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Review 1.

Haxonite revisited, $\text{NiFe}_{22}\text{C}_6$: new crystal-chemical formulae and Fe-Ni ordering as a structure-stabilizing factor

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ABSTRACT

Haxonite is the second most common carbide in meteorites following cohenite. However, unlike the latter, haxonite has no synthetic counterpart, hence its structure type and chemical formula were suggested based on the similarity of the X-ray powder diffraction pattern with that of a *tau carbide* (synthetic analogue of isovite). During the study of the mineralogy of the Barbianello meteorite (iron ungrouped, Ni-rich ataxite), we identified both cohenite and haxonite within the 2-cm single-crystal host rod of taenite matrix. Both carbides form irregular-angular crystals associated with nickelporphide, but have never been found in one inclusion together. Cohenite and haxonite vary considerably in Ni content (<1 and 5 wt. %, respectively), while the associated nickelporphide and taenite have a constant Ni composition (~27 and 52 wt. %, respectively). The Ni content in haxonite from the Barbianello meteorite is close to ~1.1 atom per formula unit (apfu), which is a typical value for all previously studied haxonites (~1.1 - 1.3 apfu). Notably, no Ni-free haxonite crystals are known. Based on single crystal X-ray diffraction data, we demonstrated that Ni orderly occupies a single crystallographic site (M1, 4a). The dominance of Ni in a single crystallographic site also leads to the ideal formula of haxonite being $^{M1}\text{Ni}^{M2-M4}\text{Fe}_{22}\text{C}_6$. We hypothesize that the presence of Ni stabilizes haxonite crystal structure and makes haxonite common in Ni-rich irons. We propose that other factors promoting haxonite formation include the presence of a precursor Ni-rich phase and relatively low crystallization temperatures.

Keywords: haxonite; cohenite; carbide; Cr_{23}C_6 ; $\text{NiFe}_{22}\text{C}_6$; iron meteorite; nickel-rich ataxite.

INTRODUCTION

Natural carbides have been known since the 19th century (e.g., Weinschenk 1889) and are a small group of minerals, including 12 species to date (Ralph et al. 2025). The formation of carbides is possible only in oxygen-poor reducing conditions typical for the Earth's core (e.g., Wood 1993; Sagatov et al. 2020; Komabayashi et al. 2024) and rarely occur in the Earth's crust (e.g., Ryabov et al. 1985; Ulff-Møller 1985; Vereshchagin et al. 2025). Notably, such conditions are common for various metal-rich meteorites, where a third of the known carbides were discovered (e.g., Weinschenk 1889; Scott 1971; Ma and Rubin 2019).

Haxonite is the second most common carbide in meteorites after cohenite (e.g., Buchwald 1975; Goldstein et al. 2017; Rubin and Ma 2021). Haxonite was discovered in IAB iron meteorites (Scott 1971) and subsequently was found in IIAB, IIIAB and IIIE irons (e.g., Buchwald 1975; Scott and Goldstein 2012; Wittmann and Garvie 2019), carbonaceous and ordinary chondrites (e.g., Taylor et al. 1981; Brearley and Jones 1998; Brusnitsyna et al. 2015), asteroid 25143 Itokawa (Harries and Langenhorst 2018) and low mantle diamond (Kaminsky and Wirth 2011).

Haxonite and cohenite may occur together, but the former is much more abundant in Ni-rich irons (Buchwald 1975; Goldstein et al. 2017), indicating the significant role of Ni in its formation. However, no stable carbide is known in Fe-Ni-C system (e.g., Paek et al. 2021), making natural haxonite the only source of data on its physical properties and formation conditions. It is worth noting, that haxonite is the only meteoritic carbide (and probably the only iron meteorite mineral) that does not have a synthetic analogue of the same composition (although structural analogues are known, see below). Besides, haxonite crystal structure has never been studied experimentally: only unit cell parameters (e.g., Scott, 1971) and computational simulations are available to date (e.g., Fang et al. 2010; Liu et al. 2015).

This paper is devoted to the discovery of haxonite in the ungrouped iron meteorite, as well as a detailed description of its crystal structure. Besides, some genetic features of haxonite are discussed.

MATERIALS AND METHODS

Barbianello meteorite

Barbianello (total weight 860 g), found in ~1960 in Lombardia, Italy, is a Ni-rich ataxite (~27 wt. % Ni), which belongs to chemically ungrouped iron meteorites (Fioretti and Zipfel 2004). Barbianello characterizes by diverse mineral assemblages including native Fe (kamacite, α -Fe), taenite (γ -Fe), tetrataenite (FeNi), schreibersite (Fe₃P), nickelpyrosphide (Ni₃P) and allabogdanite (Fe₂P) (Fioretti and Zipfel 2004; Britvin et al. 2019). No carbides were previously reported in Barbianello iron and no data on its bulk C content is available. The bar-like cut section of the Barbianello, 2 × 2 × 20 mm, previously studied by Britvin et al. (2019) was used in this study.

