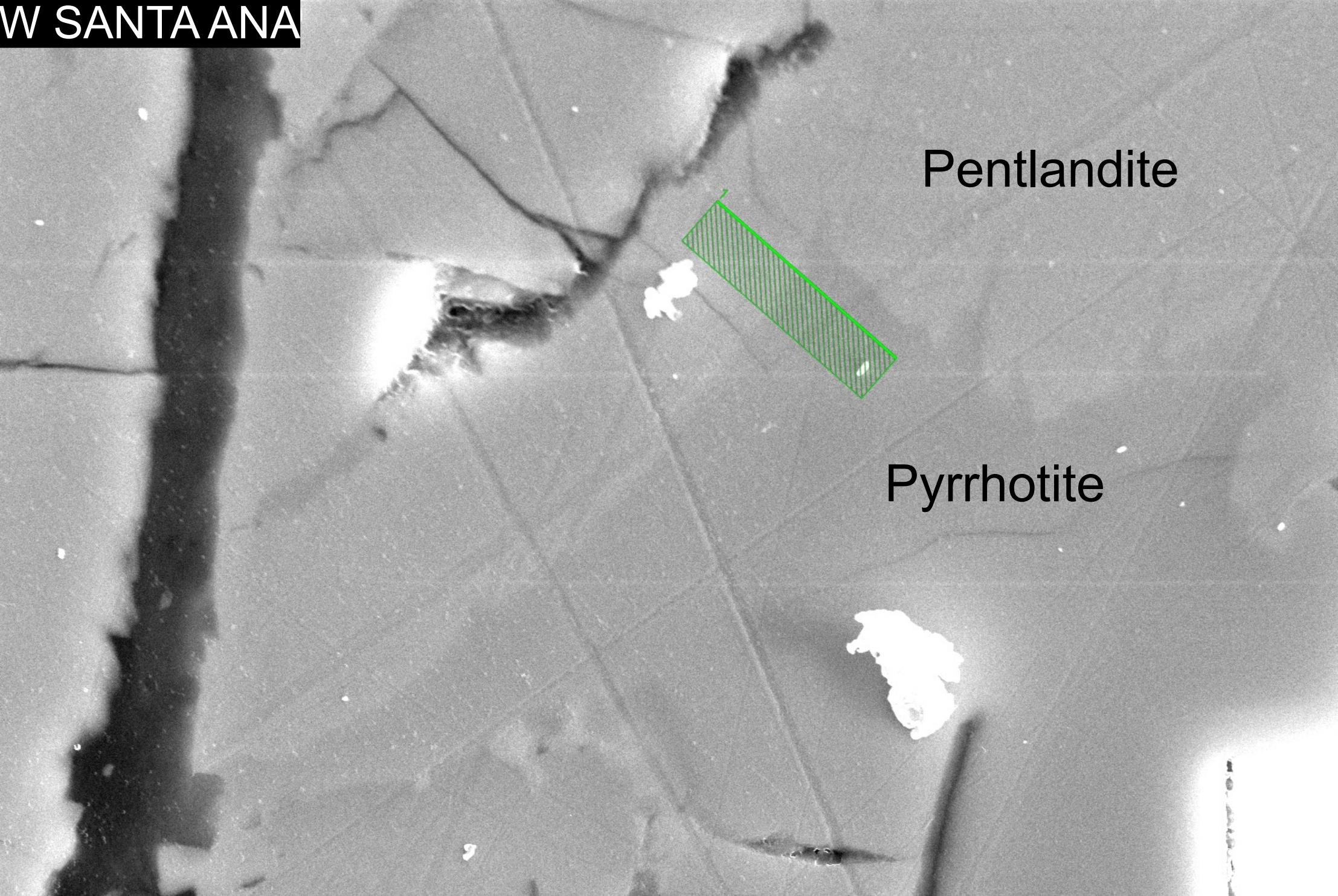


**Sulfide mineralogy of igneous basic rocks (ophites) from the External Zone of the Betic Cordillera**

José M. González-Jiménez, Idael F. Blanco-Quintero, Lola Yesares, Claudio Marchesi, Amira R. Ferreira,  
Igor González-Pérez, Erwin Schettino, Fernando Gervilla

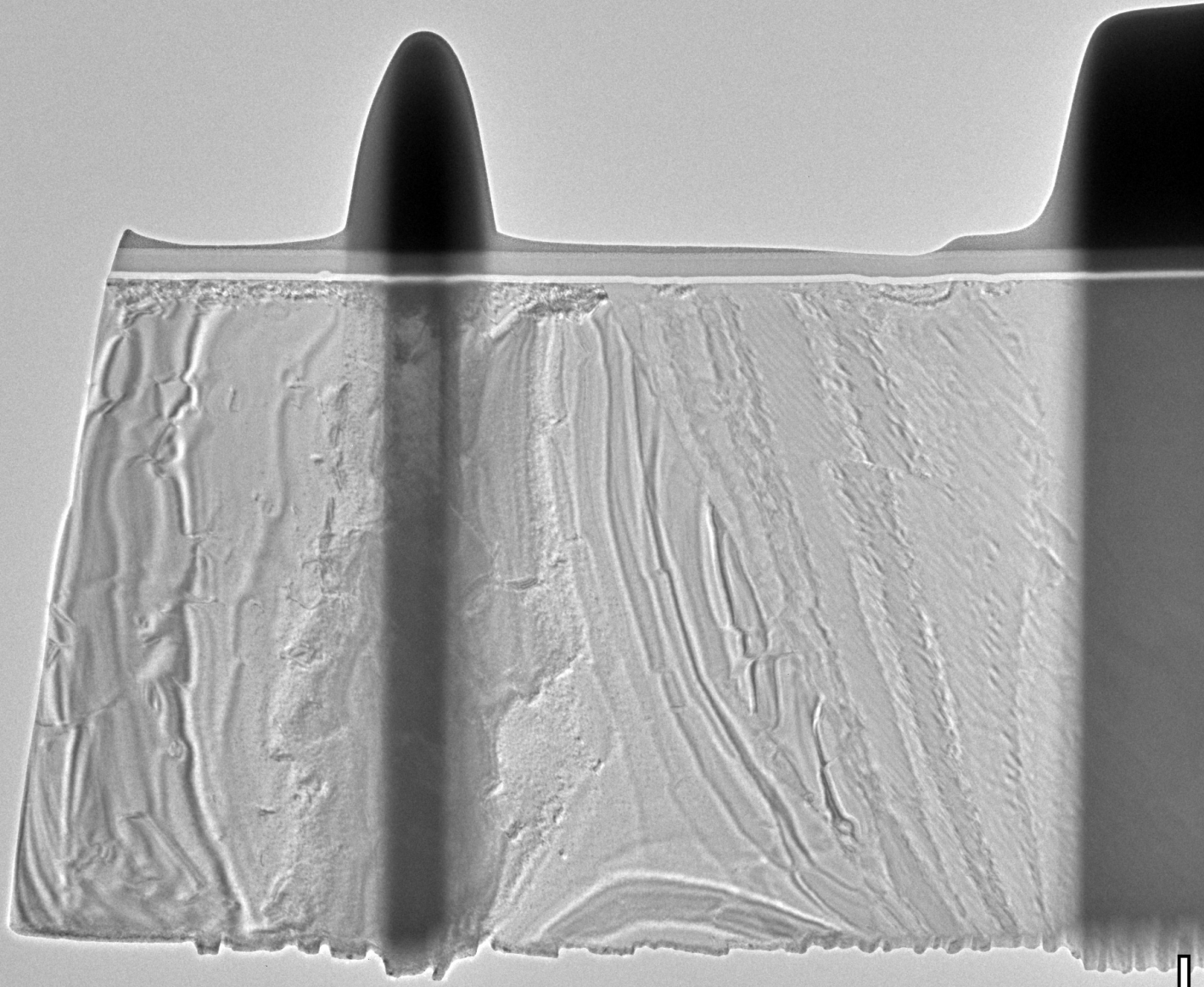
**Supplementary Information File S5**  
**Nanostructural analysis of magmatic sulfides**



