

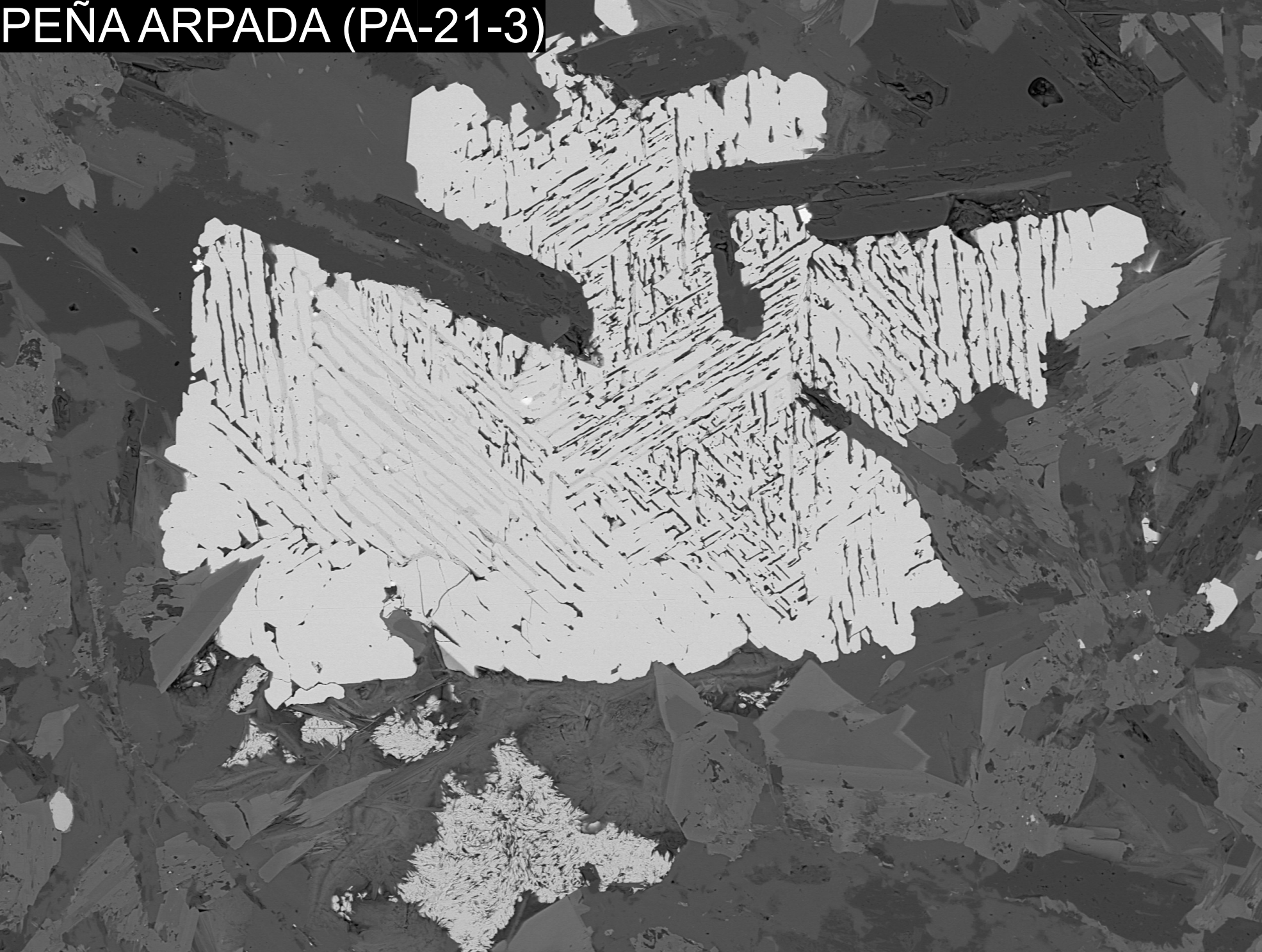
**Sulfide mineralogy of igneous basic rocks (ophites) from the External Zone of the Betic Cordillera**