Analytical techniques

The optical properties of minerals were studied by ore microscopy by means of a DLMP polarizing light microscope (Leica, Germany). Elemental composition and phase morphology were studied using a S-3400 N (Hitachi, Japan) scanning electron microscope (SEM) equipped with an AzTec Energy X-Max 20 (Oxford Instruments, UK) energy-dispersive X-ray (EDS) and a WAVE 500 (Oxford Instruments, UK) wavelength-dispersive X-ray (WDS) spectrometers. Routine analyses and elemental mapping were conducted in EDS mode, while grains of considerable size were analyzed by WDS. The conditions for EDS analysis were: 20 kV accelerating voltage, 1 nA beam current, and 30 s data-collection time (excluding dead time). WDS analysis was acquired with 20 kV, 5 nA, 30 s per element and 2×15 s background acquisition time. Pure Co, Ni and Cr metals ($K\alpha$ lines), pyrite (Fe $K\alpha$ and S $K\alpha$), and InP (P $K\alpha$) were used as analytical standards. The structural type of minerals, their crystallinity and mutual orientations were studied *in situ* by electron backscatter

diffraction (EBSD). EBSD measurements were performed with an HKL Nordlys Nano (Oxford Instruments, UK) EBSD detector, operated at 30 kV and 0.5-2 nA and equipped on the abovementioned S-3400N (Hitachi, Japan) SEM. The samples were polished with progressively smaller polycrystalline diamond suspensions with an ending step of Ar ion plasma etching for 10 min at the final stage (IonFab 300 (Oxford Instruments, UK)) to remove the amorphized layer. EBSD orientation maps were presented as color-coded images using the standard techniques of color-coded IPF-Z plots. Phase maps were presented as color-coded images using a user-defined color scheme. Phase structures were determined by matching the respective EBSD patterns with the reference structural models obtained from the Inorganic Crystal Structure Database (ICSD). The single crystal X-ray diffraction (SCXRD) analysis was performed using a XtaLAB Synergy-S (Rigaku Oxford Diffraction, Japan) diffractometer equipped with a HyPix-6000HE detector operated with monochromated MoK α radiation ($\lambda[\text{MoK}\alpha] = 0.71073 \text{ \AA}$) at 50 kV and 40 mA. The single crystal with the approximate size of $4 \times 3 \times 3 \text{ }\mu\text{m}$ was mounted on the quartz glass fiber using paraton-*n* and used for SCXRD studies. More than a hemisphere of three-dimensional data was collected (Supplementary electronic material, Crystallographic Information Files). The data were integrated and corrected for background, Lorentz, and polarization effects. The empirical absorption correction based on spherical harmonics implemented in the SCALE3 ABSPACK algorithm was applied in the CrysAlisPro program (Agilent 2012). The SHELXL package (Sheldrick 2015) was used for all structural calculations.

RESULTS AND DISCUSSION

Optical properties and appearance

Carbides in Barbianello occur as inclusions (up to 100 μm in size) in nickel-rich metal (taenite; Table 1). Typically, the inclusions consist of two chemically distinct phases – carbide (cohenite or haxonite) and phosphide (nickelphosphide). Different carbides have never been found

in one inclusion together. Carbides form irregular-angular crystals, while nickelporphide fills the marginal parts of the inclusions or "floats" inside the carbide (Figure 1). It is noteworthy that carbide-phosphide inclusions are located within single crystal of taenite (Figure 1). Previously, euhedral kamacite single crystals were found within same taenite single crystal (Britvin et al. 2019).

Both haxonite and cohenite were detected *in situ* in host metal by EBSD. EBSD analysis revealed that haxonite is cubic (space group $Fm\bar{3}m$; mean angular deviation (MAD) – 0.2-0.3; number of indexed bands (NIB) – 11-12), while cohenite is orthorhombic (space group $Pbnm$; MAD – 0.1-0.2; NIB 12). Haxonite was found to form single crystals up to 20 μm in size, while cohenite forms crystals up to 40-50 μm . The largest crystal of haxonite was extracted from the metal for a detailed study of its crystal structure using SCXRD.

Previously haxonite was found in various iron meteorites as "carbide roses" – specific intergrowths with native iron (kamacite), taenite and schreibersite (Buchwald 1975). This kind of assemblages is also common for other isostructural carbides (e.g., Abbasi et al. 2022; Sterkhova et al. 2022). Besides, haxonite is commonly found in spheroidized and pearlitic plessite as a precipitate enclosing taenite spherules and lamellae, respectively (e.g., Buchwald 1975; Goldstein et al. 2017; Wittmann and Garvie 2019). Cohenite can form both acicular crystals and worm-shaped aggregates (e.g., Buchwald 1975; Goldstein et al. 2017; Vereshchagin et al. 2024). Thus, the identification of the carbides cannot be carried out solely on the basis of its morphology. Besides, in reflected light, the carbides are almost indistinguishable by reflectance (Figure 1).

