Allabogdanite, (Fe,Ni)₂P, a new mineral from the Onello meteorite: The occurrence and crystal structure

SERGEY N. BRITVIN,¹NIKOLAY S. RUDASHEVSKY,²SERGEY V. KRIVOVICHEV,^{3,*} PETER C. BURNS,⁴ AND YURY S. POLEKHOVSKY¹

¹Department of Mineral Deposits, St. Petersburg State University, University Emb. 7/9, St. Petersburg 199034, Russia
 ²Mekhanobr-Analyt join-stock company, Vasilievsky ostrov, 21 line, 2, St. Petersburg 199026, Russia
 ³Department of Crystallography, St. Petersburg State University, University Emb. 7/9, St. Petersburg 199034, Russia
 ⁴Department of Civil Engineering and Geological Sciences, University of Notre Dame, Notre Dame IN 46556-0767, U.S.A.

ABSTRACT

Allabogdanite, (Fe,Ni)₂P, is a new mineral from the Onello iron meteorite (Ni-rich ataxite). It occurs as thin lamellar crystals disseminated in plessite. Associated minerals are nickelphosphide, schreibersite, awaruite, and graphite. Crystals of the mineral, up to $0.4 \times 0.1 \times 0.01$ mm, are flattened on (001) with dominant $\{001\}$ faces, and other faces that are probably $\{110\}$ and $\{100\}$. Mirror twinning resembling that of gypsum is common, with possible twin composition plane {110}. Crystals are light straw-yellow with bright metallic luster. Polished (001) sections look silverywhite against an epoxy background. In reflected light in air, the mineral has a creamy color, with distinct anisotropy from light to dark creamy tint. No bireflectance was observed. $R_1/R_2(\lambda, nm)$ in air: 48.4/37.2(440), 46.7/36.8(460), 47.0/37.6(480), 47.5/38.1(500), 47.6/38.8(520), 48.2/39.2(540), 49.0/39.9(560), 49.6/40.7(580), 50.1/41.6(600), 50.5/41.9(620), 51.9/43.0(640), 52.3/44.3(660), 53.3/ 45.0(680), 54.4/46.2(700). No cleavage or parting was observed. Moh's hardness is 5-6; the mineral is very brittle, and its calculated density 7.10 g/cm³. Its chemical composition (determined by microprobe methods, average of nine analyses) is: Fe 57.7, Ni 20.7, Co 1.4, P 20.4, Total 100.2 wt%, corresponding to $(Fe_{1.51}Ni_{0.50}Co_{0.03})_{2.04}P_{0.96}$ (three atoms per formula unit). Crystal structure: R1 =0.040 for 138 unique observed $(|F_0| \ge 4\sigma_F)$ reflections. Orthorhombic, *Pnma*, unit-cell parameters refined from powder data: a = 5.748(2), b = 3.548(1), c = 6.661(2) Å, $V = 135.8(1), Å^3, Z = 4$; unitcell parameters refined from single-crystal data: a = 5.792(7), b = 3.564(4), c = 6.691(8) Å, and V =138.1(3) Å³. Strongest reflections in the X-ray powder diffraction pattern are [d in Å, (I) (hkl)]: 2.238(100)(112), 2.120(80)(211), 2.073(70)(103), 1.884(50)(013), 1.843(40)(301), 1.788(40)(113), 1.774(40)(020). The mineral is named for Alla Bogdanova, Geological Institute, Kola Science Centre of Russian Academy of Sciences.