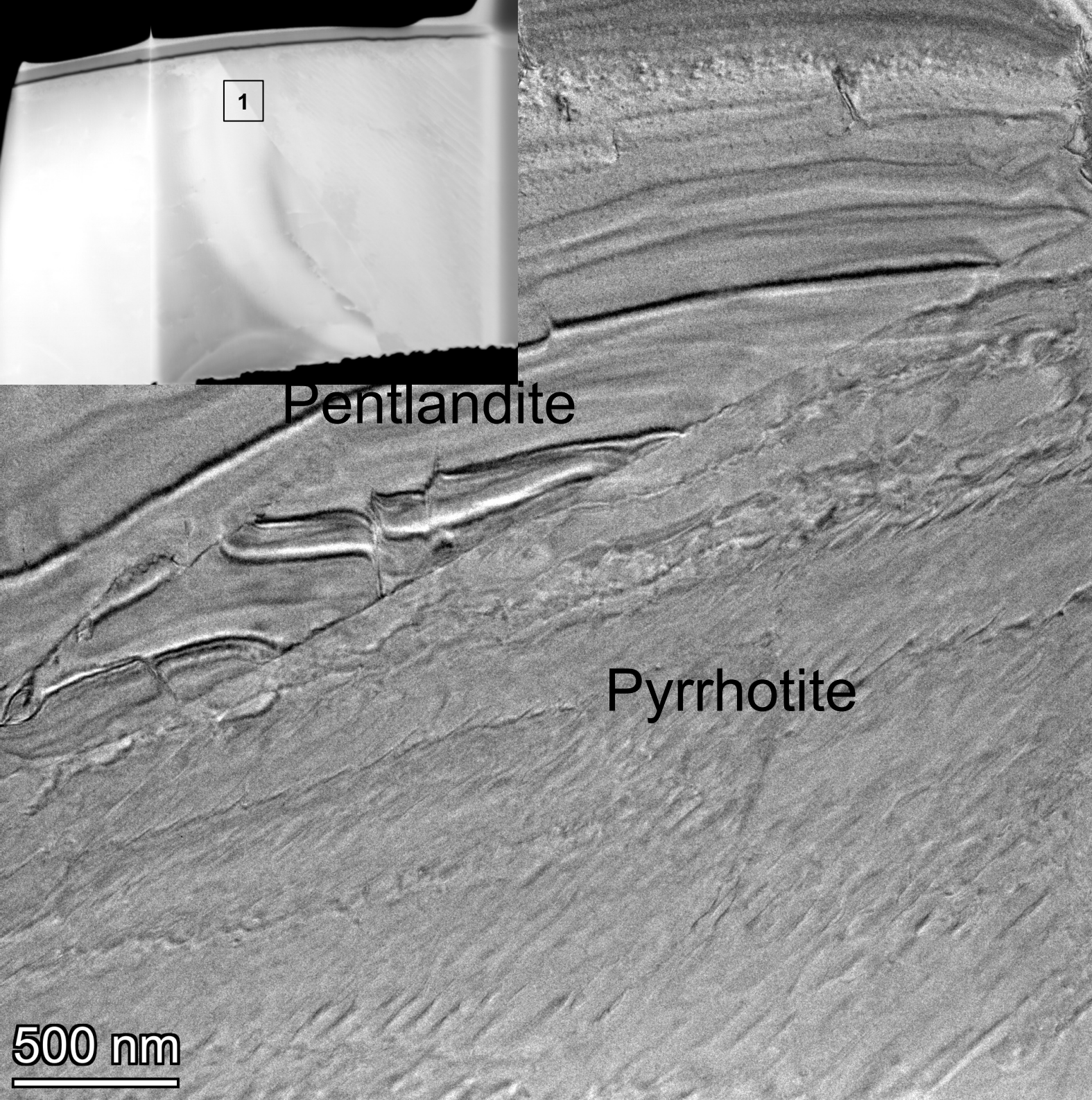
Pentlandite

Pyrrhotite





2  $\mu\text{m}$



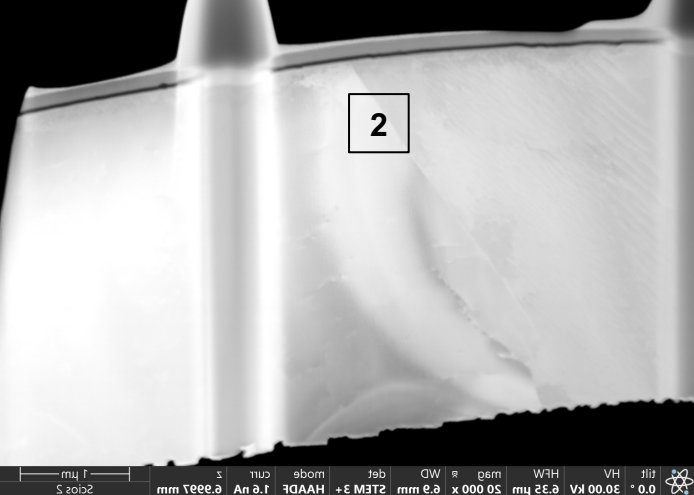
1

Pentlandite

Pyrrhotite

500 nm





Pentlandite

Pyrrhotite

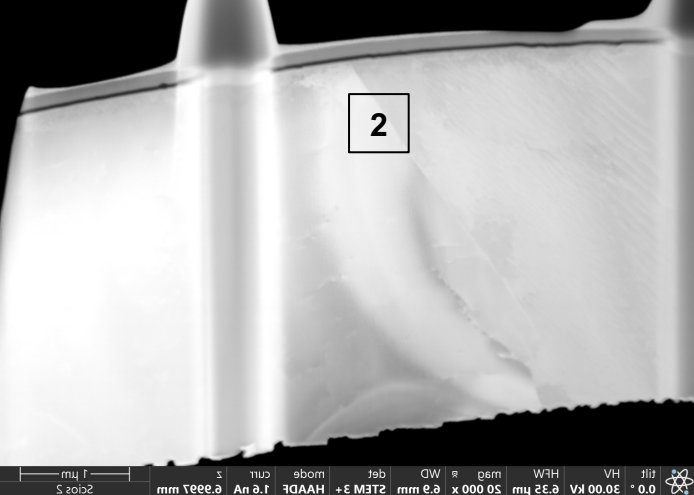
20 nm

5 nm<sup>-1</sup>

Pentlandite (FeNi)<sub>9</sub>S<sub>8</sub> (cubic; Fm3m)

Spot#	d-Spacing (nm)	(hkl)	Ideal d-Spacing (Å)
1	0.298055	(222)	2.9269-2.9458
2	0.304621	(311)	3.0570-3.0768
3	0.305403	(311)	3.0570-3.0768
4	0.291302	(222)	2.9269-2.9458
5	0.355458	(220)	3.5847-3.6078
6	0.357288	(220)	3.5847-3.6078
7	0.208034	(422)	2.0696-2.0830
8	0.208580.	(422)	2.0696-2.0830
9	0.177867	(440)	1.7923-1.8039





Pentlandite

Pyrrhotite

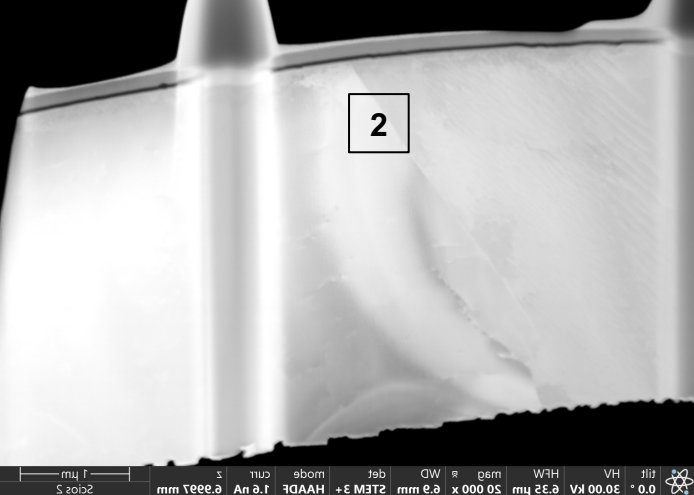
20 nm

5 nm<sup>-1</sup>

Pyrrhotite (Fe<sub>7</sub>S<sub>8</sub>) (monoclinic; C2/C; polytype 4C)  
Pentlandite (FeNi)<sub>9</sub>S<sub>8</sub> (cubic; Fm3m)