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 S6**

**Nanostructural analysis of post-magmatic sulfides**

PEÑA ARPADA (PA-21-3)



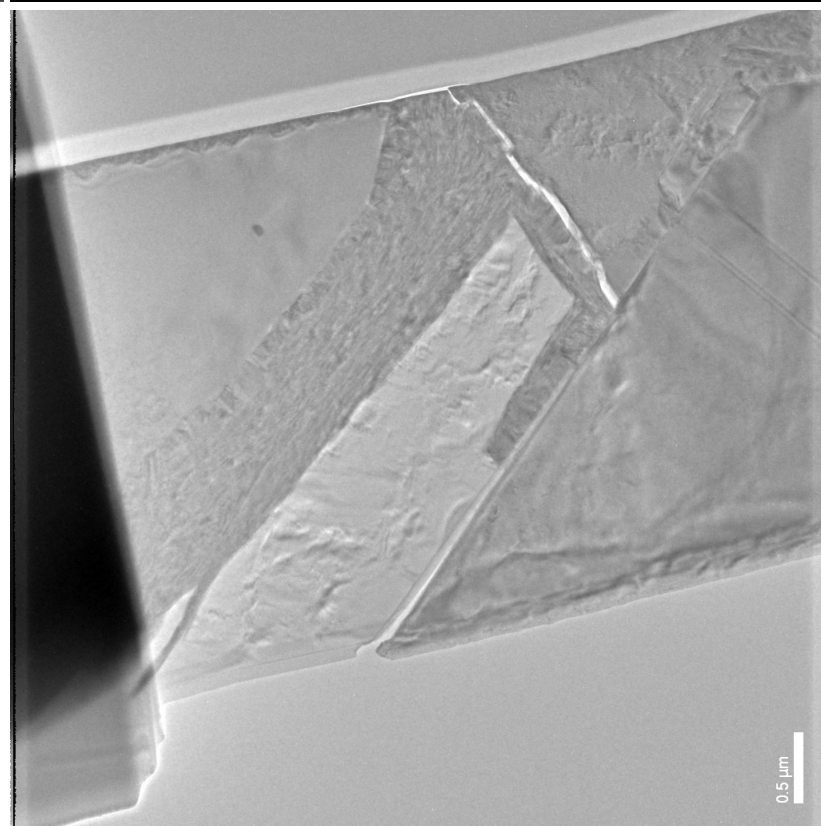
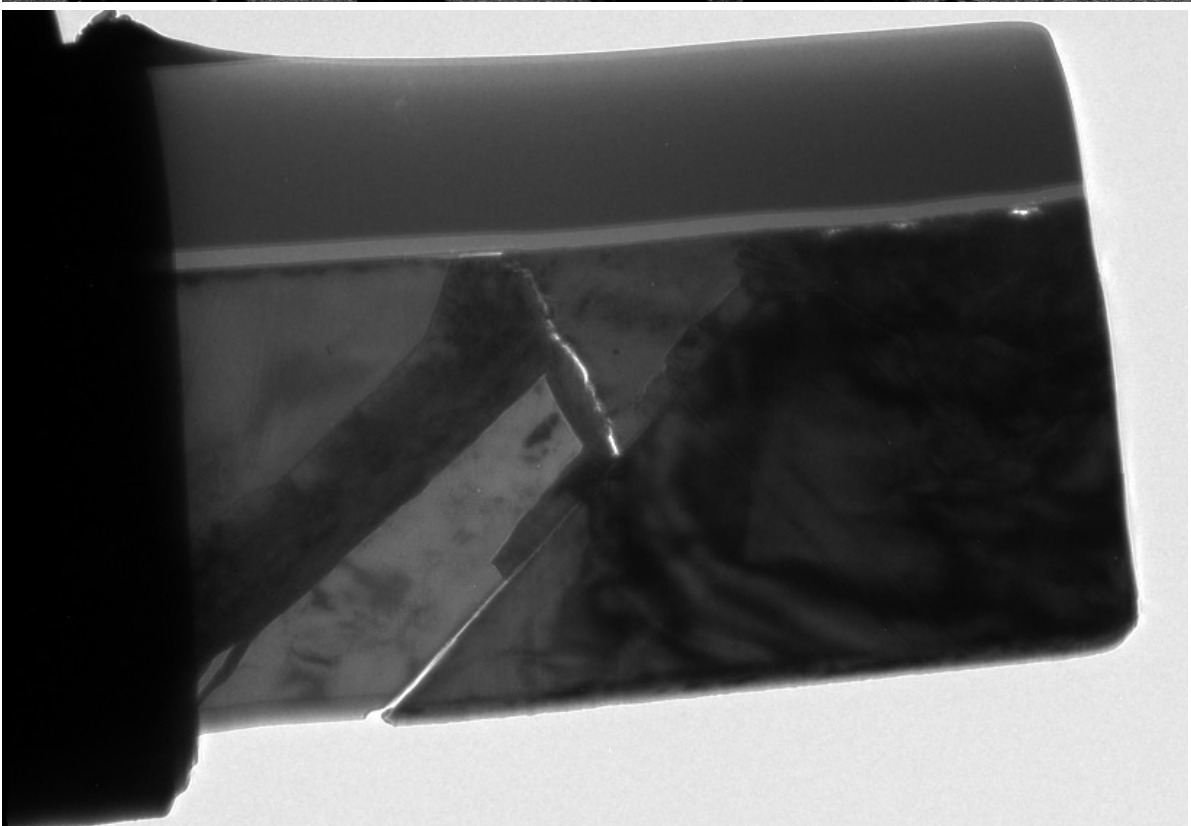
