

LETTER

Steinhardtite, a new body-centered-cubic allotropic form of aluminum from the Khatyrka CV3 carbonaceous chondrite

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ABSTRACT

Steinhardtite is a new mineral from the Khatyrka meteorite; it is a new allotropic form of aluminum. It occurs as rare crystals up to ~10 μm across in meteoritic fragments that contain evidence of a heterogeneous distribution of pressures and temperatures during impact shock, in which some portions of the meteorite reached at least 5 GPa and 1200 °C. The meteorite fragments contain the high-pressure phases ahrensite, coesite, stishovite, and an unnamed spinelloid with composition Fe_{3-3x}Si_xO₄ (x ≈ 0.4). Other minerals include trevorite, Ni-Al-Mg-Fe spinels, magnetite, diopside, forsterite, clinoenstatite, nepheline, pentlandite, Cu-bearing troilite, icosahedrite, khatyrkite, cupalite, taenite, and Al-bearing taenite. Given the exceedingly small grain size of steinhardtite, it was not possible to determine most of the physical properties for the mineral.

A mean of 9 electron microprobe analyses (obtained from two different fragments) gave the formula Al_{0.38}Ni_{0.32}Fe_{0.30}, on the basis of 1 atom. A combined TEM and single-crystal X-ray diffraction study revealed steinhardtite to be cubic, space group *Im* $\bar{3}$ *m*, with *a* = 3.0214(8) Å, and *V* = 27.58(2) Å³, *Z* = 2. In the crystal structure [*R*₁ = 0.0254], the three elements are disordered at the origin of the unit cell in a body-centered-cubic packing (α -Fe structure type). The five strongest powder-diffraction lines [*d* in Å (*hkl*)] are: 2.1355 (100) (110); 1.5100 (15) (200); 1.2329 (25) (211); 0.9550 (10) (310); 0.8071 (30) (321).

The new mineral has been approved by the IMA-NMNC Commission (2014-036) and named in honor of Paul J. Steinhardt, Professor at the Department of Physics of Princeton University, for his extraordinary and enthusiastic dedication to the study of the mineralogy of the Khatyrka meteorite, a unique CV3 carbonaceous chondrite containing the first natural quasicrystalline phase icosahedrite.

The recovery of the polymorph of Al described here that contains essential amounts of Ni and Fe suggests that Al could be a contributing candidate for the anomalously low density of the Earth's presumed Fe-Ni core.

Keywords: Aluminum, chemical composition, TEM, X-ray diffraction, new mineral, steinhardtite.

INTRODUCTION

In the course of a detailed investigation of fragments belonging to the Khatyrka meteorite (Steinhardt and Bindi 2012; MacPherson et al. 2013; Bindi and Steinhardt 2014), we found a metallic AlNiFe mineral (Hollister et al. 2014) that turned out to have the characteristics of a new mineral species.

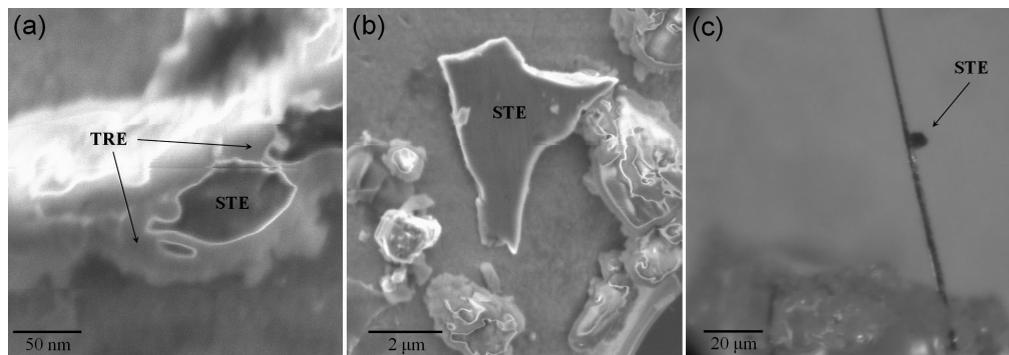
Here we report the structural and chemical study leading to the

description of this new mineral, which was named steinhardtite after Paul J. Steinhardt, Professor at the Department of Physics of Princeton University and Director of the Princeton Center for Theoretical Science, for his extraordinary and enthusiastic dedication to the study of the mineralogy of the Khatyrka meteorite, a unique CV3 carbonaceous chondrite hosting the first natural quasicrystal icosahedrite (Bindi et al. 2009, 2011, 2012). Moreover, decagonal quasicrystalline alloys have been described in the Al-Ni-Fe system (e.g., Lemmerz et al. 1994; Parshin et al. 2009), thus representing an added reason for the dedication: Steinhardt's pioneering contribution to the theoretical development of quasispe-