Spot#	d-Spacing (nm)	(hkl)	Ref. d-Spacing (Å)
1	0.514939	(200) <sub>Pn</sub>	5.1023
2	0.484741	(200) <sub>Pn</sub>	5.1023
3	0.472792	(-112) <sub>Po</sub>	4.7026
4	0.212368	(204) <sub>Po</sub>	2.1246
5	0.209554	(204) <sub>Po</sub>	2.1246
6	0.234879	(312) <sub>Po</sub>	2.3457
7	0.147931	(-627) <sub>Po</sub>	1.4790
8	0.147887	(-627) <sub>Po</sub>	1.4790

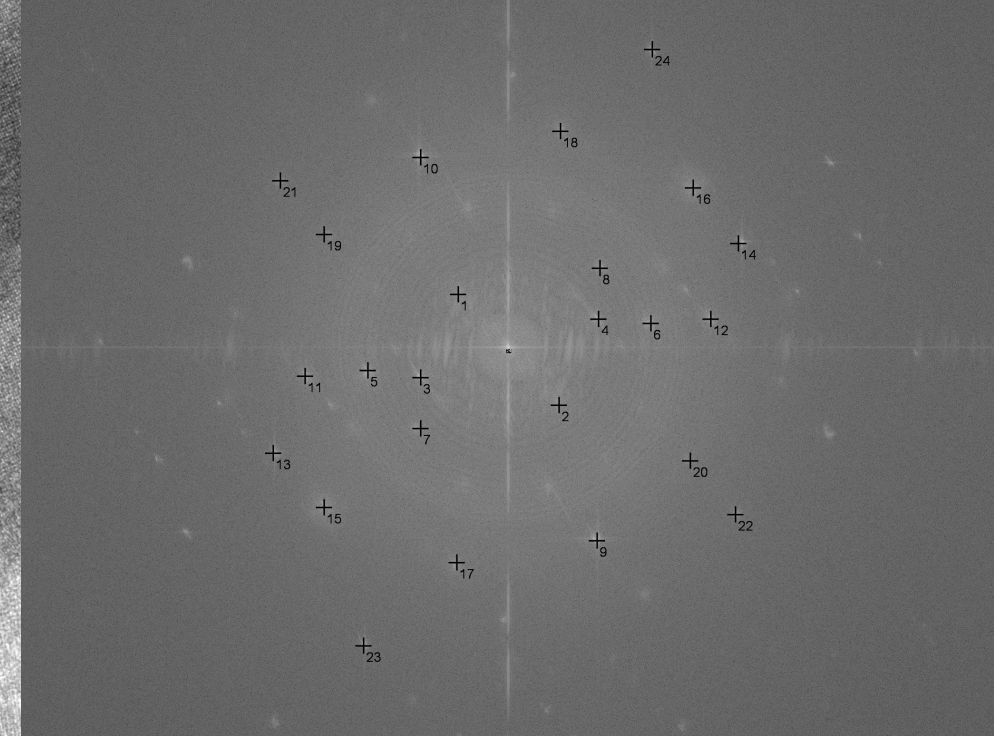




Pentlandite

Pyrrhotite

20 nm



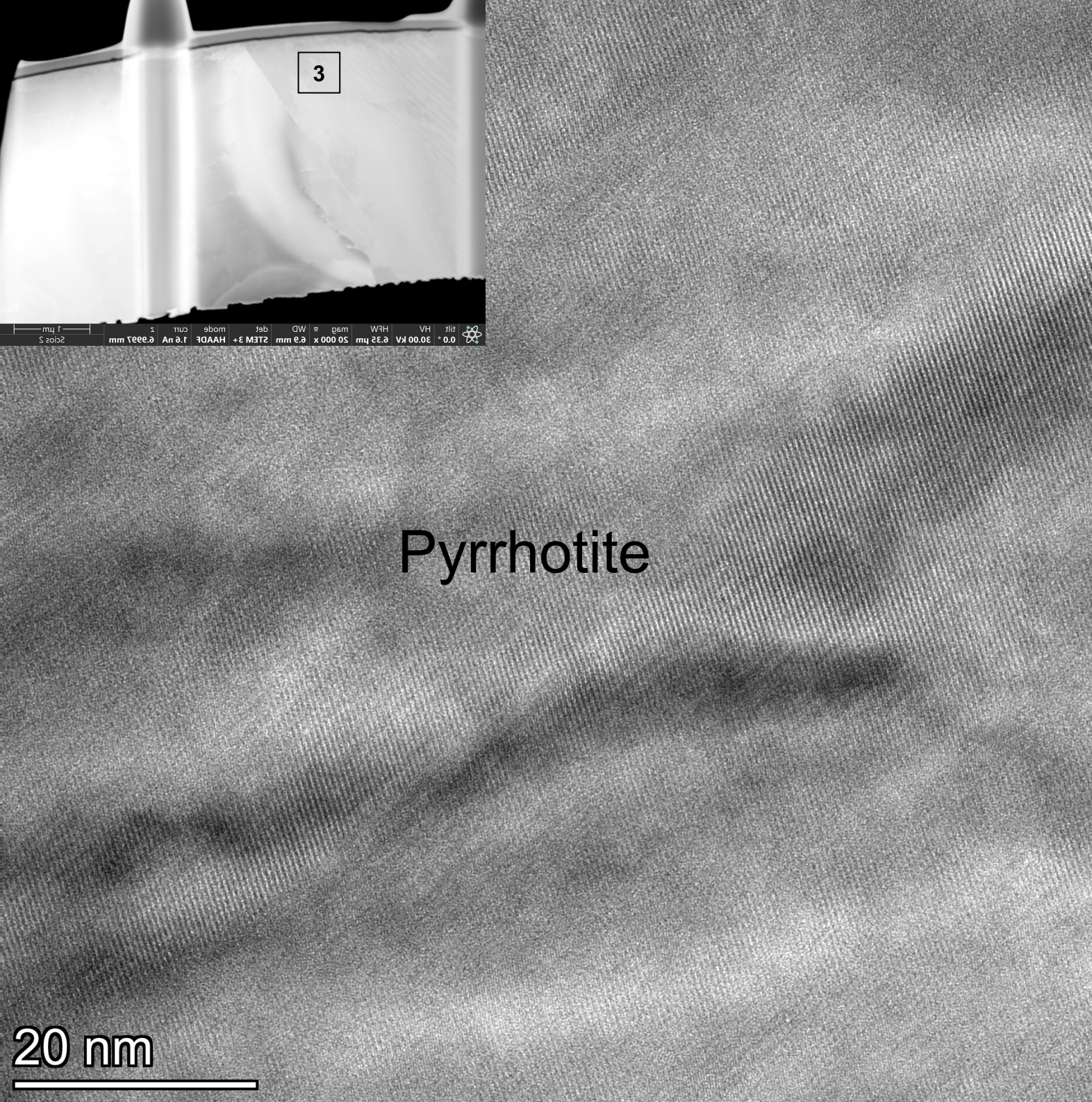
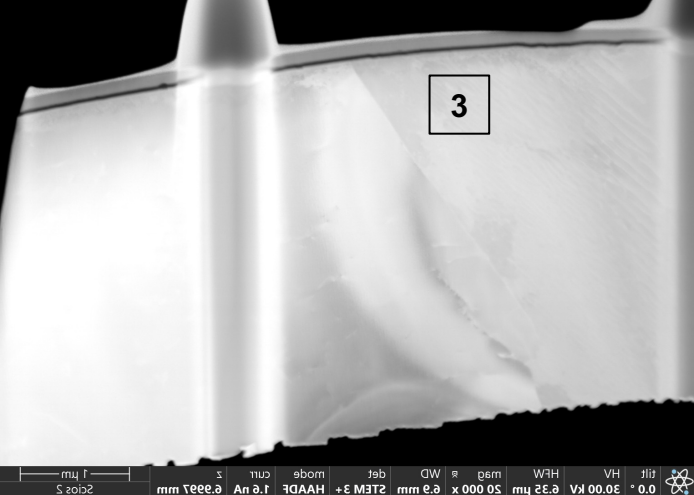
Pyrrhotite ( $\text{Fe}_7\text{S}_8$ ) (monoclinic;  $C2/C$ ; polytype 4C)

Pentlandite ( $\text{FeNi}_9\text{S}_8$ ) (cubic;  $\text{Fm}3\text{m}$ )