INTRODUCTION

The Onello iron meteorite was found in 1997 in the alluvium of the Bol'shoy Dolguchan River, Onello River basin, Aldan shield, Sakha-Yakutia, Russia (62° 20' N, 137° 40' E) and belongs to a group of nickel-rich ataxites. Its characteristic feature is a high mean Ni content (22.2 wt%), which is rare in nature, with just a few representatives known (Buchwald 1975). In total, 43 fragments of the Onello iron meteorite were recovered during gold washing in an area of about 3 km²; the weight of all fragments is 153.5 g (Kopylova et al. 1999). In December, 1997, a piece of this meteorite, at that time unnamed and labeled as "unknown iron from the Aldan River, Sakha-Yakutia, Russia" was obtained by the authors (S.N.B. and N.S.R.) from a local geologist. An interesting association of phosphide minerals was noted in the meteorite, including nickelphosphide, (Ni,Fe)₃P, schreibersite, (Fe,Ni)₃P, and the mineral initially designated as "barringerite," (Fe,Ni)₂P (Britvin et al. 1999b). Barringerite is a rare species discovered in the Ollague pallasite (Buseck 1969). The mineral is isostructural with synthetic Fe₂P, an end-member of the Fe₂P-Ni₂P solid-solution series (Novotny and Henglein 1948). Buchwald (1975) suggested that barringerite was formed during artificial annealing of the meteoritic iron and, as a consequence, is not a mineral. Later, terrestrial and lunar occurrences of barringerite were reported by Chen et al. (1983) and Brandstätter et al. (1991), respectively (see also: Nazarov et al. 1998). Both the chemical composition and the powder X-ray diffraction (XRD) pattern were obtained for terrestrial barringerite, but reports of the lunar mineral did not include any structural data, owing to small amounts of the material available.

Detailed study of the species designated "barringerite" from the Onello meteorite revealed that it is a new polymorph of (Fe,Ni)₂P that crystallizes in the Co₂Si (or anti-PbCl₂) structure type (Geller 1955; Rundquist and Jellinek 1959; Rundquist and Nawapong 1966) and, as such, is a new mineral. The mineral is named allabogdanite, in honor of Alla N. Bogdanova (b. 1947), crystallographer from the Geological Institute, Kola Science Center of Russian Academy of Sciences, Apatity, Kola

^{*} E-mail: skrivovi@mail.ru

peninsula, Russia, for her contributions to the study of new mineral species. Both the mineral and the name have been approved by the Commission on New Minerals and Mineral Names of the International Mineralogical Association (CNMMN IMA). Allabogdanite is the fourth natural species that belongs to the Co₂Si structure type, along with rhodarsenide, (Rh,Pd)₂As (Tarkian et al. 1997; Quesnel and Heyding 1962), palladodymite, (Pd,Rh)₂As (Britvin et al. 1999a), and florenskyite, FeTiP (Ivanov et al. 2000). The holotype specimen of the mineral has been deposited at the Mineralogical Museum, Department of Mineralogy, St. Petersburg State University, catalogue no. 1/18632.

OCCURRENCE AND PHYSICAL PROPERTIES

The fragment of the Onello meteorite used in this study was originally about 5 g in weight and $0.5 \times 1 \times 1.5$ cm in size. It had a dull black surface due to an outer crust of graphite, 0.5-1 mm thick. Fe-Ni-hydroxides, a result of terrestrial alteration, form an internal 0.5–1 mm zone between the graphite crust and the metal matrix. For subsequent study, the specimen was cut into slices. Polished sections were etched for 15 s with light nital (2 mL of 65% HNO3 per 98 mL of pentanol-2) to reveal the matrix microstructure and to resolve phosphide inclusions. The matrix was found to consist of microgranular plessite (taenite-kamacite aggregate, mean ~23 wt% Ni and ~0.7% Co), with small (up to 50 μ m), rare patches of awaruite (72–76%) Ni, ~0.5% Co). Allabogdanite, nickelphosphide, and schreibersite occur as minute grains and crystals randomly disseminated in plessite; their cross-sections cover less than 1% of a polished matrix surface. Because crystals of allabogdanite (Fig. 1) were too thin for any in-situ measurements, we extracted grains by chemical dissolution of the matrix. A slice of the meteorite was treated by boiling in 20% HCl until the unaltered metal was free of the oxide-graphite crust. The clean metal plate was then washed in water and boiled again in 20% HCl, until the matrix was completely dissolved. After washing with distilled water and acetone, the insoluble residue was dried in air. All three phosphides remained unaltered in the residual concentrate.