Chemical composition and crystal structure

Haxonite and cohenite in Barbianello can be easily distinguished by Ni content: its concentration in haxonite is almost uniform, oscillating at the level of ~5 wt. % (~1.1 atoms per formula unit (*apfu*)), while cohenite contains ~ 1.5 wt. % Ni (~0.05 *apfu*; Table 1). Our observations

are in good agreement with previous studies where the concentration of Ni in haxonite is about 5 ± 0.4 wt. Ni % (~ 1.1 - 1.3 apfu; Table 1) and is significantly higher than Ni content in cohenite, ~ 1 - 2 wt. Ni (< 0.1 apfu; Taylor et al. 1981; Scott and Goldstein 2012; Wittmann and Garvie 2019). It's important to note that the nickel content of haxonite remains constant regardless of the Ni content of host metal (kamacite / taenite) or its association with nickelporphide (which contains almost an order of magnitude more Ni; Table 1).

The crystal structure of haxonite was fully refined for the first time based on SCXRD data (Supplementary crystallographic information data). Haxonite is cubic (space group $Fm\bar{3}m$), $a = 10.5536(6)$ Å (Supplementary electronic material). Previously only unit cell parameters for the mineral were calculated (Scott 1971; Table 2), while all the other crystallographic data were modeled using first-principles calculations (e.g., Fang et al. 2010, 2012; Liu et al. 2015; Medvedeva et al. 2015). We succeeded in allocation of Fe and Ni into independent M1-M4 crystallographic sites. This issue had previously been addressed and solved for minerals of the schreibersite-nickelporphide series (Britvin et al. 2021a) and perryite (Britvin et al. 2021c).

The crystal structure of haxonite can be described as NaCl-type packing of cubo-octahedra and cubes, consisting of 8 Fe₄ atoms with M1 (M1=Ni, Fe) atoms located in the center and 12 Fe₃ atoms around it (Bowman et al. 1972; Figure 2a). Due to the cubic symmetry, cubo-octahedra are regular with the edge length of cube equal 2.454 Å (Table 3). Alternatively, haxonite crystal structure can be described, as consisting of five types of clusters around each site (M1, Fe₂, Fe₃, Fe₄, C). As it was mentioned above, M1 atom is surrounded by 12 Fe₃ atoms, forming regular cubo-octahedra (Figure 2b). Fe₂ atom has 4 contacts with Fe₄ and 12 contacts with Fe₃ (Figure 2c). Fe₃ atoms have the most complex coordination and are surrounded by all types of atoms, forming complex 14-fold coordination polyhedra (Figure 2d). It has 1, 2, 5 and 4 contacts with M1, Fe₂, Fe₃ and Fe₄ atoms, respectively and 2 contacts with C atoms. Fe₄ atoms are surrounded by all atoms

except M1 forming complex 13-fold polyhedra (Figure 2e). The coordination of C atoms can be described as square antiprism with the 4 contact with Fe3 and 4 contact with Fe4 atoms (Figure 2f).

Notably, haxonite has a direct chromium counterpart – isovite, Cr_{23}C_6 (Generalov et al. 1998), which is also the most common carbide in Cr-based alloys, where it is called the *tau carbide* (τ -carbide) and whose crystal structure is well studied (e.g., Bowman et al., 1972; Yakel, 1987). Both haxonite and isovite belongs to the M_{23}X_6 family compounds with general crystal chemical formula $\text{M}_1\text{M}_2\text{M}_3\text{M}_4\text{X}_6$, where $\text{M}=\text{Cr, Fe, Ni, etc.}$, $\text{X}=\text{C, B, P, etc}$ (Table 2). M_{23}X_6 family includes ~100 compounds, including diverse carbides, borides, phosphides, silicides and germanides (e.g., Griбанov et al. 1994; Eriksson et al. 2007; Veremchuk et al. 2009; Table 2). We were unable to find any data on synthetic binary Fe_{23}C_6 and Ni_{23}C_6 carbides, while both Fe_{23}B_6 and Ni_{23}B_6 are known (Table 2) indicative of the crystal-chemical control on the stability of M_{23}X_6 compounds. The absence of experimental data on the binary M_{23}X_6 phosphides, germanides or silicides evidences that simultaneous occurrence of structurally heterogeneous cations (e.g., both early and late transition metals) is essential for stabilizing this structure type.