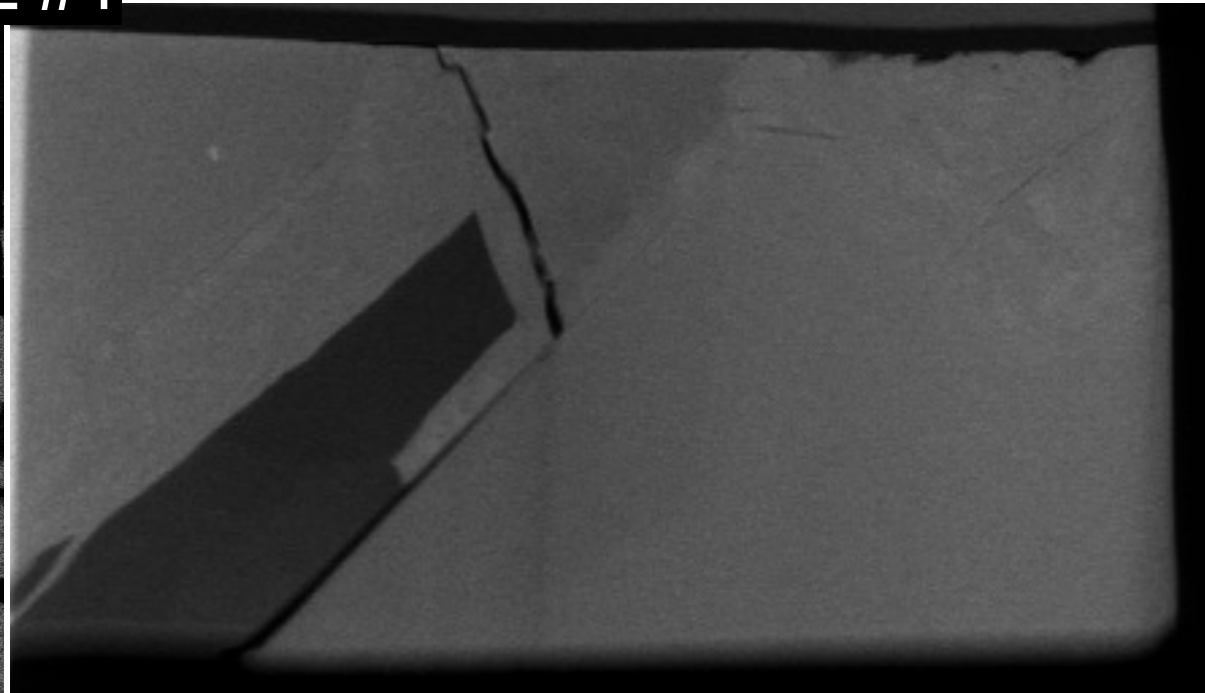
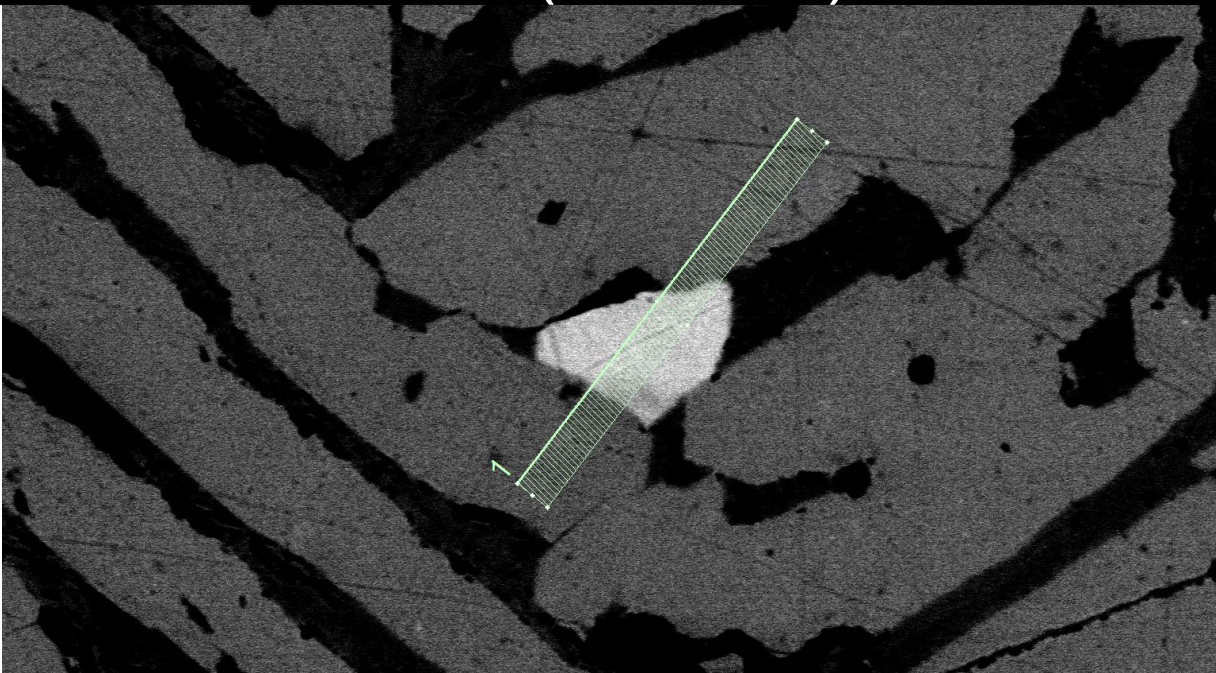
BED-C 15.0 kV WD 9.8 mm Std.-PC 80.0 HighVac.  x230