Allabogdanite and nickelphosphide were found to be non-



FIGURE 1. Allabogdanite crystal in plessite matrix. Etched. Secondary electron image. Scale bar 10 μm.

ferromagnetic, and they were easily separated from schreibersite using a magnet. Allabogdanite crystals, with very shiny faces, could easily be distinguished from nickelphosphide laths that are always naturally corroded and recrystallized (Britvin et al. 1999b). Allabogdanite was found to be a dominant phase among the phosphides in the sample. It forms thin lamellar crystals up to $0.4 \times 0.1 \times 0.01$ mm. On the basis of the powder XRD study of oriented samples, the lamellae are flattened on (001) with dominant {001} faces. Other faces could not be measured with certainty because they are always somewhat curved, but they are probably {110} and {100}. The crystals are usually hypomorphous with pseudo-monoclinic habit. Mirror twins resembling those of gypsum crystals are very common, with twin composition plane possibly {110} (Fig. 2). The color of the crystals is light straw-yellow and the mineral has a bright metallic luster. Polished (001) sections look silvery-white against an epoxy background. In reflected light in air, the mineral has a creamy color against the plessite background, with distinct anisotropy from light to dark creamy tint. No bireflectance was observed. Reflectance values (Table 1) have been measured in air on {001} faces of crystals glued and polished on a glass plate. Other sections could not be used for measurements because crystals of the mineral are too thin. No cleavage or parting was observed. Moh's hardness is estimated as 5-6 by scratching the crystals between the glass plates.

TABLE 1. Reflectance of allabogdanite measured in air

λ (nm)	R ₁	R ₂	λ(nm)	R ₁	R ₂	
440	48.4	37.2	580	49.6	40.7	
460	46.7	36.8	600	50.1	41.6	
480	47.0	37.6	620	50.5	41.9	
500	47.5	38.1	640	51.9	43.0	
520	47.6	38.8	660	52.3	44.3	
540	48.2	39.2	680	53.3	45.0	
560	49.0	39.9	700	54.4	46.2	



FIGURE 2. Allabogdanite twin glued on a glass plate. Backscattered electron image. Scale bar 33 μ m.

Microhardness VHN measurements were not possible due to the very high brittleness of allabogdanite crystals and their thin lamellar habit. Density calculated from the empirical formula is 7.10 g/cm³.

CHEMICAL COMPOSITION

Nine microprobe analyses on nine different crystals, both loose and embedded in the parent matrix, were carried out using a LINK AN-10000 EDS analyzer attached to a CamScan 4 scanning electron microscope, at 20 kV accelerating voltage and 3 nA beam current (Table 2). Fe, Ni, and Co metals, and GaP were used as standards. No other elements with atomic number greater than 11 were detected. The composition of allabogdanite is uniform from grain to grain with an Fe:Ni atomic ratio close to 3. The formula was calculated on the basis of Fe + Ni + Co + P = 3. The average analysis corresponds to the empirical formula (Fe_{1.51}Ni_{0.50}Co_{0.03})_{2.04}P_{0.96}, ideally (Fe,Ni)₂P.

CRYSTALLOGRAPHY

Our attempts to obtain reliable powder diffraction data using an automated diffractometer were unsuccessful due to the lamellar habit of the allabogdanite crystals, which resulted in severe (001) preferred orientation, giving very strong 004 and 002 reflections. A powder X-ray diffraction (XRD) pattern was acquired using a 114.6 mm Debye-Scherrer camera, Mn-filtered FeK α -radiation, 40 kV, 20 mA, and 32 h exposure time (Table 3). The mineral is orthorhombic with space group *Pnma*. Cell parameters refined from powder data by the least-squares method are: a = 5.748(2), b = 3.548(1), c = 6.661(2) Å, V =135.8(1) Å³, and Z = 4. The measured powder pattern is in good agreement with one calculated using experimental atomic coordinates and the PowderCell for Windows 1.0 program (Kraus and Nolze 1997).