We suggest that nickel has a crucial role in the stabilization of the $(\text{Fe,Ni})_{23}\text{C}_6$ structure, and therefore, incorporation of nickel promotes the haxonite formation. Our data indicate that nickel preferentially occupies the M1 (4a) site in the haxonite structure (Ni site share is ~70 %). Previously, it was shown that the M1 site in M_{23}C_6 compounds is the first to be populated by the “guest” atom (e.g., Fe in $(\text{Cr,Fe})_{23}\text{C}_6$ or Cr in $(\text{Fe,Cr})_{23}\text{C}_6$) (Yakel 1987; Xie et al. 2006; Liu et al. 2015; Medvedeva et al. 2015; Table 3). Moreover, it was reported that the stability of M_{23}C_6 -type compounds is generally achieved by the introduction of the guest atom into the M1 site (e.g., Liu et al. 2015; Medvedeva et al. 2015). As a consequence, preferential M1 site occupancy by nickel affects the correct presentation of the crystal chemical formula of haxonite. Based on the results of our study, the recommended formula of the mineral can be expressed as $^{\text{M1}}\text{Ni}_1^{\text{M2}}\text{Fe}_2^{\text{M3}}\text{Fe}_{12}^{\text{M4}}\text{Fe}_8\text{C}_6$ or simply $\text{NiFe}_{22}\text{C}_6$.

Carbides in Ni-rich ataxites

Barbianello belongs to Ni-rich ataxites, a structural class of Ni-rich (>12 wt. Ni) iron meteorites which appear structureless (with no Widmanstaetten structure) on the macro level (Buchwald 1975). A less than 30 Ni-rich ataxites are currently known, and most of them have been poorly studied using the modern methods, with only general descriptions given (e.g., Henderson and Perry 1954; Buchwald 1975; Nagata et al. 1987). However, the significant similarities in the mineralogy of Barbianello (~27 wt. % Ni; ungrouped) with some other Ni-rich (> 20 wt. %) ataxites of group IAB (e.g., Freda (~23 wt. % Ni) or San Cristobal (~26 wt. % Ni)) are noteworthy. In all cases taenite form single crystals up to several cm long with relatively small inclusions of kamacite, phosphides and carbides (e.g., Scott 1971; Scott and Bild 1974; Buchwald 1975). Besides, Barbianello, San Cristobal and Freda contain both cohenite and haxonite (e.g., Scott and Bild 1974; Buchwald 1975; Scott and Goldstein 2012). However, some Ni-rich ataxites of group IAB contain edscottite instead of haxonite (e.g., Wedderburn; Ma and Rubin 2019) or lack carbides (e.g., Tishomingo; Goldstein et al. 2017).

IMPLICATIONS

The appearance of carbides in iron meteorites is of great interest because it allows to reconstruct their primary composition and formation conditions (e.g., Buchwald 1975; Scott and Goldstein 2012). The formation of cohenite in various types of irons is fairly well studied and explained, while the formation of haxonite remains largely unclear (e.g., Buchwald 1975; Scott and Goldstein 2012). It is known that the nucleation and growth of carbide precipitates depend on chemical composition, thermal history and temperature, as well as interface interactions with other components (e.g., Fang et al. 2010).

We suggest that the formation of haxonite in iron meteorites is primarily controlled by the abundance of nickel in the chemical environment. Our data, along with previous studies of meteoritic carbides (e.g., Scott and Goldstein 2012) and theoretical calculations (e.g., Fang et al. 2010), indicate that Ni stabilizes the haxonite crystal structure. Notably, the rise of Ni content in bulk meteorite metal does not lead to further increase of Ni content in coexisting haxonite (Table 1). For example, the chemical composition of haxonite from Barbianello (~23 wt. % Ni in metal matrix) and Canñn Diablo (~7 wt. % Ni in metal) is almost identical (Table 1). Previously, Harries and Langenhorst (2018), based on experimental studies and ab initio calculations of Fang et al. (2016) also suggested that the Fe/Ni ratio in haxonite is rather non-informative about the formation temperature and the parental phases of haxonite. It seems that the crystal structure of haxonite reaches its capacity limit for Ni at ~1 apfu, and Ni₂₃C₆ can not be formed even in Ni-richest irons. Moreover, the constant content of Ni in haxonite, i.e., ~1 apfu, is mandatory for its existence, resulting in its ideal formula NiFe₂₂C₆.

The second important factor controlling haxonite nucleation is interface interactions with other components (interface energy). Small mismatch between unit cell parameters of haxonite and taenite could promote haxonite formation (e.g., Fang et al. 2010). This agrees with the fact that haxonite in iron meteorites is found to be mainly surrounded by taenite rather than kamacite (e.g., Buchwald 1975; Scott and Goldstein 2012). Besides, carbon prefers to concentrate in taenite rather than in kamacite at high temperatures (Reed-Hill 1973). Consequently, growth of kamacite from Ni-, C-rich taenite on cooling may cause Ni-rich carbide to precipitate (Romig and Goldstein 1978).