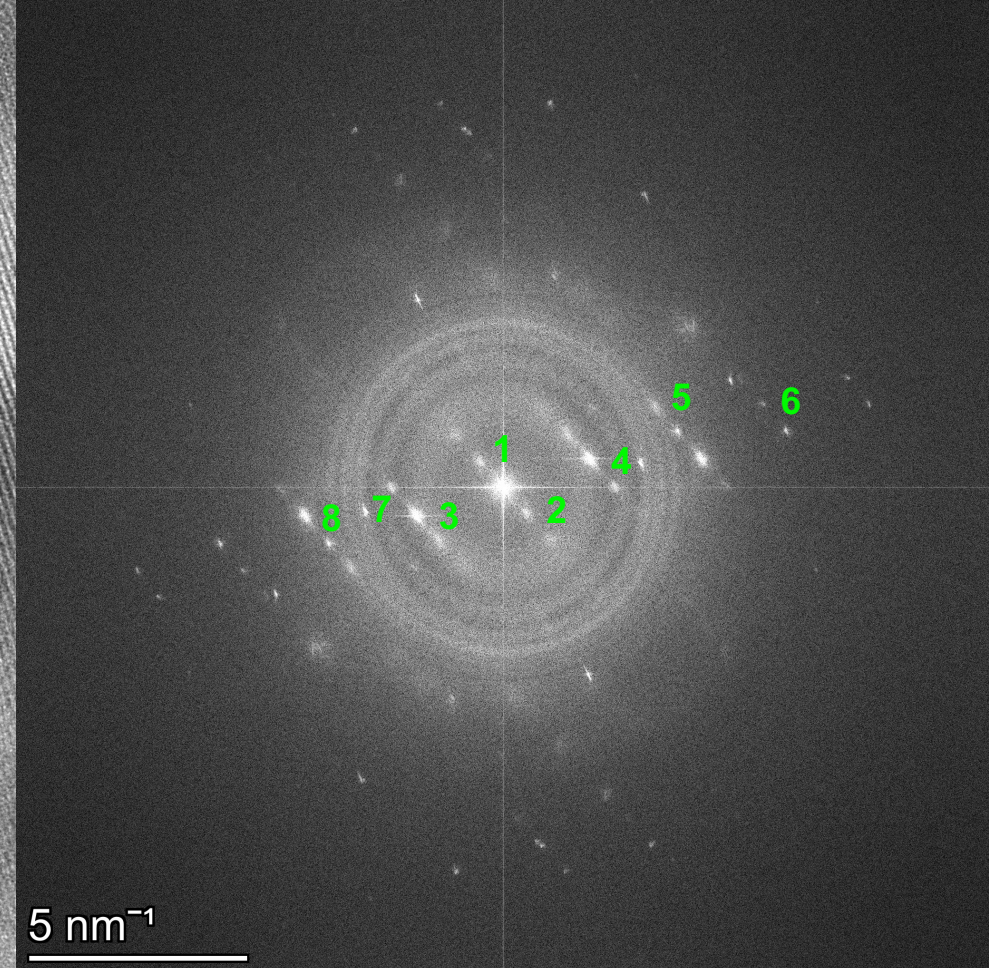
Bornite ( $\text{Cu}_5\text{FeS}_4$ ) (cubic;  $\text{F-}43\text{m}$ )

Spot#	d-Spacing (nm)	(hkl)	Ideal d-Spacing (Å)
1	0.601231	(111) <sub>Pn</sub>	5.8538-5.8916
3	0.467591	(-112) <sub>PO</sub>	4.7026
4	0.46133	(-112) <sub>PO</sub>	4.7026
5	0.305823	(311) <sub>Pn</sub>	3.0570-3.0768
7	0.362334	(220) <sub>Pn</sub>	3.5847-3.6078
8	0.360398	(220) <sub>Pn</sub>	3.5847-3.6078
9	0.203696	(422) <sub>Pn</sub>	2.0696-2.0830
10	0.208398	(422) <sub>Pn</sub>	2.0696-2.0830
11	0.212077	(204) <sub>PO</sub>	2.1246
12	0.212845	(204) <sub>PO</sub>	2.1246
19	0.201879	(-133) <sub>Pn</sub>	2.0215-2.0128
20	0.20247	(-133) <sub>Pn</sub>	2.0215-2.0128
23	0.13087	(800) <sub>Bn</sub>	1.3375
24	0.131641	(800) <sub>Bn</sub>	1.3375



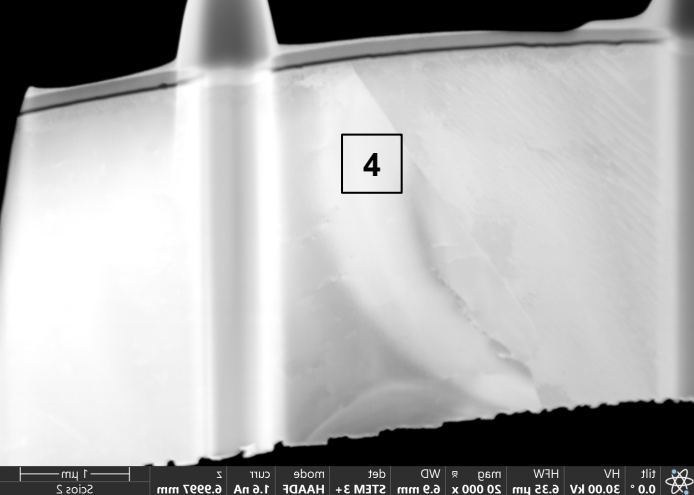


Pyrrhotite



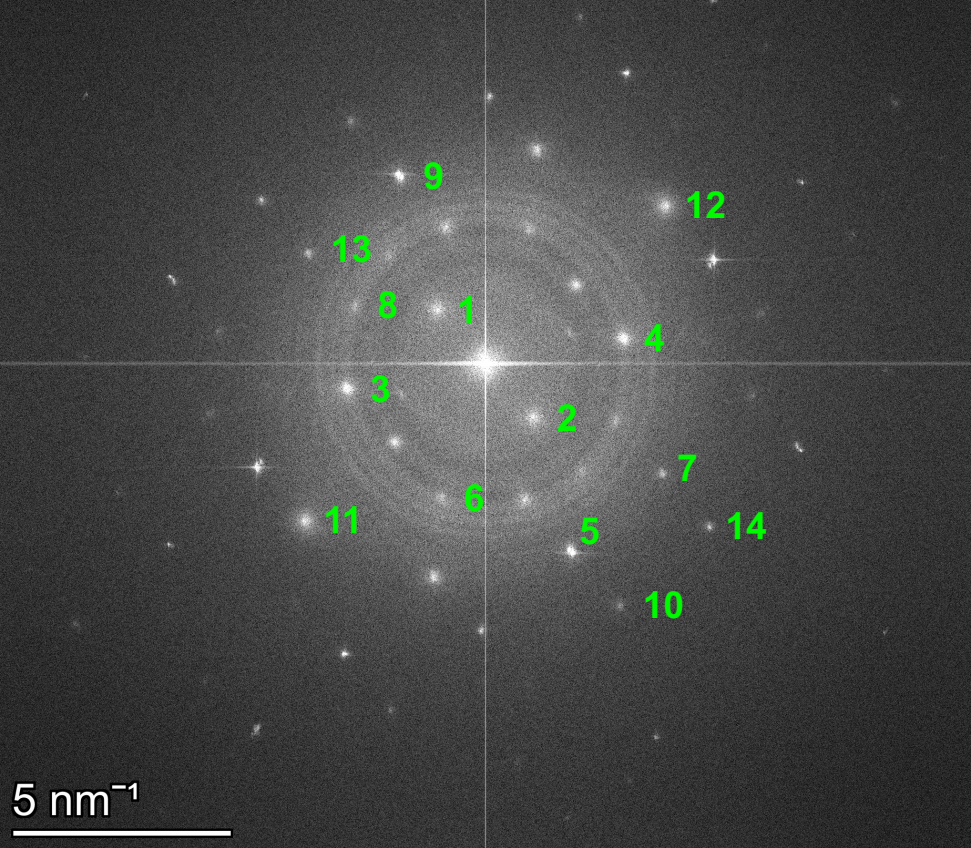
Pyrrhotite (Fe <sub>7</sub> S <sub>8</sub> ) (monoclinic; C2/C; polytype 4C)			
Spot#	d-Spacing (nm)	(hkl)	Ref. d-Spacing (Å)
1	1.231368	{001}	12.8958
2	1.171447	{001}	11.8656
3	0.46077	(-112)	4.6860-4.7026
4	0.47761	(-112)	4.6860-4.7026
5	0.530896	(-202)	5.3052
6	0.312805	(-313)	3.1336
7	0.308396	(310)	3.1093
8	0.212871	(204)	2.1246