CRYSTAL STRUCTURE

Data collection, structure solution, and refinement

A single crystal of allabogdanite was mounted on a Bruker three-circle CCD-based X-ray diffractometer operated at 50 kV and 40 mA. More than a hemisphere of three-dimensional data were collected using monochromatic MoK α X-rays, with frame widths of 0.3° in ω , and with 30 s integration for each frame. The unit-cell parameters (Table 4) were refined with 455 reflections using least-squares techniques. The intensity data were reduced and corrected for Lorentz, polarization, and background effects using the Bruker program SAINT. Absorption correc-

 TABLE 2. Chemical composition of allabogdanite

tion was done on the basis of 258 strong reflections; the crystal was modeled as a (001) plate. Reflections with plate-glancing angles of less than 3° were discarded, which lowered R_{int} from 11.1 to 9.3%. The Bruker SHELXTL Version 5 system of programs was used for the determination and refinement of the

TABLE 3. Powder X-ray diffraction data for allabogdanite*

I _{obs}	$d_{\rm obs}$	$I_{\rm calc}$	$d_{\rm calc}$	h	k	Ι		I _{obs}	d _{obs.}	$I_{\rm calc}$	$d_{\rm calc}$	h	k	Ι
10	4.32	2	4.352	1	0	1		40	1.277	17	1.278	3	2	1
20	3.33	2	3.331	0	0	2		30	1.247	{ 8	1.248	2	2	3
10	3.13	1	3.131	0	1	1				10	1.247	0	1	5
		3	2.882	1	0	2		20	1.236	4	1.237	4	1	2
30	2.750	7	2.750	1	1	1		20	1.212	{61	.214	0	2	4
100	2.238{	100	2.237	1	1	2				17	1.212	3	2	2
		49	2.233	2	1	0				7	1.209	2	0	5
10	2.177	11	2.176	2	0	2				1	1.206	4	0	3
80	2.120	75	2.117	2	1	1				3	1.188	1	2	4
70	2.073	32	2.071	1	0	3		30	1.185	26	1.185	3	1	4
50	1.884	29	1.882	0	1	3		30	1.144	{ 9	1.144	2	1	5
		7	1.855	2	1	2				2	1.141	1	3	1
40	1.843	25	1.841	3	0	1				1	1.133	5	0	1
40	1.788	18	1.789	1	1	3				3	1.123	3	2	3
40	1.774	42	1.774	0	2	0		30	1.116	1	1.117	4	2	0
40	1.758	10	1.757	2	0	3		10	1.102	5	1.101	4	2	1
30	1.662{	6	1.665	0	0	4		30	1.092	{18	1.094	1	3	2
		18	1.661	3	0	2				9	1.094	2	3	0
20	1.634	5	1.634	3	1	1				6	1.090	1	0	6
10	1.598	3	1.599	1	0	4				4	1.088	4	0	4
20	1.574	6	1.575	2	1	3				2	1.087	5	0	2
		1	1.511	1	2	2		20	1.079	{18	1.079	2	3	1
		1	1.510	2	2	0				32	1.079	5	1	1
		1	1.458	1	1	4				11	1.059	4	2	2
		2	1.451	3	0	3				8	1.047	1	2	5
		3	1.405	4	0	1		20	1.045	{10	1.045	3	1	5
30	1.374	5	1.375	2	2	2				12	1.044	0	3	3
40	1.346{	16	1.347	1	2	3				2	1.042	1	1	6
		1	1.343	3	1	3				3	1.039	2	3	2
		1	1.332	4	1	0				2	1.040	4	1	4
10	1.319	5	1.319	4	0	2				2	1.039	5	1	2
		4	1.306	4	1	1				9	1.036	2	0	6
10	1.298	3	1.298	1	0	5		10	1.027	10	1.027	1	3	3
* Calc	* Calculated pattern generated using cell parameters refined from pow-													

der data: a = 5.748(2), b = 3.548(1), c = 6.661(2) Å, V = 135.8(1) Å³, and Z = 4.

TABLE 4. Crystallographic data for allabogdanite

a (Å)	5.792(7)	Crystal size (mm)	$0.16 \times 0.02 \times 0.01$
b (Å)	3.564(4)	Radiation	Μο <i>Κ</i> α
c (Å)	6.691(8)	Total Ref.	677
$V(Å^3)$	138.1(3)	Unique Ref.	183
Space group	Pnma	Unique $ F_0 \ge 4\sigma_F$	138
μ (cm ⁻¹)	264.70	R	0.040
D _{calc} (g/cm ³)	7.10	wR	0.049
Unit-cell contents	4[(Fe,Ni)2P]	S	0.945

Note: $R = \Sigma (|F_o|-|F_c|)/\Sigma |F_o|$; $\Sigma = [\Sigma w (|F_o|-|F_c|)2/(m-n)]^{1/2}$, for *m* observations and *n* parameters. $w = 1/[\sigma^2(F_o^2) + (0.0192P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$.