The third important factor is the formation temperature and cooling rate. Our data and previously published studies indicate that haxonite is a fairly common carbide found in the metal of various types of iron meteorites (including IAB, IIAB, IIIAB, IIIE and ungrouped irons; e.g., this study; Buchwald 1975; Scott and Goldstein 2012). It is thought that iron meteorites have cooled slowly and to have reached thermodynamic equilibrium (e.g., Buchwald 1975; Goldstein et al.

2009). However, haxonite (and cohenite) are thermodynamically unstable at all temperatures at one atmosphere, ultimately decomposing to native Fe (“kamacite”) and graphite (e.g., Buchwald 1975; Fang et al. 2010). Moreover, no $M_{23}C_6$ ($M=Fe, Ni$) carbides were found in B-, Cr-free steels and no stable carbide is known in Fe-Ni-C system at one atmosphere pressure (e.g., Paek et al. 2021). Besides, all artificial “haxonites” (typically found in Cr-rich Fe-Ni alloy) lack chemical composition and detail description (e.g., Nachez et al. 2006). It was suggested that the complexity of the crystal structure and the unique coordination of Ni, Fe and C in $(Fe, Ni)_{23}C_6$ hamper its formation during the non-equilibrium steel fabrication and manipulation processes (Fang et al. 2010). Thus, haxonite is the only meteoritic carbide (and probably the only iron meteorite mineral) that does not have a synthetic analogue of the same composition.

It is known that $M_{23}C_6$ carbides are formed during heat treatment by transformation of carbides with a lower M/C ratio ($M_3C \rightarrow M_{23}C_6$ / $M_7C_3 \rightarrow M_{23}C_6$ / $M_6C \rightarrow M_{23}C_6$; Gorunov 2020; Song et al. 2022; Sterkhova et al. 2022). For example synthetic isovite $(Cr, Fe)_{23}C_6$ could be formed at relatively low temperatures (below 700 °C) *via* intermediate phase, which accumulates Cr / Mo / V from metal (Baltušnikas et al. 2016; Wiecek et al. 2017). Long annealing (~100 h) of M_7C_3 carbide at elevated temperatures (~1000 °C) also leads to its full transformation to $M_{23}C_6$ carbide (Kondrat'ev et al., 2015). Besides, it was shown that Cr/Fe ratio in $(Cr, Fe)_{23}C_6$ is temperature dependent: Fe-rich $M_{23}C_6$ carbide is formed at elevated temperatures (above 700 °C; Medvedeva et al., 2015).

Based on these data, we can assume that haxonite formed in several stages. In the first stage (at temperatures ~700-1000 °C), a nickel-rich metastable $(Ni, Fe)_7C_3$ or $(Ni, Fe)_3C$ carbide was formed from Ni-, C-rich iron melt. The upper temperature limit corresponds to the temperatures of formation of $(Fe, Cr)_{23}C_6$ carbide in steels (e.g., Kondrat'ev et al., 2015). Bulk nickel content above 7 wt. % promotes the formation of Ni-rich carbide (e.g., Buchwald 1975; Scott and Goldstein 2012).

In the second stage (~400-700 °C), this precursor phase transforms into haxonite or cohenite. The lower temperature corresponds to the decomposition temperature of Ni₃C (e.g., Leng et al., 2008). The discovery of two different carbides (haxonite / cohenite) close together (e.g., this study) indicates the localized nature of the stabilizing conditions required for the formation of haxonite. It is possible that its formation is due to irregularly distributed micro-impurities or structural defects of precursor phase. It is difficult to imagine that cooling rates could differ significantly over distances of a few millimetres or less.

We would also like to note that pressure does not play a significant role in the formation of haxonite. Allabogdanite, previously discovered in the Barbianello meteorite, was thought to have formed under high pressure (Britvin et al. 2019). However, subsequent studies have demonstrated the role of trace elements in stabilizing allabogdanite and the possibility of its formation at ambient pressures (e.g., Litasov et al. 2020; Kong et al. 2024). Nevertheless, the presence of allabogdanite can be considered an indicator of secondary alteration, as the mineral is unstable when heated above 600 °C (Britvin et al. 2021b; Kong et al. 2024).