NOR 0517 July 13 2023

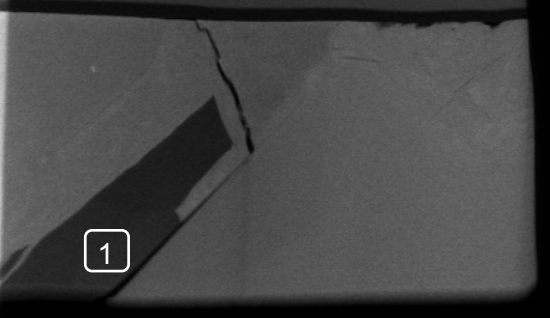
 100  $\mu\text{m}$



# PEÑA ARPADA (PA-21-3) THIN-FOIL #1







$\alpha$ -Quartz  
(SiO<sub>2</sub>)

10 nm

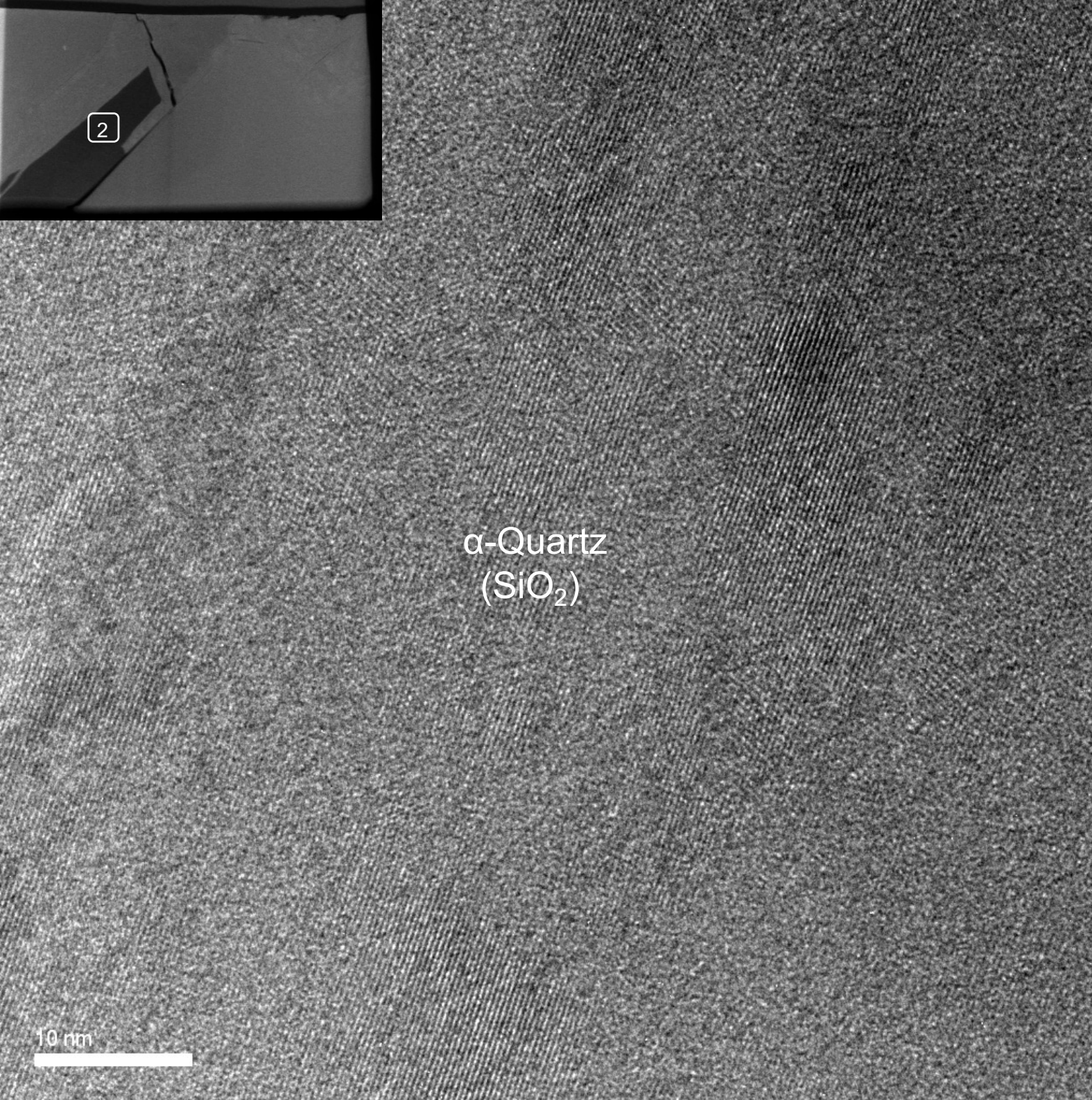
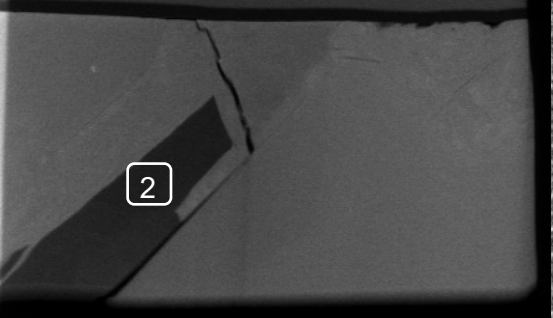
FFT (1)