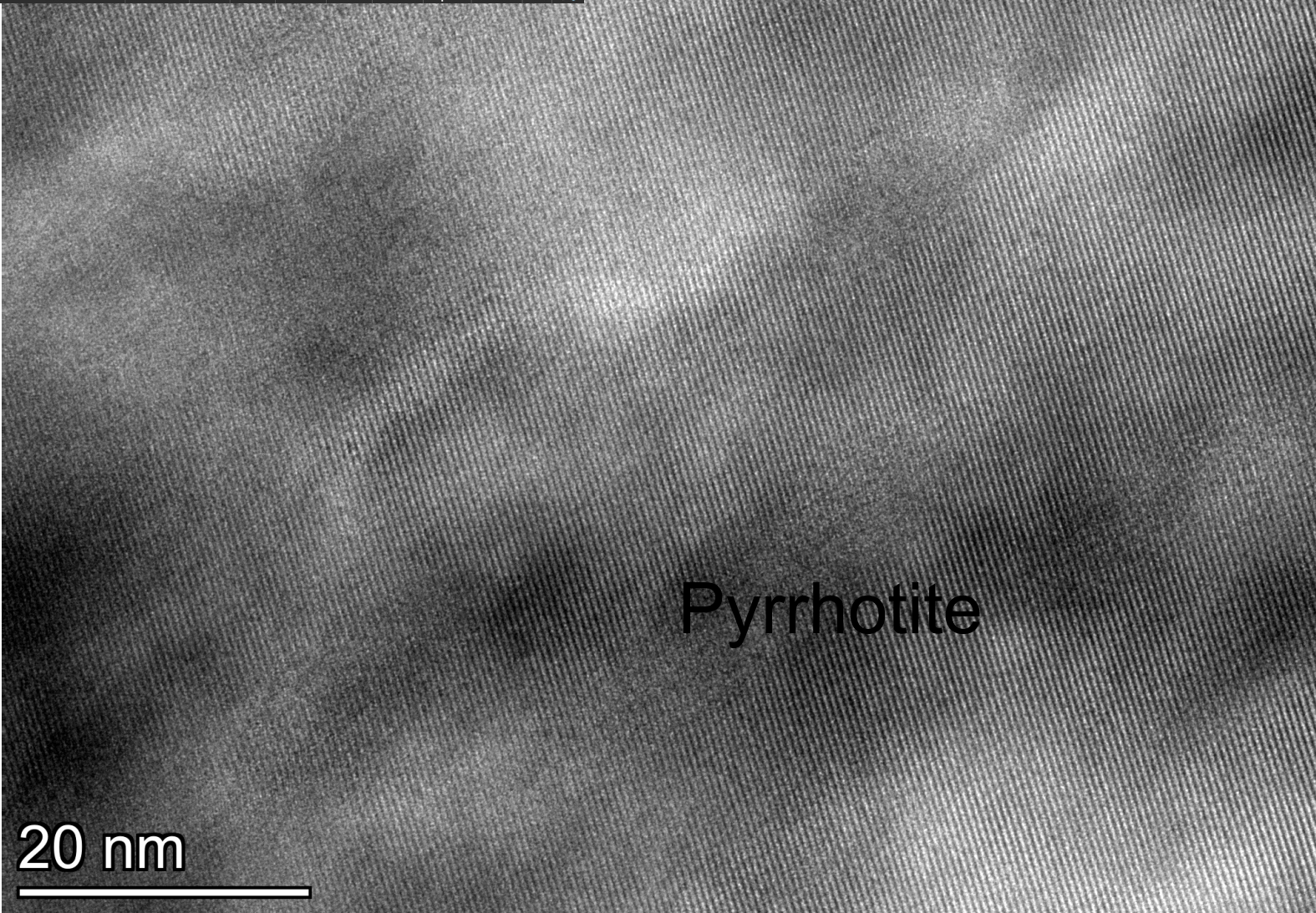
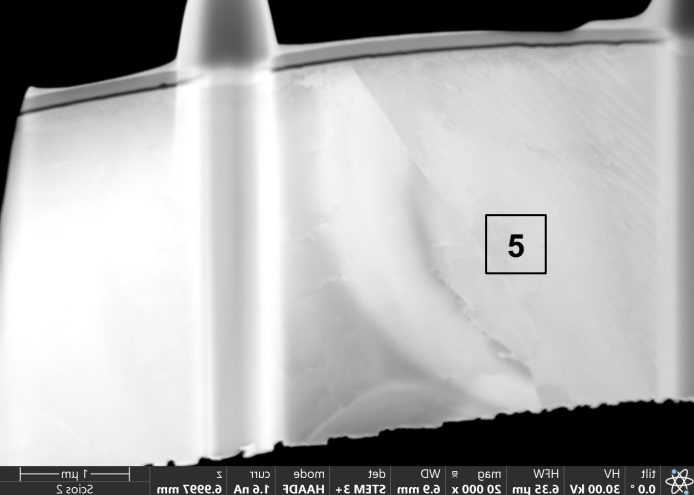
# Pentlandite

20 nm

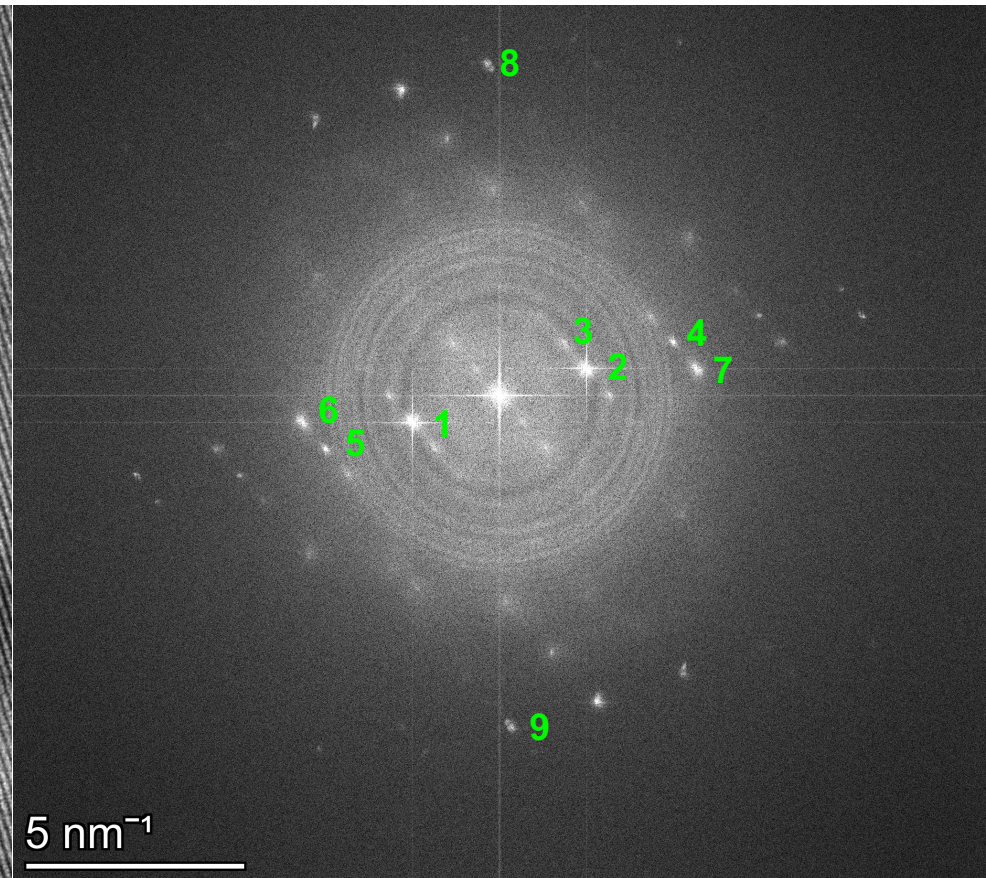


Pentlandite (FeNi) <sub>9</sub> S <sub>8</sub> (cubic; Fm3m)			
Spot#	d-Spacing (nm)	(hkl)	Ideal d-Spacing (Å)
1	0.594419	(111)	5.8538-5.8916
2	0.569116	(111)	5.8538-5.8916
3	0.305972	(311)	3.0570-3.0768
4	0.304598	(311)	3.0570-3.0768
5	0.29855	(222)	2.9269-2.9458
6	0.299393	(222)	2.9269-2.9458
7	0.305389	(311)	3.0570-3.0768
8	0.308573	(311)	3.0570-3.0768
9	0.209475	(422)	2.0696-2.0830
10	0.206015	(422)	2.0696-2.0830
11	0.179149	(440)	1.7923-1.8039
12	0.182742	(440)	1.7923-1.8039
13	0.209096	(422)	2.0696-2.0830
14	0.209247	(422)	2.0696-2.0830