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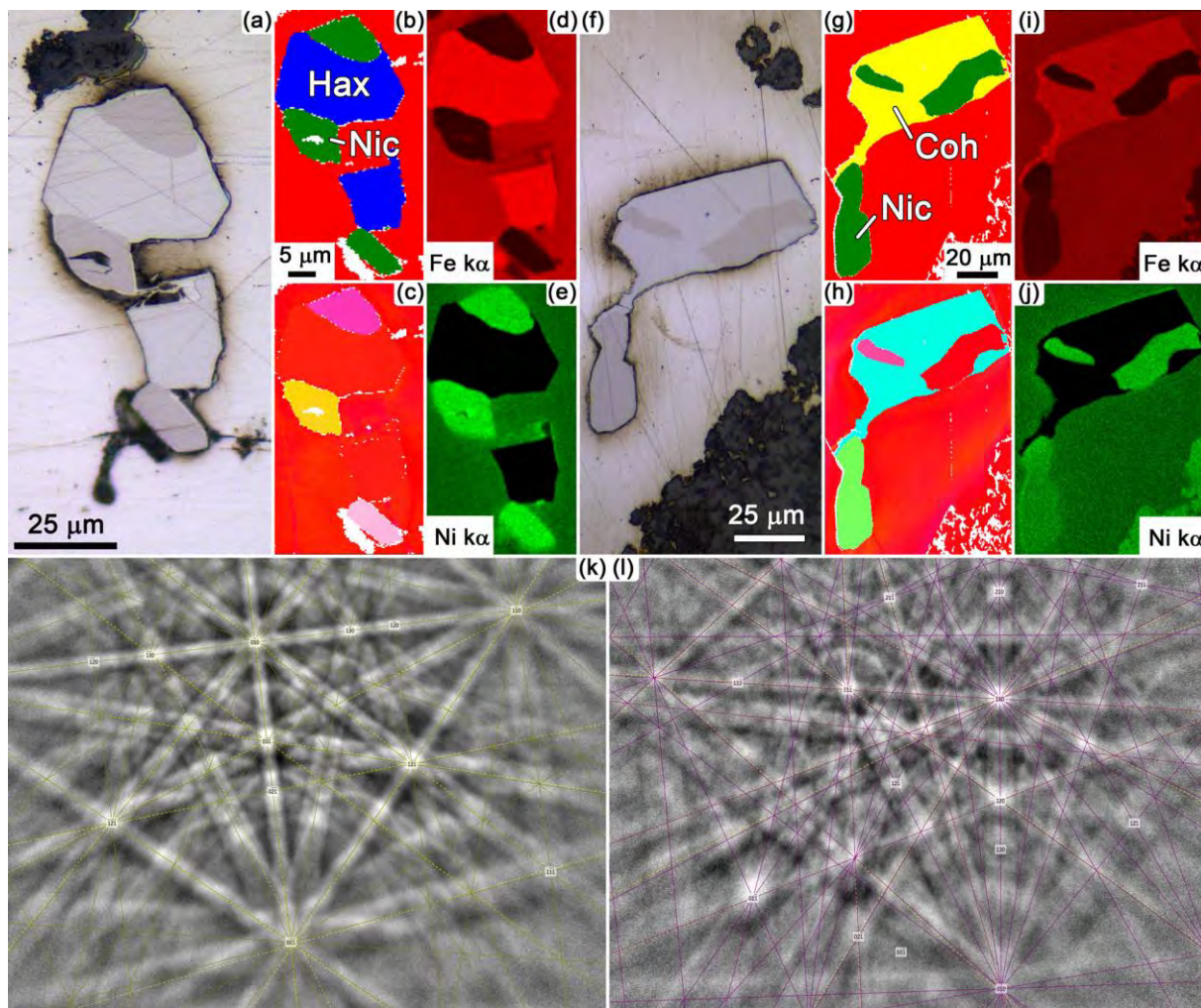
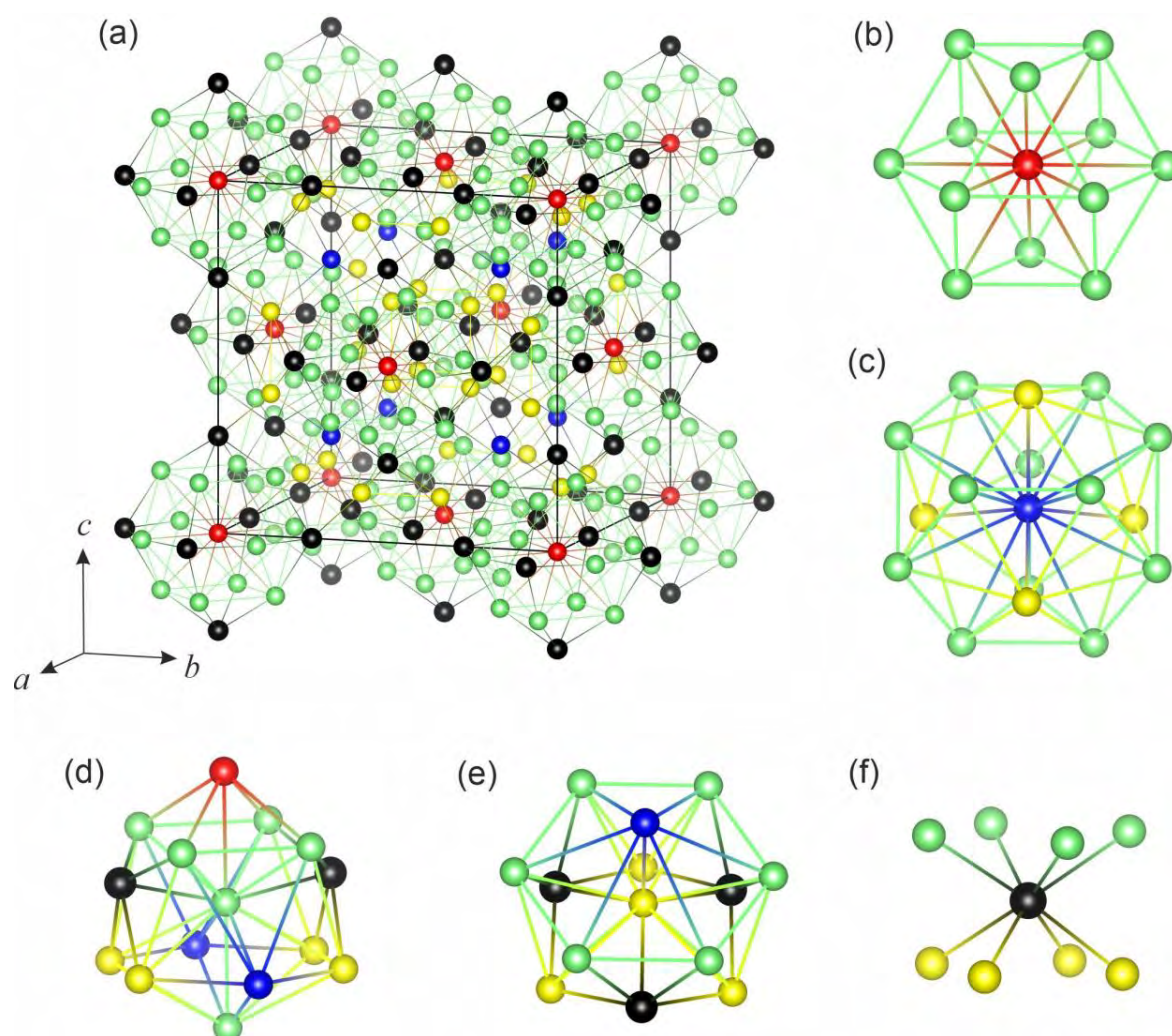


