STOICHIOMETRY, STRUCTURE AND TWINNING OF GODLEVSKITE AND SYNTHETIC LOW-TEMPERATURE Ni-EXCESS NICKEL SULFIDE

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ABSTRACT

New electron-microprobe data for godlevskite from Noril’sk indicate a 9:8 (metal:sulfur) stoichiometry, consistent with the recent determination of its structure in space group C2221, and a formula of (Ni8.7Fe0.3)S8. Powder-diffraction intensity data confirm that low-temperature Ni-excess nickel sulfide is the synthetic equivalent of godlevskite, and also has a formal composition of Ni8S8; α-Ni7S6 disproportionate on annealing at 297°C to Ni6S6 and Ni3S2. The twin law for godlevskite from Noril’sk is established as: composition plane (101), twin axis normal to (101). The structure of godlevskite and synthetic Ni8S8 is a hybrid of the structural elements of pentlandite, millerite, and α-Ni7S6; unlike millerite, α-Ni7S6 and heazlewoodite, the structure does not contain 3-fold clusters (Ni3) of short Ni–Ni distances.

Keywords: godlevskite, Ni-excess nickel sulfide, Ni8S8, twinning, crystal structure, Noril’sk.

INTRODUCTION

Study of the stoichiometry, symmetry and phase relations of the Ni-excess nickel sulfide phases has been complicated by the small compositional differences between proposed phases, lack of single-crystal products, and some confusion in reporting. In their detailed review of the binary system Ni–S, Kullerud & Yund (1962) noted that the many phases which had been reported in the composition interval 30 to 33 wt.% S included: Ni6S6 (Schenck & Forst 1939, Lundqvist 1947, Rosenqvist 1954, Sokolova 1956), Ni5S6 (Peyronel & Pacilli 1942, Lundqvist 1947, Rosenqvist 1954), and Ni6S8 (Sokolova 1956). The experiments of Kullerud & Yund (1962) suggested the existence of two stable phases with 7:6 (metal:sulfur) stoichiometry (α-Ni7S6 and β-Ni7S6) and disproved the proposed phases with 6:5 and 9:8 stoichiometry. Kullerud & Yund reported that the low-temperature phase β-Ni7S6 transforms to α-Ni7S6 at 379°C in the presence of excess Ni3S2, and at 400°C with excess α-NiS. Because the present paper argues that the low-temperature phase does not have ideal 7:6 stoichiometry, this phase will be referred to as "β-Ni7S6", low-temperature Ni-excess nickel sulfide, or Ni6S8. The alpha designation for the high-temperature phase will be retained to avoid further confusion.

Lundqvist (1947) reported that the high-temperature phase has orthorhombic symmetry (a 11.22, b 16.56, c 3.27 Å). Fleet (1972) confirmed the orthorhombic symmetry [a 3.274(1), b 16.157(7), c 11.359(4) Å, Bmmb] and determined the crystal structure. Surprisingly, the structure of α-Ni7S6 has an ideal 6:5 stoichiometry, the 7:6 stoichiometry being accommodated by partial occupancy of the Ni positions. Three of the Ni positions are disordered, but a tendency for ordering was indicated by weak reflections of a superstructure. This was confirmed by the existence of various superstructures: 2a, 2b, 2c; 2a, 2b, 3c; and 2a, 2b, 4c (Putnis 1976), and 2a, 2b, 2c (Parise & Moore 1981).

Neither Lundqvist (1947) nor Kullerud & Yund (1962) were able to index the powder pattern of the low-temperature Ni-excess nickel sulfide phase. Lundqvist (1947) noted that the possibility of a degenerate pentlandite structure (with ideal Ni5S6 stoichiometry) could not be excluded. Further progress was made with the discovery of godlevskite in the Noril’sk and Talnakh Cu–Ni sulfide deposits in northern Siberia by Kulagov et al. (1969). These authors showed that godlevskite is a Ni-excess nickel sulfide with an orthorhombic space group (C2221, Cmm2, Amm2, or Cmmm) and an X-ray powder pattern similar to that reported by Kullerud & Yund (1962) for low-temperature Ni-excess nickel sulfide.
The low Fe content of godlevskite (Table 1) is consistent with the limited solid solution of Fe in the synthetic phase (Misra & Fleet 1973). Almost immediately after the Kulagov et al. study, Naldrett et al. (1972) reported godlevskite from the Texmont mine, Ontario. Their systematic study reaffirmed the conclusion of Kulagov et al. (1969) concerning the equivalence of godlevskite and low-temperature Ni-excess nickel sulfide. Following the experimental work of Kullerud & Yund (1962), both of these groups of investigators assumed the ideal stoichiometry of godlevskite to be 7:6, even though the mean composition derived from the electron-microprobe data of Kulagov et al. indicated a stoichiometry closer to 1:1. Very recently, and after some 17 years of intermittent study of low-temperature Ni-excess nickel sulfide and godlevskite, Fleet (1987) determined the crystal structure of godlevskite and established the ideal stoichiometry as Ni$_5$S$_4$. There has been renewed interest in the thermodynamic properties and phase relations of the system Ni–S in recent years (e.g., Lin et al. 1978, Sharma & Chang 1980, Cemic & Kleppa 1986), but these investigations have no bearing on the present study.