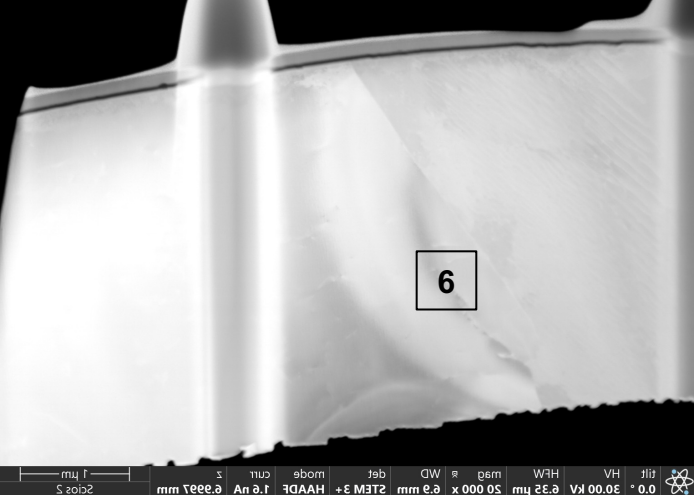


Pyrrhotite

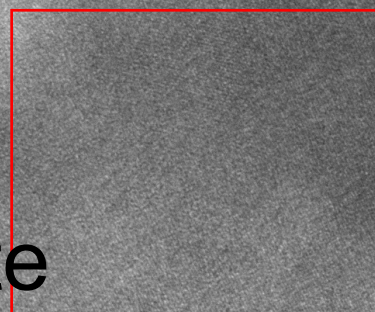


Pyrrhotite (Fe <sub>7</sub> S <sub>8</sub> ) (monoclinic; C2/C; polytype 4C)			
Chalcopyrite (CuFeS <sub>2</sub> ) (tetragonal; I42d)			
Spot#	d-Spacing (nm)	(hkl)	Ref. d-Spacing (Å)
1	0.471036	(-112) <sub>Po</sub>	4.7026
2	0.480821	(-112) <sub>Po</sub>	4.7026
3	0.530071	(-202) <sub>Po</sub>	5.3052
4	0.240795	(-315) <sub>Po</sub>	2.3702-2.3767
5	0.237625	(-315) <sub>Po</sub>	2.3702-2.3767
6	0.220301	(-421) <sub>Po</sub>	2.1959-2.2076
7	0.218549	(-421) <sub>Po</sub>	2.1959-2.2076
8	0.131675	(008) <sub>Cp</sub>	1.3024-1.3027
9	0.130936	(008) <sub>Cp</sub>	1.3024-1.3027