Figure 1. Haxonite (Hax), cohenite (Coh) and nickelporphide (Nic) in Barbianello iron: (a, f) – optical microscopy; (b, g) – EBSD, phase maps; (c, h) – EBSD, grain orientation maps (IPF-Z plots); (d-e, i-j) – SEM-EDS elemental maps (Fe and Ni, respectively), (k) – example of haxonite EBSD pattern indexation using theoretical Kikuchi pattern generated from meteoritic haxonite structure (Scott, 1972); (l) – example of cohenite EBSD pattern indexation using theoretical Kikuchi pattern generated from Fe_3C . Note: bright color on d / i and e / j indicates high Ni and Fe content, respectively.

456



457

458 **Figure 2.** The crystal structure of haxonite: general view (a) and clusters around M1 (b), Fe2 (c),
459 Fe3 (d), Fe4 (e) and C (f) atoms. Red, blue, green, yellow and black spheres show M1 (M = Ni, Fe),
460 Fe2, Fe3, Fe4 and C atoms, respectively.

461

Table 1. Selected chemical compositions and calculated mineral formulae of haxonite and associated minerals in various meteorites.

Mineral	Hax	Coh	Tae	Nic	Hax	Coh	Fe	Hax	Hax	Hax
Meteorite	Barbianello				Canyon Diablo			Semarkona	Allen Hills A77278	Colonia Obrera
Major constituents (wt. %)										
C*	5.31	6.67	-	-	5.29	6.65	-	5.26	5.27	5.28
P	-	-	-	15.52	-	-	-	0.1	-	-
Si	-	-	-	-	-	-	-	-	0.1	-
Fe	89.42	90.93	72.75	32.73	89.50	91.10	93.30	88.1	88.6	89.1
Co	0.74	0.76	0.82	0.78	0.18	0.07	0.68	0.55	0.15	0.30
Ni	4.81	1.43	27.22	52.25	4.91	1.69	6.40	5.4	5.1	5.03
Cr	-	-	-	-	-	-	-	0.12	0.50	-
Sum	100.28	99.79	100.79	101.28	99.88	99.51	98.40	99.31	99.77	99.71
Chemical formula (apfu)**										
C	6	1			6	1		6	6	6
P				1.01						
Si										
Fe	21.72	2.93	0.73	1.18	21.82	2.95	0.93	21.61	21.68	21.76
Co	0.17	0.02	0.01	0.03	0.04	0.00	0.01	0.12	0.02	0.07
Ni	1.11	0.04	0.26	1.79	1.14	0.05	0.06	1.26	1.17	1.17
Cr								0.01	0.13	
Sum	23	3	1	4	23	3	1	23	23	23
Reference	This study				Hilton et al., 2020; Scott, 1971			Taylor et al., 1981		Wittmann and Garvie, 2019