In the present paper, new compositional data for godlevskite and low-temperature Ni-excess nickel sulfide indicate that the true composition of both phases is Ni$_5$S$_4$. New X-ray powder data for the synthetic phase establish its true equivalence to godlevskite, and various crystal-chemical and crystallographic aspects are discussed.

**Godlevskite**

**Petrographic aspects, twinning, powder pattern and chemical composition**

In the Noril’sk and Talnakh deposits, godlevskite occurs in bornite mineralization accompanying veins and massive accumulations of chalcopyrite (Kulagov et al. 1969). The host rocks are andesites and basalts, gabbro-dolerites and sandstones. Associated nickel sulfide minerals include millerite and pentlandite. In polished section, the godlevskite from Noril’sk and Talnakh is characterized by aggregates of twinned grains that form “elbow”-bend outlines.

In the Texmont mine, godlevskite occurs in close association with pentlandite, heazlewoodite and millerite, these forming irregular blebs of sulfide in serpentinized peridotite (Naldrett et al. 1972). Twinning (polysynthetic) has been observed but it is not a common feature.

The present observations were made on two samples from Noril’sk, obtained from A.E. Kulagov along with brief descriptions. In the first sample, which was the most extensively studied, godlevskite occurs with bornite, millerite, pentlandite and “nickel leaf pentlandite” (pers. comm., 1972). In the second sample, a small amount of godlevskite occurs with bornite. The study of this sample was limited to a few grain fragments removed for X-ray precession study. In the first sample, a small rock chip with a maximum diameter of 2 cm, godlevskite accounts for about 10 vol.% of all sulfides. It occurs in a matrix of chalcopyrite, as large twinned grains up to 0.4 mm in diameter (Fig. 1a), and as fine disseminations. Godlevskite is readily distinguished by its characteristic twinning, reflection pleochroism, and anisotropic colors. The reflection pleochroism is the same as described by Naldrett et al. (1972), pale cream to pinkish cream. Bornite is intimately intergrown with the aggregates of larger grains and forms a discontinuous rim against the chalcopyrite matrix (Fig. 1a). Individual laths of godlevskite are incipiently to completely replaced by millerite, as described by Kulagov et al. (1969).

As observed in polished section, twinned aggregates of godlevskite consist of either two lath-like individuals joined by a single composition plane forming an “elbow”, as described by Kulagov et al. (1969), or as several individuals arranged in a cross or butterfly outline. All grains examined by X-ray precession are twinned on a coarse scale consistent with the texture observed in polished section. The twin operation places c* near coincidence with a (004 of the twinned crystal coincides with 400 of the untwinned crystal, etc.; cf. Table 2). Where both twin individuals are present in equal proportions, single-crystal diffraction patterns have a pseudotetragonal appearance (cf. Table 3). However, twinning is readily detected by the presence of extra reflections at extinction positions for the C-centered lattice. Because of the near-equality of a and c (and a* and c*) and the C2221 space group, it was not possible to distinguish between the twin laws possible, using the precession photographs alone. Several twinned grains were removed from a polished section, and their orientation determined by X-ray
precession. Careful study showed that the lath-like individuals (Fig. 1a) are elongate parallel to the a axis, and the twin composition plane is (101). Therefore, the twin axis is normal to (101). This twin law for godlevskite is different from that relevant to poly-synthetic twinning in low-temperature Ni-excess nickel sulfide when transformed from α-Ni$_7$S$_6$, for which the twin axis is normal to (011) (Putnis 1976).