					Analyses					
	1	2	3	4	5	6	7	8	9	Average
					Wt%					
Fe	58.2	58.3	58.3	58.4	57.2	57.2	57.5	57.7	56.8	57.7
Ni	20.4	20.7	19.8	20.4	21.4	21.3	20.9	20.9	20.7	20.7
Co	1.5	1.3	1.4	1.5	1.4	1.3	1.3	1.3	1.3	1.4
Р	20.3	20.4	21.0	20.1	19.9	20.1	20.4	20.4	21.2	20.4
Total	100.4	100.7	100.5	100.4	99.9	99.9	100.1	100.3	100.0	100.2
				Ato	oms per form	ula unit				
Fe	1.51	1.51	1.50	1.52	1.50	1.49	1.49	1.50	1.47	1.50
Ni	0.50	0.51	0.49	0.50	0.53	0.53	0.52	0.52	0.51	0.51
Co	0.04	0.03	0.03	0.04	0.03	0.03	0.03	0.03	0.03	0.03
Р	0.95	0.95	0.98	0.94	0.94	0.95	0.96	0.95	0.99	0.96

crystal structure. Systematic absences of reflections indicated space group *Pnma*, in agreement with the space group for other compounds that belong to Co₂Si structure type. The structure was solved by direct methods and refined up to R1 = 0.040 for 138 unique observed ($|F_o| \ge 4\sigma_F$) reflections. The final model included all atomic positional parameters, anisotropic-displacement parameters for all atoms, and a refinable weighting scheme of the structure factors. The final atomic coordinates and anisotropic displacement parameters are reported in Table 5, and selected interatomic distances are listed in Table 6.

Coordination of atoms and cation ordering

There are two symmetrically independent metal atoms (M) in the structure. The M1 atom is tetrahedrally coordinated by four P atoms, whereas the M2 atom is coordinated by five P atoms arranged at the vertices of a tetragonal pyramid. The single symmetrically unique P atom has nine metal neighbors and its coordination polyhedron can be described as a trigonal prism with three rectangular faces capped by three additional M atoms.

As noted above, the Fe:Ni ratio is close to 3 in allabogdanite. Because the X-ray scattering factors of Fe and Ni are similar, it is impossible to study cation ordering in detail using X-ray data. However, refinement of the site occupancies of the cation positions shows that the site-scattering factor for the M2 position with tetragonal pyramidal coordination is slightly lower than that for the M1 position. This difference may indicate that at least partial ordering exists in allabogdanite, with Fe atoms occupying preferably M1 sites.

Structure description

Allabogdanite belongs to the family of compounds with the Co₂Si or anti-PbCl₂ structure type (Geller 1955; Rundquist and Nawapong 1966; Pearson 1972; Kripyakevich 1977). This structure type can be described in several ways (Pearson 1972; Kripyakevich 1977; Sommer and Hoppe 1977; Vegas et al. 2001). The simplest is to depict it as an array of PNi₆ trigonal

prisms (cf., Vegas et al. 2001), although this description ignores the ninefold coordination of the P atoms. The prisms share their triangular faces to form columns parallel to the *b* axis that are linked by the sharing of edges to form sheets parallel to (001). The sheets are shifted by b/2.

RELATIONSHIPS TO OTHER MINERALS AND INOR-GANIC COMPOUNDS

There are no known polymorphs of Ni₂P and Fe₂P that belong to the Co₂Si structure type (Novotny and Henglein 1948; Samsonov and Vereikina 1961; Fruchart et al. 1969). Fruchart et al. (1969) studied the crystallographic properties of solid solutions of the phosphides M_2P (M = Cr, Mn, Fe, Co, Ni) and found that Mn₂P, Fe₂P, and Ni₂P are hexagonal and belong to the Ni₂In structure type (as does barringerite), whereas Co₂P is orthorhombic and isostructural with Co2Si. Solid solutions between two hexagonal end members, such as Fe₂P with Ni₂P, may exhibit orthorhombic (Co2Si-type) structures, due to cation ordering. Chenevier et al. (1987) studied the high temperature orthorhombic-hexagonal phase transition of iron manganese phosphide, FeMnP. Above 1473 K, FeMnP has the hexagonal Fe₂P (barringerite) structure with disordered metal atoms. The degree of disorder decreases with temperature and, at 1413 K, a hexagonal-orthorhombic transition takes place. The low-temperature FeMnP phase belongs to the Co2Si struc-