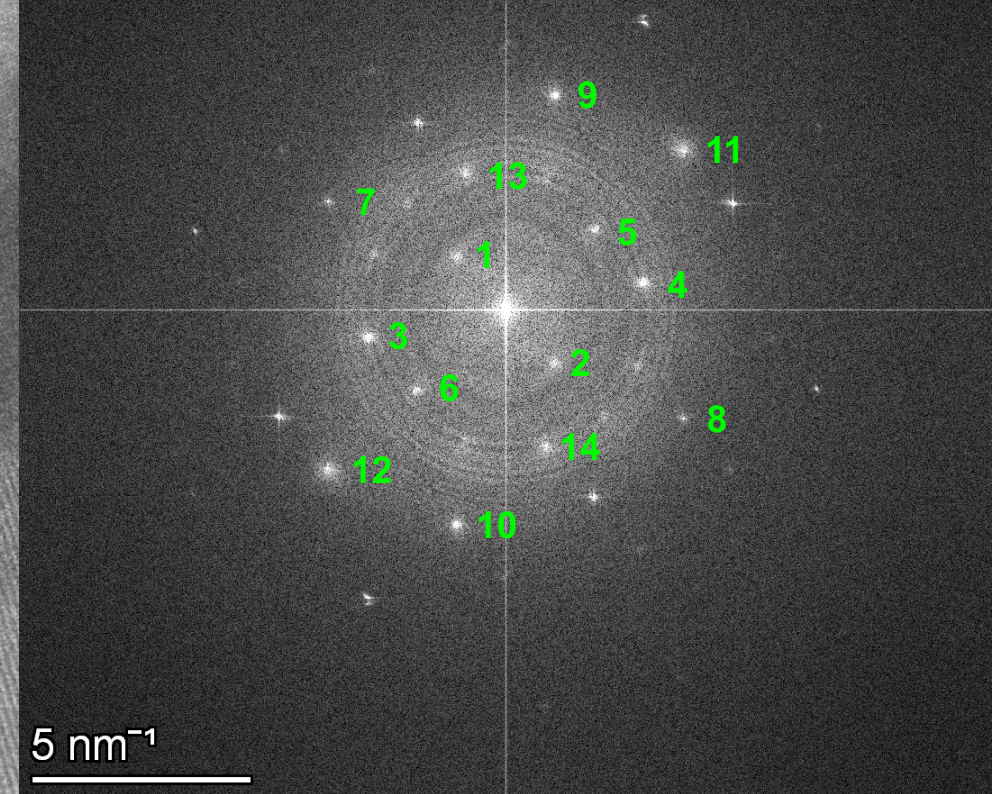


Pentlandite



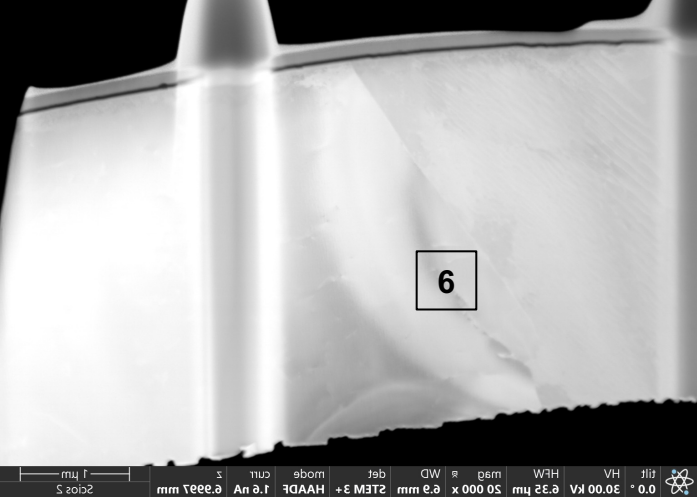
Pyrrhotite

20 nm

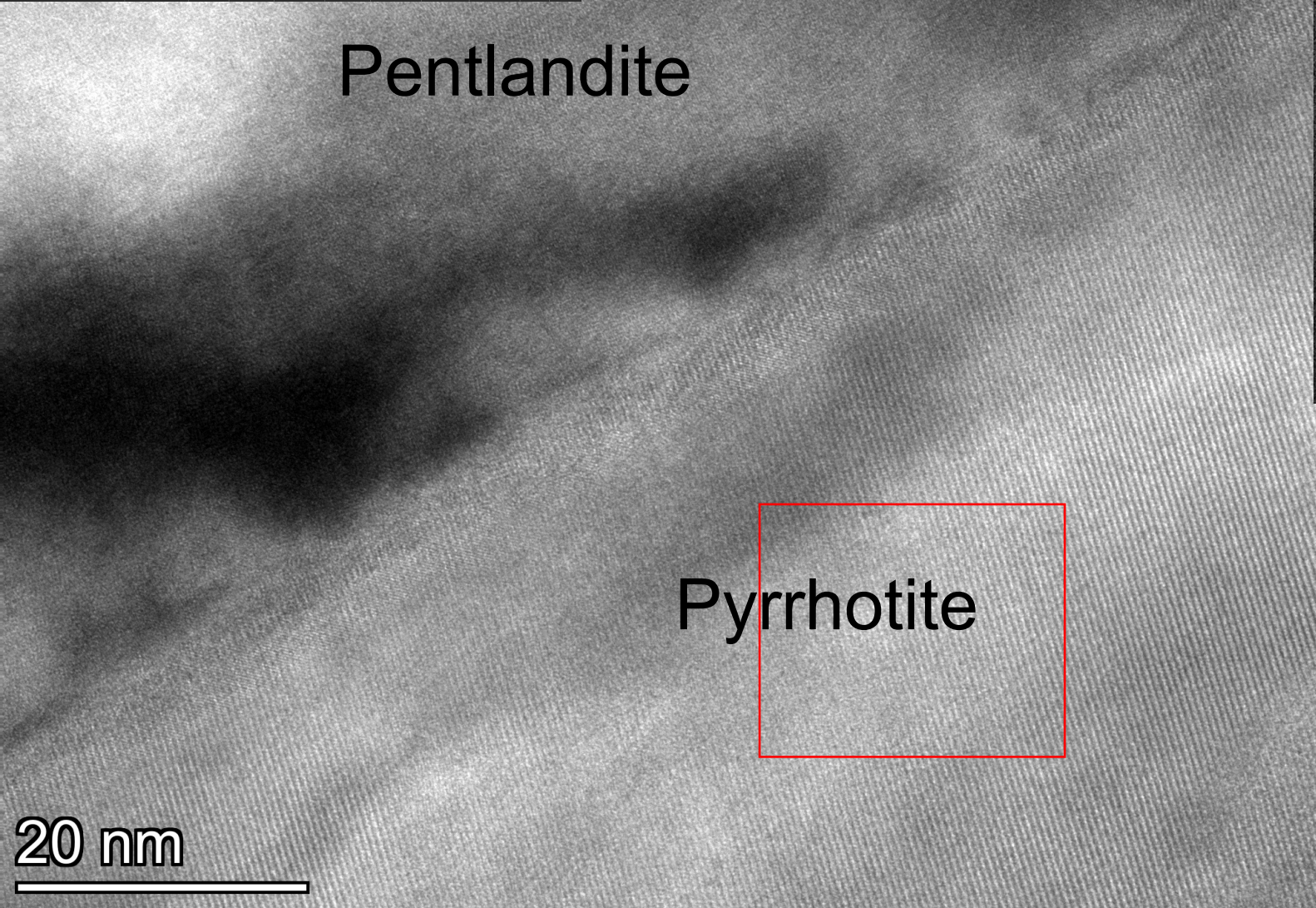


Pentlandite (FeNi) <sub>9</sub> S <sub>8</sub> (cubic; Fm3m)			
Chalcopyrite (CuFeS <sub>2</sub> ) (tetragonal; <i>I</i> 42 <i>d</i> )			
Spot#	d-Spacing (nm)	(hkl)	Ideal d-Spacing (Å)
1	0.602232	(111)	5.8538-5.8916
2	0.581329	(111)	5.8538-5.8916
3	0.304694	(112) <sub>Cp</sub>	3.0385-3.0387
4	0.303621	(112) <sub>Cp</sub>	3.0385-3.0387
5	0.365277	(220)	3.5847-3.6078
6	0.347047	(220)	3.5847-3.6078
7	0.209806	(422)	2.0696-2.0830
8	0.20995	(422)	2.0696-2.0830
9	0.199718	(333)	1.9513-1.9639
10	0.194856	(333)	1.9513-1.9639
11	0.185201	(204) <sub>Cp</sub>	1.8365-1.8561
12	0.183313	(204) <sub>Cp</sub>	1.8365-1.8561
13	0.29789	(222)	2.9269-2.9458
14	0.29249	(222)	2.9269-2.9458