The X-ray powder-diffraction data of Kulagov et al. (1969, Table 4) have been reindexed using powder-pattern data calculated with POWDR2 (D. K. Smith, Pennsylvania State University) and the crystal-structure data of Fleet (1987): powder lines were indexed on the basis of both position and intensity. The refined unit-cell parameters (Table 3) are in good agreement with the single-crystal data of Fleet (1987).

An electron-microprobe analysis of godlevskite from Noril’sk was carried out with the JEOL JXA-8600 Superprobe at the University of Western Ontario, using synthetic NiS and FeS and metallic Cu-Ni$_7$S$_6$ synthesized at Noril’sk. This synthetic twinning in low-temperature Ni-excess nickel sulfide when transformed from Cu-Ni$_7$S$_6$, for which the twin axis is normal to (011) (Putnis 1976).

The refined unit-cell parameters (Table 3) are in good agreement with the single-crystal data of Fleet (1987).

Table 1. Powder diffraction data for low-temperature Ni$_7$S$_6$ compositions for godlevskite from Noril’sk

<table>
<thead>
<tr>
<th>d(A)</th>
<th>hkl</th>
<th>peak d(A)</th>
<th>hkl</th>
</tr>
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<tr>
<td></td>
<td></td>
<td></td>
<td></td>
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<tr>
<td>3.864</td>
<td>16</td>
<td>4.047</td>
<td>16</td>
</tr>
<tr>
<td>4.177</td>
<td>17</td>
<td>4.408</td>
<td>18</td>
</tr>
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<td>4.684</td>
<td>1</td>
<td>4.906</td>
<td>1</td>
</tr>
<tr>
<td>5.159</td>
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<td>5.548</td>
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<tr>
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<td>10</td>
<td>6.408</td>
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<td>7.084</td>
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<td>7.147</td>
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<tr>
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<td>1</td>
<td>7.408</td>
<td>1</td>
</tr>
<tr>
<td>8.084</td>
<td>1</td>
<td>8.408</td>
<td>1</td>
</tr>
</tbody>
</table>

Recognizing now that both the crystal structure and the reanalysis of godlevskite from northern Siberia indicate a 9:8 stoichiometry (and not 7:6), it is appropriate to reinterpret the analytical data of Naldrett et al. (1972, Table 2). The reported value of the metal/sulfur ratio for godlevskite from Texmont is intermediate between those for 9:8 and 7:6 stoichiometries. Furthermore, the compositions for the other binary nickel sulfide phases from Texmont (heazlewoodite and millerite) are slightly metal-rich compared to their ideal stoichiometries (3:1.97 versus 3:2 and 1:0.99 versus 1:1, respectively). Applying the discrepancy for the reported heazlewoodite composition as a linear calibration correction to the godlevskite data gives an apparent minimum metal/sulfur ratio for godlevskite from Texmont of 1.127, which is close to the ideal value for 9:8 stoichiometry (Table 1). Thus there is reason to suspect that the analytical data of Naldrett et al. (1972) for godlevskite from Texmont may not indicate a significant departure from the ideal 9:8 stoichiometry.

It is fully appreciated that the accuracy of electron-microprobe analyses is predicated on meaningful calibration. The standard NiS and FeS of the present study were prepared under exacting laboratory co-
Table 3. UNIT-CELL PARAMETERS (Å) FOR GODLEVSKITE FROM NORIL'SK AND SYNTHETIC Ni₅S₆.

<table>
<thead>
<tr>
<th></th>
<th>a</th>
<th>b</th>
<th>c</th>
</tr>
</thead>
<tbody>
<tr>
<td>godlevskite</td>
<td>9.3359(7)</td>
<td>11.2185(10)</td>
<td>9.4300(6)</td>
</tr>
<tr>
<td></td>
<td>9.328(6)</td>
<td>11.209(7)</td>
<td>9.429(6)</td>
</tr>
<tr>
<td></td>
<td>9.18</td>
<td>11.29</td>
<td>9.47</td>
</tr>
<tr>
<td>Ni₅S₆</td>
<td>9.306(6)</td>
<td>11.222(7)</td>
<td>9.415(6)</td>
</tr>
<tr>
<td></td>
<td>9.327(3)</td>
<td>11.230(4)</td>
<td>9.366(3)</td>
</tr>
</tbody>
</table>

single crystal¹
powder²
powder²

¹ Fleet (1987), ² Table 1, ³ indexed by Kulagov et al. (1969).
⁴ twinned single crystal.