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► **FIGURE 1.** SEM-BSE images of three small steinhardtite grains. (a) Steinhardtite (STE) is enclosed by trevorite (TRE); (b) a separate grain exhibiting tabular morphology; (c) a small grain attached to a carbon fiber that was used for the X-ray single-crystal diffraction study.



riodic structures (e.g., Levine and Steinhardt 1984).

The mineral and its name have been approved by the Commission on New Minerals, Nomenclature and Classification, IMA (2014-036). The holotype material is deposited in the mineralogical collections of the Museo di Storia Naturale, Università di Firenze (Italy), under catalog number 3142/I.

OCCURRENCE

Steinhardtite was found in one of the meteoritic fragments (labeled number 126; see Hollister et al. 2014 for more details) recovered from an expedition to the Koryak Mountains in far eastern Russia in 2011 (Steinhardt and Bindi 2012; Bindi and Steinhardt 2014) as a result of a search for material that would provide information on the origin of the quasicrystal mineral icosahedrite (Bindi et al. 2009, 2011, 2012; Hollister et al. 2014). The recovered fragments have meteoritic (CV3-like) oxygen isotopic compositions (MacPherson et al. 2013; Hollister et al. 2014).

In the meteoritic fragments, which present a range of evidence indicating that an impact shock generated a heterogeneous distribution of pressures and temperatures in which some portions of the meteorite reached at least 5 GPa and 1200 °C, steinhardtite occurs as small grains, one of which is surrounded by trevorite (Fig. 1a). The grains of steinhardtite are generally anhedral and do not contain inclusions or intergrowths of other minerals. The maximum grain size of steinhardtite identified so far is about 10 μm. Given the exceedingly small size, it was not possible to determine properties like color, streak, luster, hardness, cleavage, parting, fracture, or density. The calculated density (for $Z = 2$), using the empirical formula and the unit-cell volume from single-crystal data (see below), is 5.52 g/cm³. Other minerals identified in the meteorite fragments include trevorite, diopside, forsterite, ahrensite, clinostatite, nepheline, coesite, stishovite, pentlandite, Cu-bearing troilite, icosahedrite, khatyrkite, cupalite, taenite, Al-bearing taenite, Ni-Al-Mg-Fe spinels, magnetite, and an unnamed spinelloid with composition Fe_{3-x}Si₄O₄ ($x \approx 0.4$).

EXPERIMENTAL METHODS

X-ray diffraction and structure refinement

A crystal of steinhardtite $8 \times 9 \times 10 \mu\text{m}$ across (Fig. 1c) was mounted on a 0.005 mm diameter carbon fiber (which was, in turn, attached to a glass rod) and checked on a CCD-equipped Oxford Diffraction Excalibur 3 single-crystal diffractometer. Despite the extremely small size of the crystal (to the limit for conventional in-house experiments), the diffraction quality was satisfactory and several reflections were collected. The refined unit-cell dimensions are: $a = 3.0214(8) \text{ \AA}$ and $V = 27.58(2) \text{ \AA}^3$. Intensity integration and standard Lorentz-polarization corrections were done with the

CrysAlis RED software package (Oxford Diffraction 2006). The program ABSPACK in CrysAlis RED (Oxford Diffraction 2006) was used for the absorption correction.

