	404	1	< 1		
1.546	{521 440}	3 4	4	3 5	4	1.085	722	1	< 1		
1.457	600	6	4	9	5	1.026	434	2	1		
1.441	313	25	18	38	21	1.019	514	< 1	$\ll$ 1		
1.439	432	13	11	20	12	1.003	831	< 1	$\ll$ 1		
1.420	512	< 1	$\ll$ 1	< 1	< 1	0.9987	524	2	< 1		
1.382	{611 620}	9 12	13	15 20	16	0.9962	751	< 1	< 1		
1.367	522	14	9	26	13	0.9797	444	< 1	$\ll$ 1		
1.333	621	$\ll$ 1	$\ll$ 1	< 1	$\ll$ 1	0.9652	910	3	1		
1.321	413	2	2	3	2	0.9595	841	1	< 1		
1.319	442	$\ll$ 1	$\ll$ 1	< 1	3	0.9560	604	2	< 1		
1.318	541	14	9	33	15	0.9538	901	1	< 1		
						0.9503	614	< 1	$\ll$ 1		
						0.9481	{832 911}	< 1 2	< 1		
						0.9339	624	2	< 1		
						0.9318	761	1	< 1		
						0.9144	415	2	< 1		
						0.9113	851	2	< 1		
						0.9095	335	1	< 1		

Table 4 (Continued)

		CuK α_{1-2}		CrK α_{1-2}				CuK α_{1-2}		CrK α_{1-2}	
		Relative Intensities Flat Absorption		Relative Intensities Flat Absorption				Relative Intensities Flat Absorption		Relative Intensities Flat Absorption	
d-Spacings (A)	HKL	Integrated	Peak Height	Integrated	Peak Height	d-Spacings (A)	HKL	Integrated	Peak Height	Integrated	Peak Height
0.9064	931	1	< 1			0.8450	{1021 006	3 2	2		
0.9020	912	< 1	$\ll$ 1			0.8396	535	1	< 1		
0.8978	823	< 1	$\ll$ 1			0.8380	{913 942	7 3	3		
0.8879	{922 762	< 1 2	< 1			0.8337	772	< 1	$\ll$ 1		
0.8829	770	1	< 1			0.8293	206	2	< 1		
0.8769	505	2	1			0.8282	615	2	< 1		
0.8758	644	1	< 1			0.8259	{1031 216	1 < 1	< 1		
0.8750	833	< 1	$\ll$ 1			0.8237	814	< 1	$\ll$ 1		
0.8715	724	2	< 1			0.8173	625	< 1	$\ll$ 1		
0.8707	753	2	1			0.8138	545	6	2		
0.8701	852	4	2			0.8116	871	< 1	$\ll$ 1		
0.8597	525	2	< 1			0.8088	933	6	2		
0.8506	734	< 1	$\ll$ 1								
0.8489	950	3	1								
0.8459	843	3	1								

The reflections listed in the tables are those with a relative integrated intensity greater than or equal to 0.5, with the exception of smaller reflections that had been previously reported in the literature. The lines listed as having an intensity value $\ll$ 1 have a calculated relative value between 0 and 0.4; those with a value of < 1 have a relative value between 0.5 and 0.9. All other relative intensity values are rounded to the nearest whole value.

Agreement between the calculated peak height intensities of α -rhombohedral boron (Table 2) and those of a previously reported powder pattern is excellent. Minor discrepancies occurred among the observed pattern,⁽¹⁹⁾ the previously reported calculated pattern,⁽⁶⁾ and the results obtained in the present calculation. The differences are believed to be due to impurities, or preferred orientation in the sample in the case of the observed pattern and positional parameter discrepancies in the case of the previously calculated pattern. The calculated pattern of α -tetragonal boron is in good agreement with a previously published calculated pattern.⁽⁶⁾ The pattern generated in the present study, however, is calculated through a d-spacing value of 0.8088, thereby adding a significant number of proposed reflections to the previously generated pattern.

Calculated patterns reveal the major contributing reflections in overlapping peaks and identify high angle lines for lattice parameter refinements. Theoretical patterns are needed for detecting the intensity variation caused by solid solution formation. They also verify that the program can produce results based on good input structure data that are comparable to experimentally observed patterns, as shown in the case of α -rhombohedral boron.

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