Crystal structure

The crystal structure of godlevskite [(Ni₈.7 Fe₀.3) S₈, C222, Z = 4, Dₓ = 5.273 g cm⁻³] is based on a distorted cubic close-packed array of 32 S atoms per unit cell, with 20 Ni atoms in tetrahedral coordination and 16 in square-pyramidal coordination (Fig. 2). There are six independent tetrahedral Ni positions [Ni(1), Ni(2), Ni(3), Ni(4), Ni(5), Ni(6)], two independent square-pyramidal Ni positions

Fig. 2. Crystal structure of godlevskite: Ni open circles, S small filled circles.
[Ni(7), Ni(8)] and four independent S positions. Completion of the crystal structure analysis (Fleet 1987) was frustrated for some time by the high pseudosymmetry, structural complexity, and compositional ambiguity. The combination of pseudosymmetry and structural complexity even limits the possibilities for diagrammatic representation. However, the ideal crystal structure does afford a useful model for developing the structural details. It is based on a cubic close-packed array of sulfur atoms, 32 per unit cell, as in pentlandite [(Fe,Ni)₉S₈], with Ni atoms in 20 of the 64 possible tetrahedral positions and 16 of the 32 possible octahedral positions. Distortion of this ideal structure (principally, stretching parallel to [010], Fig. 3, and contraction normal to [010]) modifies the NiS₆ octahedra to NiS₄ square pyramids. The NiS₄ tetrahedra are associated into three-membered chains via shared coordination edges (Fig. 4), yielding short Ni-Ni distances. Chains of Ni(1)S₄-Ni(2)S₄, Ni(3)S₄-Ni(4)S₄, and Ni(5)S₄-Ni(6)S₄ tetrahedra are parallel to, respectively, [100], [001] and [010] (Fig. 4); the last two chains form a five-membered cross centered on Ni (6). Square-pyramids of Ni (7) S₄ and Ni (8) S₄ form both 4-fold clusters and [101] chains (Figs. 2,

Fig. 3. Crystal structure of godlevskite in [010] projection, showing distortion by stretching parallel to [010] and development of square-pyramidal coordination from octahedral coordination of ideal structure. Ni in square pyramidal coordination, large circles; Ni in tetrahedral coordination, medium circles; S small circles; remote “sixth” S atoms, which complete NiS₆ octahedra, are located by stippled lines from selected Ni (7) and Ni (8) atoms.

Fig. 4. Chains and crosses of NiS₄ tetrahedra, 4-fold clusters of NiS₅ square pyramids, and short Ni-Ni distances in structure of godlevskite, cf. Figure 2. Ni open circles; S small filled circles; heavy lines, Ni-Ni < 2.60 Å; broken heavy lines, Ni-Ni = 2.60-2.75 Å.
4) by sharing pyramidal and basal edges, but most of the resulting Ni–Ni interactions are longer than 2.9 Å. The shortest Ni–Ni distances project through the bases of the square pyramids (Fig. 4). These arise because the NiS_{6} octahedra, formed by adding the sixth, more remote S atom to the NiS_{4} square pyramids, share faces with NiS_{4} tetrahedra.

**LOW-TEMPERATURE Ni-excess Nickel Sulfide (Ni_{9}S_{8})**

Low-temperature Ni-excess nickel sulfide was synthesized in 1969 and 1970, when it was assumed to have ideal 7:6 stoichiometry. The starting material was the product α-Ni_{9}S_{8} used in the study of Fleet (1972). This had been prepared by reacting Ni sponge (reduced with hydrogen at 900°C) and S crystals in an evacuated sealed silica-glass tube at 504°C for 9 days. The crushed product α-Ni_{9}S_{8} was annealed in a sealed silica-glass tube at 297°C for 49 days.

Examination, at the time of synthesis, by polished section and X-ray powder and single-crystal diffraction procedures, suggested that the annealed product was the homogeneous β-Ni_{9}S_{8} phase of Kullerud & Yund (1962). The powder pattern (Table 2) was equivalent to that of Kullerud & Yund (1962, Table 18) but remained unindexed. Grain fragments were twinned and gave pseudo-tetragonal unit-cell parameters (Table 3). An attempt at structure analysis was unsuccessful. Several subsequent attempts at structure analysis with fragments of twinned grains from Noril’sk also were unsuccessful. However, the intensity and unit-cell data obtained from the natural material permitted the original powder pattern of the Ni_{9}S_{8} bulk composition to be indexed. A TEM analysis confirmed that the diffraction pattern of low-temperature Ni-excess nickel sulfide was consistent with space groups C222, Cmcm2, Cmmn, and possibly C222_1, and that no other diffraction effects (consistent with domain structure, etc.) are present. The structural information gleaned at this time (1983) indicated a pentlandite-like (9:8) stoichiometry for both godlevskite and synthetic low-temperature Ni-excess nickel sulfide. On further examination, this was supported by the presence of excess heazlewoodite (Ni_{9}S_{8}) in the annealed Ni_{9}S_{8} bulk composition, as indicated by heazlewoodite lines in the indexed powder pattern (Table 2), heazlewoodite reflections on precession films, and heazlewoodite exsolution in the tarnished polished section.