The systematic absences indicated the space group $Im\bar{3}m$ and the structure was refined starting from the atomic coordinates reported $\alpha\text{-Fe}$ (Wilburn and Bassett 1978) using the full-matrix least-squares program SHELXL-97 (Sheldrick 2008). The scattering curve for neutral Ni was taken from the *International Tables for X-ray Crystallography* (Ibers and Hamilton 1974). The scattering power was allowed to vary (Ni vs. structural vacancy) at the (0,0,0) position. The refined value (21.8 e⁻) is in excellent agreement with the mean electron number calculated from the empirical formula (21.7 e⁻). Refinement of the anisotropic atomic displacement parameters led to an R_1 index of 0.0208 [for 11 reflections with $F_o > 4\sigma(F_o)$] and 0.0254 (for all 12 independent reflections) with 3 refined parameters. Details on the data collection and refinement are given in Table 1¹ and in the deposited CIF¹.

Chemical analyses

The same crystal used for the structural study (Fig. 1c) together with another grain of steinhardtite showing an almost tabular morphology (Fig. 1b) were analyzed by means of a JEOL JXA-8600 electron microprobe analysis in wavelength dispersion mode at 15 kV, 20 nA beam current, and 1 μm beam diameter. Variable counting times were used: 30 s for Al, Ni, and Fe, and 60 s for the minor elements Mg, Si, Cr, P, Co, Cu, Cl, Ca, Zn, and S. Replicate analyses of synthetic Al₃Ni₁₂Fe₃ were used to check accuracy and precision. The crystal fragments were found to be homogeneous within analytical error. The standards used were: metal-Al (Al), synthetic Ni₃P (Ni, P), synthetic FeS (Fe), metal-Mg (Mg), metal-Si (Si), metal-Cr (Cr), metal-Co (Co), metal-Cu (Cu), synthetic CaCl₂ (Ca, Cl), and synthetic ZnS (Zn, S). Mg, Si, Cr, P, Co, Cu, Cl, Ca, Zn, and S were found to be equal to or below the limit of detection (0.01 wt%).

Nine point analyses on different spots were performed on the two fragments. Table 2 reports the chemical analyses (means and ranges in wt% of elements), standard deviations, and atomic ratios calculated on 1 atom per formula unit.

Transmission electron microscopy

Because of the small size of the grains, the single-crystal X-ray investigation was combined with a structural study done by transmission electron microscopy. The instrument was a Philips CM200-FEG TEM operating at 200 keV with a vacuum pressure of $\sim 2 \times 10^{-7}$ Torr. The electron beam size ranged from 30 nm to 0.2 μm. The sample was placed on an Au mesh TEM grid (300 mesh, 3 mm in diameter) that was previously covered by a thin carbon layer (support film). Energy-dispersive

¹ Deposit item AM-14-1111, Table 1 and CIF. Deposit items are stored on the MSA web site and available via the *American Mineralogist* Table of Contents. Find the article in the table of contents at GSW (ammin.geoscienceworld.org) or MSA (www.minsocam.org), and then click on the deposit link.

TABLE 2. Electron microprobe analyses (means, ranges, and standard deviations in wt% of elements) and atomic ratios (on the basis of one atom) for steinhardtite

Element	wt%	Ranges	σ	Atom	Atomic ratios
Al	22.41	21.94–23.30	0.16	Al	0.38
Ni	40.90	40.01–42.10	0.26	Ni	0.32
Fe	36.23	35.06–37.29	0.19	Fe	0.30
Total	99.54	98.45–101.62			

(EDS) data were obtained using Evex NanoAnalysis System IV attached to the Philips CM200-FEG TEM. A small probe diameter of 20–100 nm was used, with a count rate of 100–300 cps and an average collection time of 180 s. The quantitative analyses were taken at 200 kV and are based on using pure elements and the NIST 2063a standard sample as a reference under the identical TEM operating conditions.

The measurement of the cubic unit-cell parameter from both the selected area diffraction patterns (Fig. 2) and the diffraction rings (Fig. 3) is only about 1% different and led to a value of 3.02(1) Å, in excellent agreement with the value measured by single-crystal X-ray diffraction [3.0214(8) Å].