Note: - – below detection limit; * – calculated based on stoichiometric ratio; ** – calculated based on the assumed total number of atoms per formula unit quoted in the Sum line; Hax – haxonite; Coh – cohenite; Tae – taenite, Nic – nickelporphide, Fe – kamacite (native Fe)

468

Table 2. Crystallographic data for haxonite and some isostructural $M_{23}X_6$ compounds*

Ideal Formula	<i>a</i>, Å	Volume, Å³	Reference (name)
Ni ₁ Fe ₂₂ C ₆	10.554	1175.4	This study (haxonite)
(Fe,Ni) ₂₃ C ₆	10.55	1174.2	Scott, 1971 (haxonite)
Cr ₂₃ C ₆	10.650	1207.9	Bowman et al., 1972 (isovite)
Mn ₂₃ C ₆	10.595	1189.3	Karen et al., 1991
Fe ₂₃ B ₆	10.761	1246.1	Idzikowski and Szajek, 2003
Ni ₂₃ B ₆	9.53	865.5	Idzikowski et al., 2004
Er ₂ Ni ₂₁ B ₆	10.652	1208.6	Veremchuk et al., 2009
Mg ₃ Ni ₂₀ P ₆	11.113	1372.4	Keimes and Mewis, 1992
Ce ₃ Pd ₂₀ Ge ₆	12.445	1927.6	Gribanov and Seropegin, 1992
Ce ₃ Pd ₂₀ Si ₆	12.161	1798.5	

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Note: * space group $Fm\bar{3}m$; $Z = 4$.

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Table 3. Crystallographic data for haxonite in comparison with (Cr,Fe)₂₃C₆ compounds (space group *Fm-3m*, *Z* = 4).

Formula	Fe _{22.3} Ni _{0.7} C ₆	Fe ₂₃ C ₆	Cr ₂₃ C ₆	Cr _{22.26} Fe _{0.74} C ₆	Cr _{21.3} Fe _{1.7} C ₆	Cr _{18.87} Fe _{4.13} C ₆	Cr _{15.64} Fe _{7.36} C ₆	Cr ₂₃ C ₆
<i>a</i> , Å	10.5536(6)	10.5146	10.6595(4)	10.6537(1)	10.6454(6)	10.6199(3)	10.5966(3)	10.650(2)
Volume, Å ³	1175.4(2)	1162.5	1211.2	1209.2	1206.4	1197.7	1189.9	1207.9
Source*	SCXRD	DFT	SCXRD	SCXRD	SCXRD	SCXRD	SCXRD	SCXRD
Contact name	distance, Å							
<i>M1-M3</i>	2.5225(3)	2.4383	2.5613(3)	2.5526(2)	2.5378(3)	2.5290(3)	2.5254(3)	2.558(5)
<i>M2-M4</i>	2.4450(3)	2.3546	2.4369(4)	2.4347(2)	2.4303(4)	2.4238(3)	2.4177(4)	2.415(5)
<i>M2-M3</i>	2.9021(2)	2.7898	2.9256(2)	2.9270(1)	2.9301(2)	2.9242(1)	2.9170(1)	2.923(2)
<i>M3-M3</i>	2.4176(5)	2.3076	2.4148(6)	2.4279(4)	2.4519(5)	2.4513(5)	2.4422(6)	2.414(9)
<i>M3-M3</i>	2.5225(3)	2.4383	2.5613(3)	2.5526(2)	2.5378(3)	2.5290(3)	2.5254(3)	2.558(5)
<i>M3-M4</i>	2.6366(4)	2.5340	2.6456(2)	2.6471(1)	2.6502(2)	2.6449(2)	2.6379(2)	2.637(7)
<i>M3-C</i>	2.109(2)	2.0399	2.130(2)	2.133(1)	2.131(1)	2.126(1)	2.122(2)	2.136(5)
<i>M4-M4</i>	2.4535(5)	2.3612	2.5159(5)	2.5154(3)	2.5164(4)	2.5112(4)	2.5066(5)	2.536(11)
<i>M4-C</i>	2.076(2)	1.9912	2.113(2)	2.106(1)	2.103(1)	2.098(1)	2.093(2)	2.110(6)
<i>M1-C</i>	2.910(4)	2.8143	2.933(3)	2.941(2)	2.944(3)	2.937(3)	2.931(3)	2.945
Reference	This study	Liu et al., 2015	Yakel, 1987	Yakel, 1987	Yakel, 1987	Yakel, 1987	Yakel, 1987	Bowman et al., 1972

471

Note: * DFT – first principle calculations; SCXRD – single crystal X-ray diffraction data