The original powder pattern was obtained with a Jagodzinski focusing powder camera and was calibrated with α-quartz (Fleet 1968) (Table 2). The intensity data were obtained recently by planimetry from a single Joyce-Loebl densitometer scan magnified by an electrostatic copier. These data, when corrected for interference by heazlewoodite lines, are in remarkably good agreement with intensities calculated by POWDR2 using the structural data for godlevskite (Fleet 1987) (Table 2). Refined unit-cell parameters for the indexed powder pattern are in better agreement with the unit-cell parameters for godlevskite than the data for the twinned single crystal (Table 2). Small remaining discrepancies with the single-crystal data for godlevskite may be attributable to the small extent of Fe substitution in the natural material (Table 1), which would be expected to result in a decrease in unit-cell volume. The heazlewoodite 110 line accounts for 26% of the intensity of the 2.875 Å line of the powder pattern for the bulk Ni_{9}S_{8} composition. The proportion of heazlewoodite present, estimated semi-quantitatively from the sums of the calculated intensities for godlevskite and of the normalized intensities for heazlewoodite, gave 13.2% (by diffraction volume).

In polished surfaces exposed to air, heazlewoodite develops a much stronger tarnish than low-temperature Ni-excess nickel sulfide (Fig. 1b). The apparent proportion of heazlewoodite in the annealed Ni_{9}S_{8} bulk composition, as observed in tarnished polished section, varies up to a maximum of about 25%. This appears to indicate that the exsolved heazlewoodite is present as flame- or ribbon-like lamellae. The weak heazlewoodite reflections in precession films were randomly oriented. The heazlewoodite lamellae are, therefore, incoherent with the matrix of low-temperature Ni-excess nickel sulfide.

**DISCUSSION**

**Structure and composition of low-temperature Ni-excess nickel sulfide**

The good agreement between the observed intensities of powder diffraction lines for low-temperature Ni-excess nickel sulfide and the calculated intensities for godlevskite (Table 2) is final confirmation of the equivalence of the synthetic and natural phases (Kulagov et al. 1969, Naldrett et al. 1972). Low-temperature Ni-excess nickel sulfide clearly has the crystal structure of godlevskite (Fleet 1987) with ideal 9:8 stoichiometry. Its formal composition is Ni_{9}S_{8}.

The present analytical data and the structure analysis of Fleet (1987) both indicate that the composition of godlevskite is very close (virtually identical) to the ideal 9:8 stoichiometry. On the other hand, both synthetic and natural pentlandite, (Fe,Ni)_{9}S_{8}, exhibit deviation from ideal 9:8 stoichiometry and are commonly slightly metal-rich (Knop et al. 1965, Harris & Nickel 1972, Misra & Fleet 1973). Theoretically, synthetic Ni_{9}S_{8} could have a composition of either Ni_{9.x}S_{8} or Ni_{9.S1-x}. However, the present experimental data suggest that, like godlevskite, equilibrated synthetic Ni_{9}S_{8} has a composition close to the ideal 9:8 stoichiometry. On annealing at
297°C, $\alpha$-Ni$_5$S$_6$ disproportionates to (Ni$_5$S$_8$ + Ni$_3$S$_2$) according to the reaction: 3$\alpha$-Ni$_5$S$_6$ = 2Ni$_5$S$_8$ + Ni$_3$S$_2$. The proportion of heazlewoodite estimated from the powder-diffraction pattern (13.2%) is in very good agreement with the proportion of exsolved heazlewoodite in the annealed Ni$_5$S$_6$ composition calculated according to this reaction (13.3 wt.%). This agreement is further supported by the proportion of heazlewoodite observed in tarnished polished section.