TABLE 6. Selected bond lengths (Å) in the crystal structure of allabogdanite

M1-P	2.197(4)	P-M1	2.197(4)							
M1-P ^{a,b}	2.254(3) 2×	P-M1 ^{g,h}	2.254(3) 2×							
M1-P°	2.273(4)	P-M1 ⁱ	2.273(4)							
		P-M2 ^j	2.338(4)							
M2-P ^d	2.338(4)	P-M2 ^{e,f}	2.452(3) 2×							
M2-P ^{e,f}	2.452(3) 2×	P-M2 ^{g,h}	2.586(3) 2×							
M2-P ^{a,b}	2.586(3) 2×									
Note: $a = -x + 1/2$, $-y + 1$, $z + 1/2$; $b = -x + 1/2$, $-y$, $z + 1/2$; $c = x + 1/2$										
2, y, $-z + 3/2$; d = x, y, z + 1; e = $-x + 1$, $-y + 1$, $-z + 2$; f = $-x + 1$, $-y$, $-z + 3/2$; f = $-x + 1$, $-y$, $-z + 3/2$; f = $-x + 1$, $-y + 1$, $-z + 2$; f = $-x + 1$, $-y + 1$, $-z + 2$; f = $-x + 1$, $-y + 1$, $-z + 2$; f = $-x + 1$, $-y + 1$, $-z + 2$; f = $-x + 1$, $-y + 1$, $-z + 2$; f = $-x + 1$, $-y + 1$, $-z + 2$; f = $-x + 1$, $-y + 1$, $-z + 2$; f = $-x + 1$, $-y + 1$, $-z + 2$; f = $-x + 1$, $-y + 1$, $-z + 2$; f = $-x + 1$, $-y + 1$, $-z + 2$; f = $-x + 1$, $-y + 1$, $-z + 2$; f = $-x + 1$, $-y + 1$, $-z + 2$; f = $-x + 1$, $-y + 1$, $-z + 2$; f = $-x + 1$, $-y + 1$, $-z + 2$; f = $-x + 1$, $-y + 1$, $-z + 2$; f = $-x + 1$, $-y + 1$, $-z + 2$; f = $-x + 1$; f										
z + 2; g = $-x + 1/2$, $-y$, $z - 1/2$; h = $-x + 1/2$, $-y + 1$, $z - 1/2$; i = $x - 1/2$, y,										
-z + 3/2;	j = x, y, z - 1.	-z + 3/2; j = x, y, z - 1.								

TABLE 5. Atomic coordinates and displacement parameters (Å²) for allabogdanite

Atom	x	у	Z	$U_{ m eq}$	<i>U</i> ₁₁	U ₂₂	<i>U</i> ₃₃	U ₂₃	<i>U</i> ₁₃	<i>U</i> ₁₂
M1*	0.3577(3)	1/ ₄	0.9357(2)	0.0095(4)	0.0129(9)	0.0084(6)	0.0072(6)	0	0.0001(5)	0
M2*	0.4693(3)	¹ / ₄	0.3324(2)	0.0111(5)	0.014(1)	0.0114(8)	0.0080(6)	0	0.0010(5)	0
Р	0.2443(5)	¹ / ₄	0.6225(3)	0.0071(8)	0.009(2)	0.007(1)	0.005(1)	0	0.0002(8)	0

* *M* = Fe_{1.50}Ni_{0.50}.