RESULTS AND DISCUSSION

Crystal structure considerations

In the crystal structure of steinhardtite, Al, Ni, and Fe are disordered at the origin of the unit-cell (0,0,0) in a body-centered-cubic (bcc) packing (α -Fe structure type). The metal-metal bond distance observed is 2.6166(7) Å ($\times 8$). Taking into account the site population and the unit-cell parameters observed for the face-centered-cubic (fcc) polymorphs of pure Ni and Fe (Wyckoff 1963; Nishihara et al. 2012), and assuming the same V /atom ratio for fcc and bcc structure for Ni, Fe, and ideality, the following unit-cell value for the pure Al polymorph (Ni- and Fe-free steinhardtite) can be derived: $a = 3.218$ Å. Such a value is in excellent agreement with that predicted ($a = 3.230$ Å) by Lechermann et al. (2005) for the bcc allotropic form of Al under room conditions.

Potential new natural quasicrystals?

Decagonal quasicrystalline alloys have been described in the Al-Ni-Fe system (e.g., Lemmerz et al. 1994; Parshin et al. 2009). The decagonal phase is thermodynamically stable in a narrow compositional range around $\text{Al}_{71}\text{Ni}_{24}\text{Fe}_5$. At a temperature of about 940 °C it transforms to $\text{Al}_{13}(\text{Fe,Ni})_4$, $\text{Al}_3(\text{Ni,Fe})_2$, and the liquid phase, and between 800 and 850 °C to $\text{Al}_{13}(\text{Fe,Ni})_4$, $\text{Al}_3(\text{Ni,Fe})$, and $\text{Al}_3(\text{Ni,Fe})_2$. For comparison to the decagonal quasicrystal, based on 100 atoms the composition of steinhardtite is $\text{Al}_{38}\text{Ni}_{32}\text{Fe}_{30}$, quite far from the theoretical composition for a

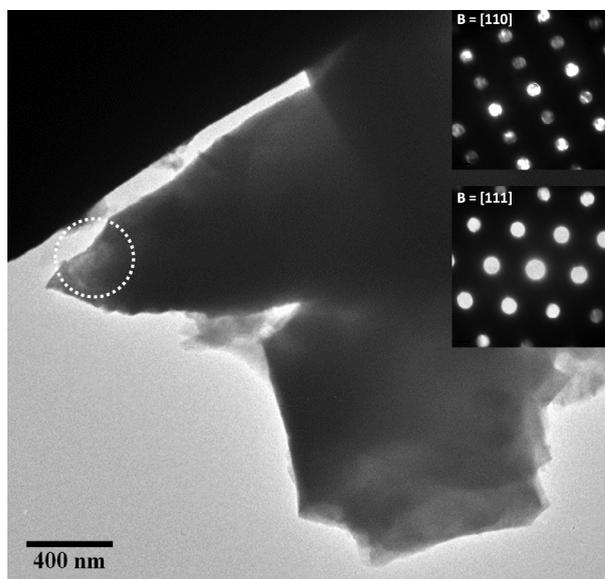


FIGURE 2. TEM image of steinhardtite. Electron diffraction patterns (zone axes are indicated) were obtained from a thin region of this granule (indicated with the white dotted circle).

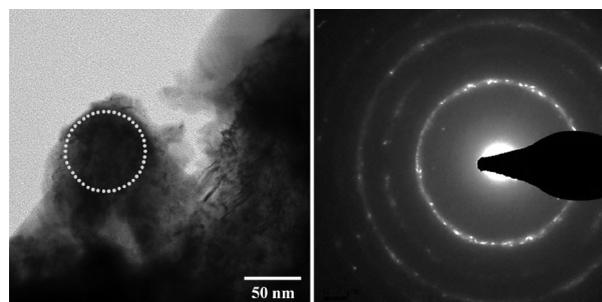


FIGURE 3. TEM image of another granule of steinhardtite. On the right are the diffraction rings, obtained from a thin region (indicated with the white dotted circle), which were indexed according to a body-centered-cubic structure, space group $Im\bar{3}m$, with $a = 3.02(1)$ Å (indexing as 110, 200, 211, 220, 310, 222, 321).

decagonal quasicrystal; but it should be kept in mind that a large variation of the Al/(Ni+Fe) ratio has been observed among the spinel phases of the Khatyrka fragments (see Hollister et al. 2014). This implies that the decagonal quasicrystal may yet be found in the Khatyrka meteorite.