2 1/nm

$\alpha$ -Quartz (SiO<sub>2</sub>) (trigonal;  $P3_221$ )

Spot#	d-Spacing (nm)	(hkl)	Ideal d-Spacing (Å)
1	0.424061	(100)	4.2552
2	0.428226	(100)	4.2552
3	0.213034	(200)	2.1276
4	0.213958	(200)	2.1276
5	0.227543	(102)/(012)	2.2813
6	0.22722	(102)/(012)	2.2813
8	0.155821	(211)/(112)	1.5415
7	0.155516	(211)/(112)	1.5415

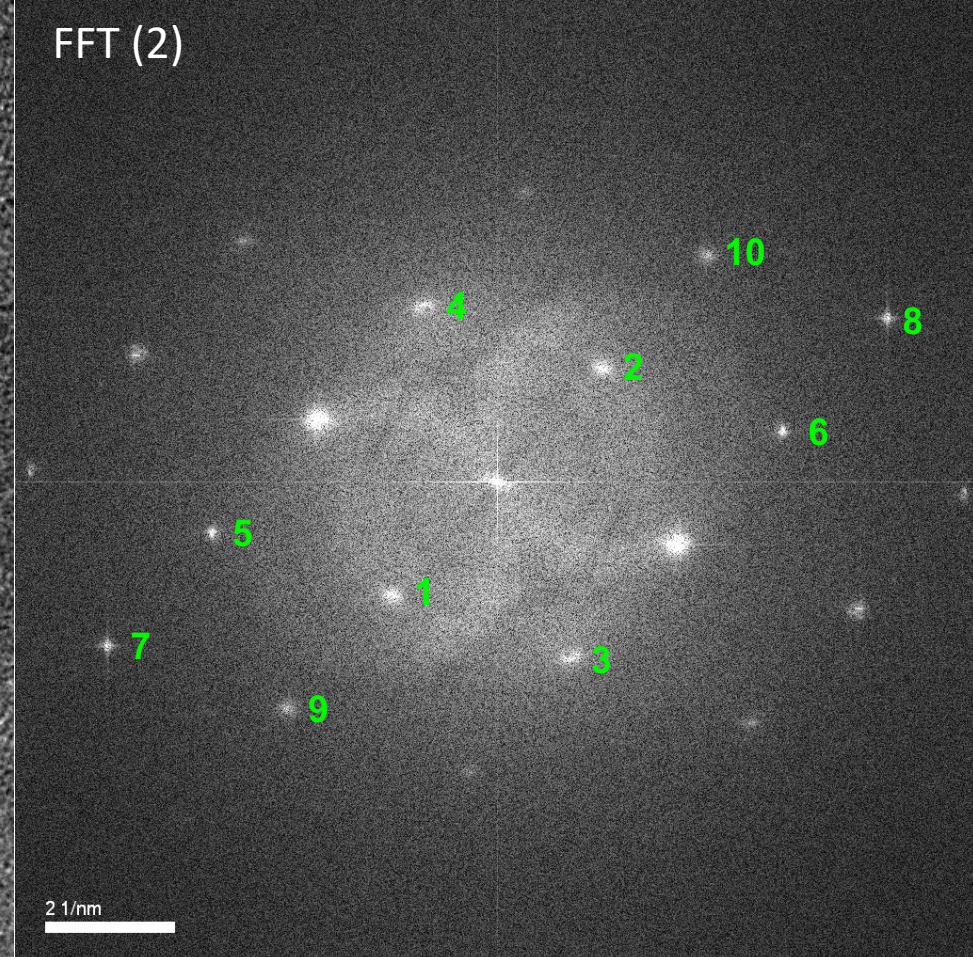




$\alpha$ -Quartz  
(SiO<sub>2</sub>)