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	Allabogdanite	Florenskyite	Synthetic Fe _{1.6} Ni _{0.2} Cu _{0.2} P	Rhodarsenide	Palladodymite	Barringerite
Reference	Ivanov et al. 2000	Kuz'ma et al. 1983	Tarkian et al. 1997	Britvin et al. 1999	Buseck 1969	
Chemical formula	(Fe,Ni)₂P	FeTiP	Fe _{1.6} Ni _{0.2} Cu _{0.2} P	(Rh,Pd)₂As	(Pd,Rh)₂As	(Fe,Ni)₂P
Structure type	Co ₂ Si	Co₂Si	Co ₂ Si	Co ₂ Si	Co ₂ Si	Fe ₂ P
Crystal system	Orthorhombic	Orthorhombic	Orthorhombic	Orthorhombic	Orthorhombic	Hexagonal
Space group	Pnma	Pnma	Pnma	Pnma	Pnma	P-62m
a	5.748 *	6.007	5.783	5.866	5.91	5.87
b	3.548	3.602	3.554	3.893	3.90	
С	6.661	6.897	6.646	7.302	7.34	3.44
V	135.8	149.2	136.6	166.8	169.2	102.6
Ζ	4	4	4	4	4	3
a:b:c	1.620:1:1.877	1.668:1:1.915	1.627:1:1.870	1.507:1:1.876	1.515:1:1.882	1.706 (<i>c:a</i>)
D _{calc} ., g/cm ³	7.10	6.83 †	7.04	11.32	11.3	7.04‡

* Cell parameters refined from powder data.

Density re-calculated from the empirical formula given in the original reference.

‡ Calculated on the basis of empirical formula. In original reference, D = 6.92 g/cm³ is calculated for pure Fe₂P.

ture type. On the basis of Mössbauer spectroscopic studies, Fruchart et al. (1969) concluded that, in the mixed Fe₂P-M₂P systems (M = Mn, Cr, Ni, Co), Mn and Cr substitute for the tetragonal-pyramidal M1 site, whereas Ni and Co substitute preferentially for the tetrahedral M2 site. This observation is in agreement with our conclusion that Fe atoms in allabogdanite may show a preference for the M1 position. It can be suggested that the orthorhombicity of allabogdanite is due to the Fe-Ni ordering. It should also be noted that allabogdanite contains a small amount of Co (Table 2) that may cause its structure to be orthorhombic.

The electronic structure of transition metal M_2P phosphides was studied by Boucekkine et al. (1991) using tight-binding extended Hückel molecular orbital (EHMO) calculations. Those authors pointed out that the second-order Jahn-Teller effect is responsible for the fact that Co_2P is orthorhombic and that the structure choice is controlled by the electronic features of metalmetal bonding. Kuz'ma et al. (1983) synthesized a series of compounds in the Fe-Ni-Cu-P system that crystallize with the Co_2Si type. In particular, the powder diffraction pattern of $Fe_{1.6}Ni_{0.2}Cu_{0.2}P$ (PDF 37-0435) is very similar to that of allabogdanite.

Only three minerals belong to the Co₂Si structure type: rhodarsenide, (Rh,Pd)₂As (Tarkian et al. 1997, Quesnel and Heyding 1962), palladodymite (Pd,Rh)₂As (Britvin et al. 1999a) and florenskyite FeTiP (Ivanov et al. 2000). Table 7 summarizes some properties of allabogdanite and related compounds.

ORIGIN OF THE MINERAL

It seems very likely that allabogdanite is a primary phase in the Onello meteorite. Most probably it crystallized at the first stages of the Fe-Ni melt crystallization. Later, some of the crystals were altered to schreibersite that forms irregular rims around some of the allabogdanite relict grains (Fig. 3). In this meteorite, schreibersite is a secondary mineral. The relationships between allabogdanite and nickelphosphide remain unclear, as they were never found as intergrowths.

It should also be noted that, if (Fe,Ni)₂P solid solutions across the whole compositional range crystallize in the Co₂P structure type, barringerite can be considered as a high-temperature poly-



FIGURE 3. Relict of allabogdanite crystal (ABG) surrounded by schreibersite rim (SCHR) in plessite matrix (PL). Black phase is a secondary Fe-Ni-hydroxide. Backscattered electron image. Scale bar 10 µm. morph of (Fe,Ni)₂P, by analogy with iron manganese phosphide, FeMnP, studied by Chenevier et al. (1987).

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