The present conclusion on the range in composition of synthetic Ni$_5$S$_8$ is at variance with the experimental work of Kullerud & Yund (1962). However, the heazlewoodite 101 (4.081 Å) and 202 (2.0404 Å) lines are visible in the powder-diffraction pattern of the low-temperature Ni$_5$S$_6$ composition published by Kullerud & Yund (1962, Fig. 6), although the apparent proportion of heazlewoodite is less than that observed in the present study.

The low-temperature phase relations of the system Ni-S as depicted in Figure 2 of Kullerud & Yund (1962) have been revised to include the proposed Ni$_5$S$_6$ stoichiometry of low-temperature Ni-excess nickel sulfide (Fig. 5). Phase relations for the proposed Ni$_5$S$_6$ phase of Lin et al. (1978) and Sharma & Chang (1980), which would replace the Ni$_3$S$_2$ composition field, have not been included. The present study has not investigated the possibility of a stable solid-solution field for compositions more Ni-rich than Ni$_5$S$_8$ above 300°C, the existence of which would explain partly the discrepancies with Kullerud & Yund (1962).

Twinning and crystal structure

The present study has shown that the characteristic elbow-like twins of godlevskite from Noril'sk and Talnakh have a (101) composition plane and twin law with twin axis normal to (011). This twin law seems to follow directly from the pseudo-tetragonal symmetry of the unit-cell (Table 3) and the high pseudo-symmetry of the crystal structure (Fig. 2). A (101) composition plane that includes the Ni(4), Ni(5), Ni(7) and Ni(8) positions (Fig. 2), for example, would yield a twin structure that preserves the integrity of the square-pyramidal and tetrahedral coordination polyhedra. The twin law with twin axis normal to (011), for polysynthetic twinning in synthetic Ni$_5$S$_6$ transformed from $\alpha$-Ni$_5$S$_6$ (Putnis 1976), must result in a more complicated twin structure (Fig. 3).

Comparison with other sulfide structures

The crystal structure of godlevskite is very much a hybrid of the structural elements of several related phases (pentlandite, millerite and $\alpha$-Ni$_5$S$_6$). Although there are similarities in the unit cells, pow-
der patterns, and arrays of S atoms of godlevskite and pentlandite, godlevskite does not have a pentlandite-derivative crystal structure. In the crystal structure of pentlandite (e.g., Hall & Stewart 1973), 32 metal (M) atoms per unit cell are in tetrahedral coordination with sulfur, and only 4 are in octahedral coordination. Short $M$-$M$ distances arise through shared tetrahedral edges, the $MS_4$ tetrahedra being associated into “cubic” clusters. In millerite (Grice & Ferguson 1974, Rajamani & Prewitt 1974), Ni is 5-fold coordinated within an approximately square-pyramidal polyhedron of S atoms (the apical S is offset from the pyramid axis). The NiS$_5$ square pyramids are associated into 3-fold clusters through the sharing of basal edges, which results in two short Ni-Ni bonds per Ni atom (e.g., Fig. 2 of Fleet 1972). In the crystal structure of $\alpha$-Ni$_5$S$_6$ (Fleet 1972), four of the Ni positions are in square-pyramidal coordination with S, and one is in tetrahedral coordination. Short Ni-Ni distances arise through shared coordination edges; the 3-fold clusters of the Ni(2)S$_5$ and Ni(5)S$_5$ square pyramids (Fig. 1 of Fleet 1972) are equivalent to the 3-fold clusters of NiS$_5$ polyhedra in the crystal structure of heazlewoodite (Ni$_5$S$_6$, Fleet 1917, Parise 1980), each Ni atom is coordinated to four S atoms, forming a NiS$_4$ tetrahedron, and to four other Ni atoms, through the sharing of edges of NiS$_5$ tetrahedra.

In summary, the structure of godlevskite has fewer tetrahedrally coordinated Ni atoms than pentlandite, and fewer Ni atoms in square-pyramidal coordination than either millerite or $\alpha$-Ni$_5$S$_6$. Short Ni-Ni distances arise both from shared NiS$_5$ coordination edges, as in pentlandite, and through the bases of NiS$_5$ square pyramids, as in millerite and $\alpha$-Ni$_5$S$_6$. Three-fold clusters of short (and presumably bonded) Ni-Ni distances (Ni$_3$ clusters), proposed as a stabilizing unit in metal-bonded nickel sulfides (Parise & Moore 1981) and present in millerite, $\alpha$-Ni$_5$S$_6$ and heazlewoodite, are not present in godlevskite.

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