10 nm

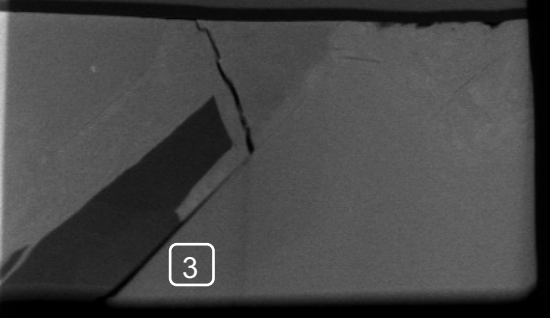
FFT (2)



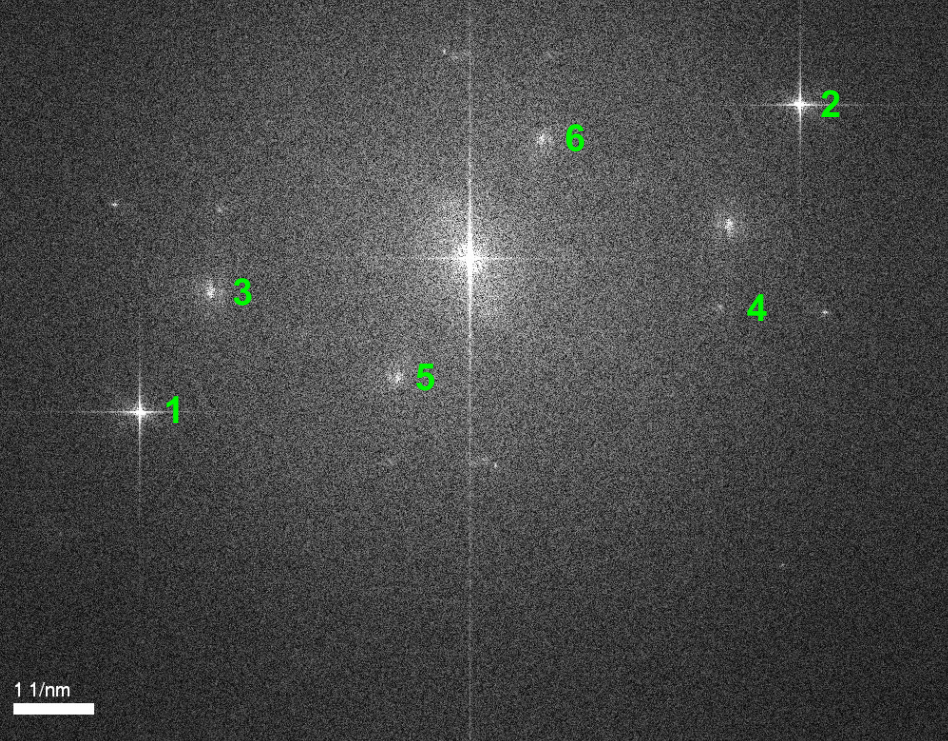
$\alpha$ -Quartz (SiO<sub>2</sub>) (trigonal;  $P3_221$ )

Spot#	d-Spacing (nm)	(hkl)	Ideal d-Spacing (Å)
1	0.428028	(100)	4.2552
2	0.431487	(100)	4.2552
3	0.339058	(011)	3.3434
4	0.342101	(011)	3.3434
5	0.225607	(102)/(012)	2.2813
6	0.225917	(102)/(012)	2.2813
7	0.154627	(211)/(112)	1.5415
8	0.15494	(211)/(112)	1.5415
9	0.210777	(200)	2.1276
10	0.211756	(200)	2.1276





FFT (3)



Pyrite ( $\text{FeS}_2$ ) (cubic; P3a)