Steinhardtite in the Al-Ni-Fe system

The composition of steinhardtite within the Al-Ni-Fe system (Chumak et al. 2008) suggests that it should exhibit the B2 structure (CsCl-type; space group $Pm\bar{3}m$) and not the A2 structure (space group $Im\bar{3}m$) as observed for the new mineral. The B2 structure is typically observed for stoichiometric composition, such as (Ni,Fe)Al. In this structure, Ni and Fe atoms share the structural positions at the cell corners (0,0,0) and Al atoms are at the centers ($\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$) (Rennhofer et al. 2003; Lechermann et al. 2005; Zhang and Du 2007). On the other hand, in the A2 structure there is a complete disorder of the three atoms (i.e., Al, Ni, and Fe) at the origin (and, consequently, at $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ given the I lattice) of the unit cell.

To the best of our knowledge, nothing is known about the effects of pressure on the Al-Ni-Fe system. Recent investigations on high-pressure torsion (HPT) processing of B2-ordered Fe-Al (Gammer et al. 2011) and Ni-Al (Klöden et al. 2008) alloys showed that when a pressure of 4–6 GPa is applied during the process an incipient cation disorder in the original B2 structure toward the formation of either nanosized domains with persistent B2 order (Gammer et al. 2011) or even of the A2 structure is observed (Sergiy Divinski, personal communication). The structural disorder of steinhardtite (pointing to the A2 structure) may have been induced by shock. At ambient pressure the B2 structure would be stable.

Origin

The incorporation of metallic Al in steinhardtite as well as in taenite has been tentatively explained by Hollister et al. (2014) with one of the two possible scenarios: (1) the Al-bearing FeNi phases might have been the initial source of the Al-bearing alloys khatyrkite, cupalite, and icosahedrite or (2) the Al-metals may have had a pre-accretion nebular origin and steinhardtite and Al-bearing taenite observed in the sample formed by reaction of shock-produced Al-melt and pre-existing taenite.

In the first hypothesis, the shock features observed locally for grains 125 and 126 of the Khatyrka meteorite (Hollister et al. 2014) would be generated by a strong increase of heat and pressure sufficient to extract Al from the FeNi metals and to initiate the local melting of metals and silicates. In the second hypothesis, the Al metals would form in some nebular process before the impact, with the impact resulting in the remelting, rapid cooling (about 10^2 – 10^3 °C s⁻¹) and solidification of the Al metals. In both scenarios, the sequence of events leading to the exchange of metallic Al that formed steinhardtite and Al-taenite can only be plausibly imagined to occur in space under low- f_{O_2} solar nebular conditions.

IMPLICATIONS

Our investigation of the different fragments of the thus far unique and remarkable Khatyrka carbonaceous chondrite (MacPherson et al. 2013) has revealed the heretofore unobserved metallic Al-bearing minerals (Hollister et al. 2014) for a carbonaceous chondrite: khatyrkite, cupalite, icosahedrite, and steinhardtite. These unique phases existed at the birth of our Solar System 4.5 billion years ago. The fact that metallic Al can be incorporated in nebular FeNi to form new mineral species like steinhardtite is a striking discovery.

It is currently accepted that the phase considered stable in the Earth's core is a body-centered-cubic structured alloy of Fe-Ni doped with lighter elements (e.g., Dubrovinsky et al. 2007; Luo et al. 2010). Moreover, first-principle theoretical (Friedli and Ashcroft 1975; Moriarty and McMahan 1982; Boettger and Trickey 1996; Pickard and Needs 2010) and experimental studies (Roy and Steward 1969; Akahama et al. 2006; Vailionis et al. 2011) have shown that pure Al converts from a face-centered-cubic to a hexagonal-close-packed structure at multimegabar pressures, and, at 0.38 TPa, a pressure slightly above that found at the center of the Earth, to a body-centered-cubic structure. Such a bcc polymorph of Al, successfully synthesized with ultrafast explosions, also has been found to be quenchable at room conditions (Vailionis et al. 2011).

These considerations, together with the presence of essential amounts of Ni and Fe in steinhardtite might reveal an additional light element, Al (beside C, O, Si, and S; Allègre et al. 2001; Côté et al. 2008) to contribute to the anomalously low density of the Earth's presumed Fe-Ni core.

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