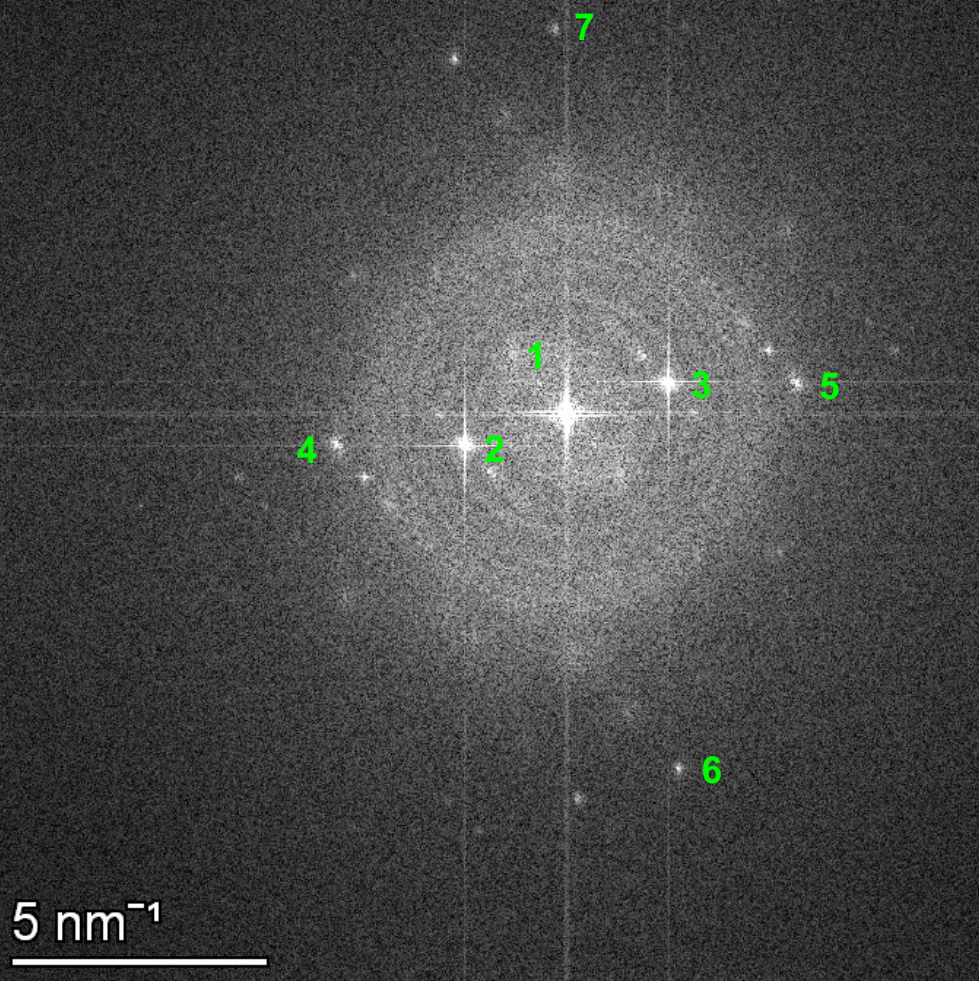




Pentlandite

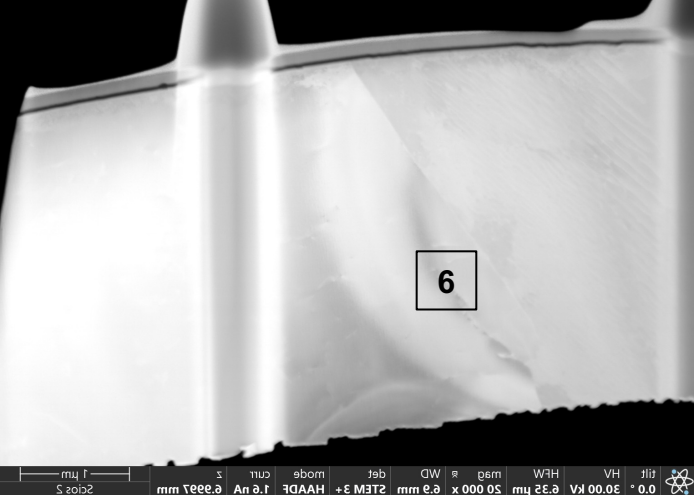


Pyrrhotite

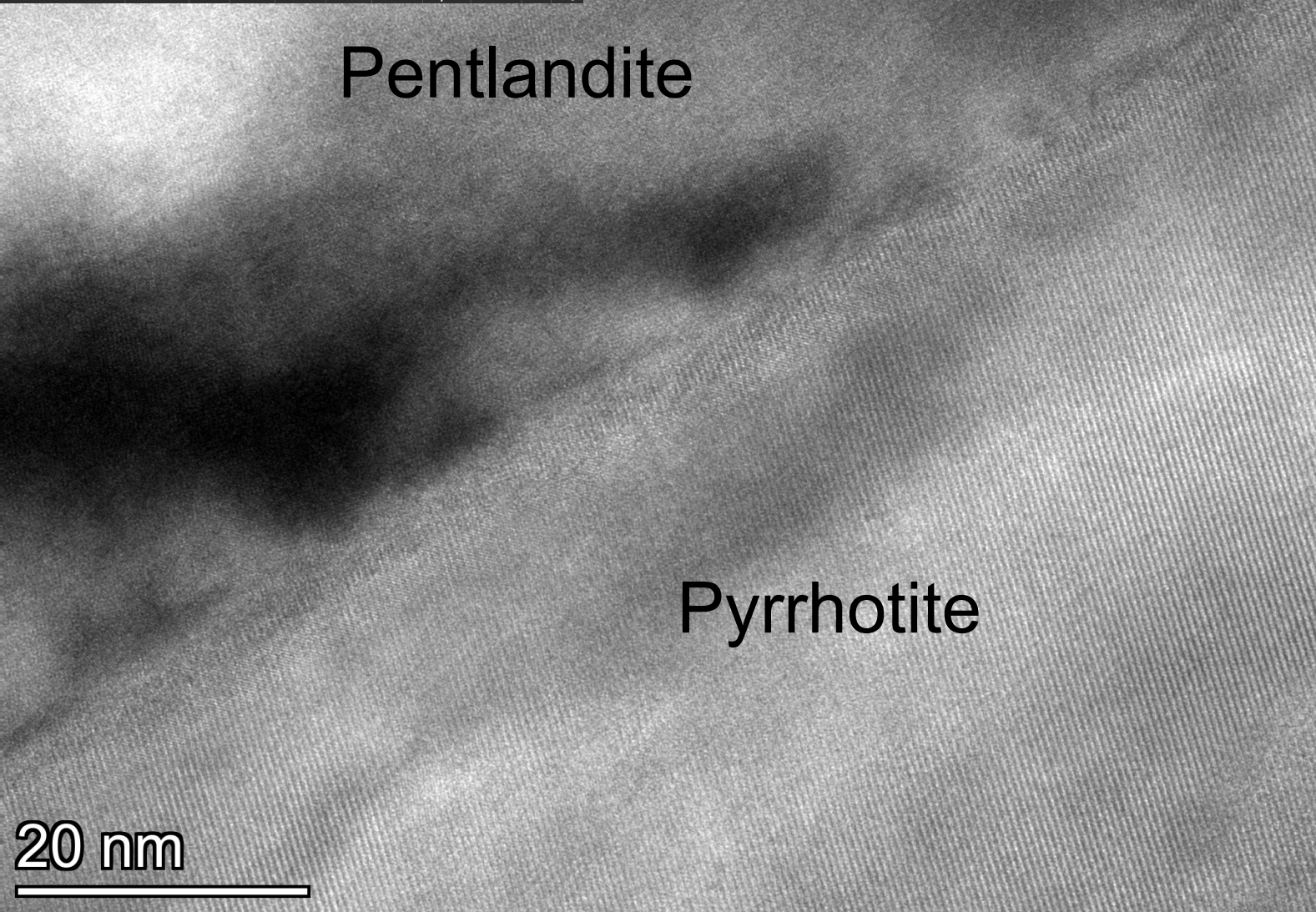


Pyrrhotite (Fe <sub>7</sub> S <sub>8</sub> ) (monoclinic; C2/C; polytype 4C)			
Pentlandite (FeNi) <sub>9</sub> S <sub>8</sub> (cubic; Fm3m)			
Bornite (Cu <sub>5</sub> FeS <sub>4</sub> ) (cubic; F4̄3m)			
Spot#	d-Spacing (nm)	(hkl)	Ref. d-Spacing (Å)
1	0.602232	(111) <sub>Pn</sub>	5.8538-5.8916
2	0.47309	(-112)	4.7026
3	0.485556	(-112)	4.7026
4	0.219033	(-421)	2.1959-2.2076
5	0.221832	(-421)	2.1959-2.2076
6	0.134774	(800) <sub>Bn</sub>	1.3375
7	0.133779	(800) <sub>Bn</sub>	1.3375

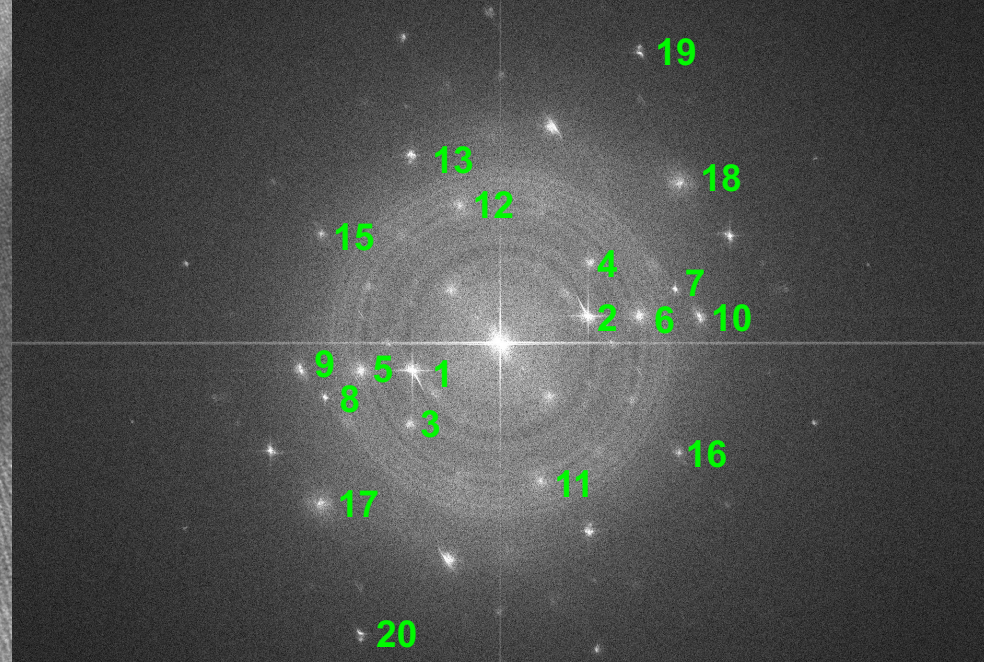




Pentlandite



Pyrrhotite



Pyrrhotite ( $\text{Fe}_7\text{S}_8$ ) (monoclinic;  $C2/C$ ; polytype 4C)

Pentlandite ( $\text{FeNi}_9\text{S}_8$ ) (cubic;  $Fm\bar{3}m$ )

Bornite ( $\text{Cu}_5\text{FeS}_4$ ) (cubic;  $F\bar{4}3m$ )

Spot#	d-Spacing (nm)	(hkl)	Ref. d-Spacing (Å)
1	0.473165	$(-112)_{\text{Po}}$	4.7026
2	0.47761	$(-112)_{\text{Po}}$	4.7026
3	0.361694	$(220)_{\text{Pn}}$	3.5847-3.6078
4	0.35476	$(220)_{\text{Pn}}$	3.5847-3.6078
5	0.304133	$(112)_{\text{Cp}}$	3.0385-3.0387
6	0.30286	$(112)_{\text{Cp}}$	3.0385-3.0387
7	0.236065	$(331)_{\text{Pn}}/(312)_{\text{Po}}$	2.3411/2.3457
8	0.236532	$(331)_{\text{Pn}}/(312)_{\text{Po}}$	2.3411/2.3457
9	0.218667	$(-421)_{\text{Po}}$	2.1959-2.2076
10	0.217234	$(-421)_{\text{Po}}$	2.1959-2.2076
11	0.307591	$(112)_{\text{Cp}}$	3.0385-3.0387
12	0.303482	$(112)_{\text{Cp}}$	3.0385-3.0387
13	0.209727	$(422)_{\text{Pn}}$	2.0830
14	0.209566	$(422)_{\text{Pn}}$	2.0830
15	0.20767	$(422)_{\text{Pn}}$	2.0830
16	0.207081	$(422)_{\text{Pn}}$	2.0830
17	0.1812	$(440)_{\text{Pn}}$	1.8039
18	0.183285	$(440)_{\text{Pn}}$	1.8039
19	0.135658	$(800)_{\text{Bn}}$	1.3375
20	0.134553	$(800)_{\text{Bn}}$	1.3375