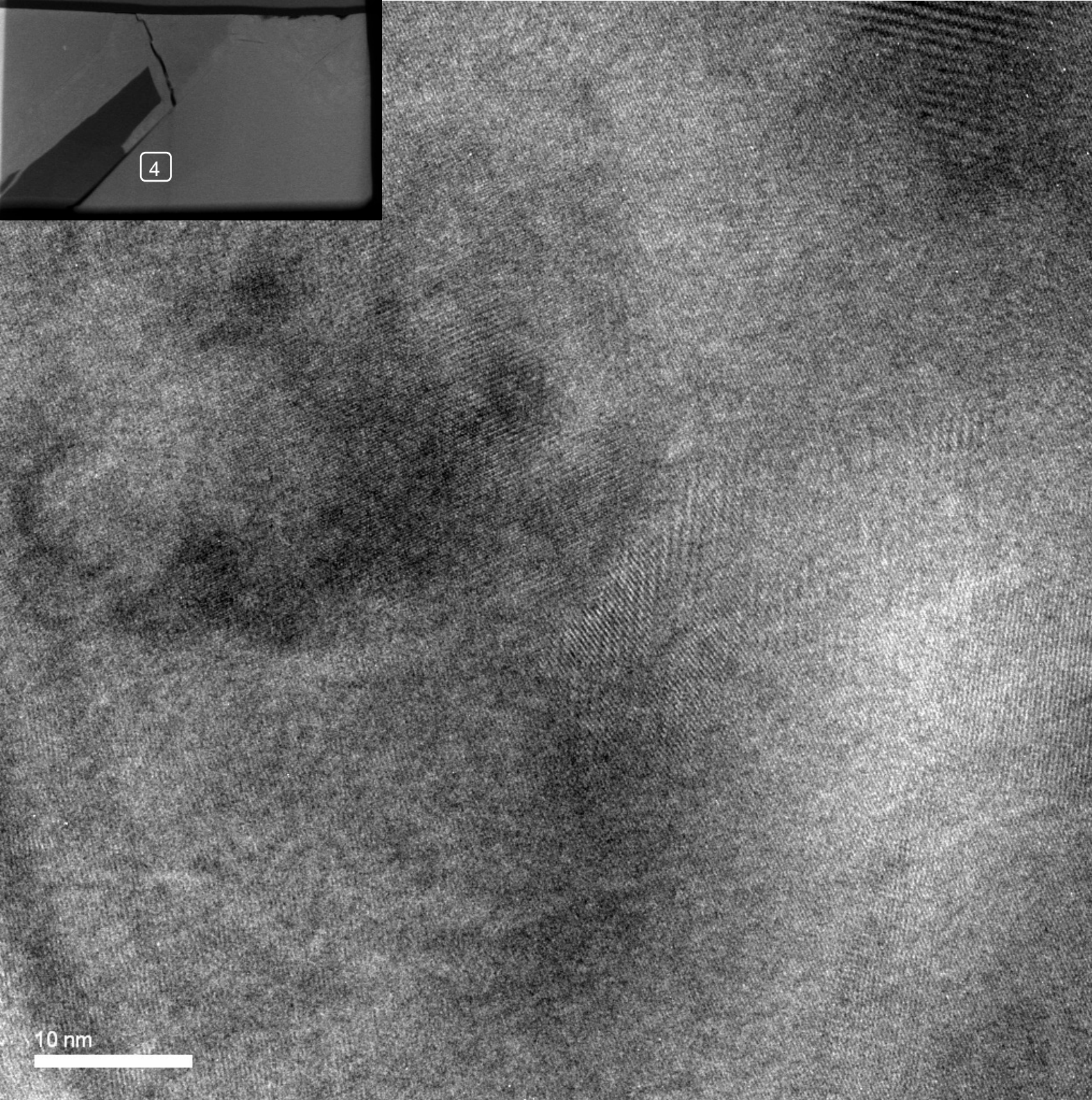
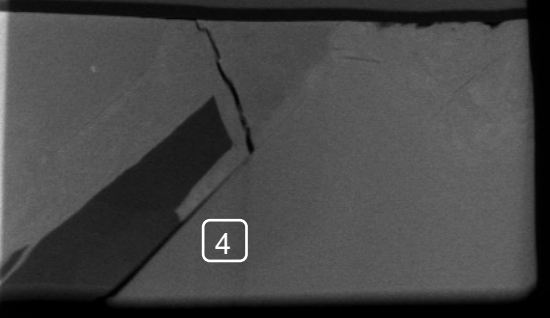
Pyrrhotite ( $\text{FeS}$ ) (monoclinic; C2/c politype 4C

& orthorhombic; Cmca polytype 5C)

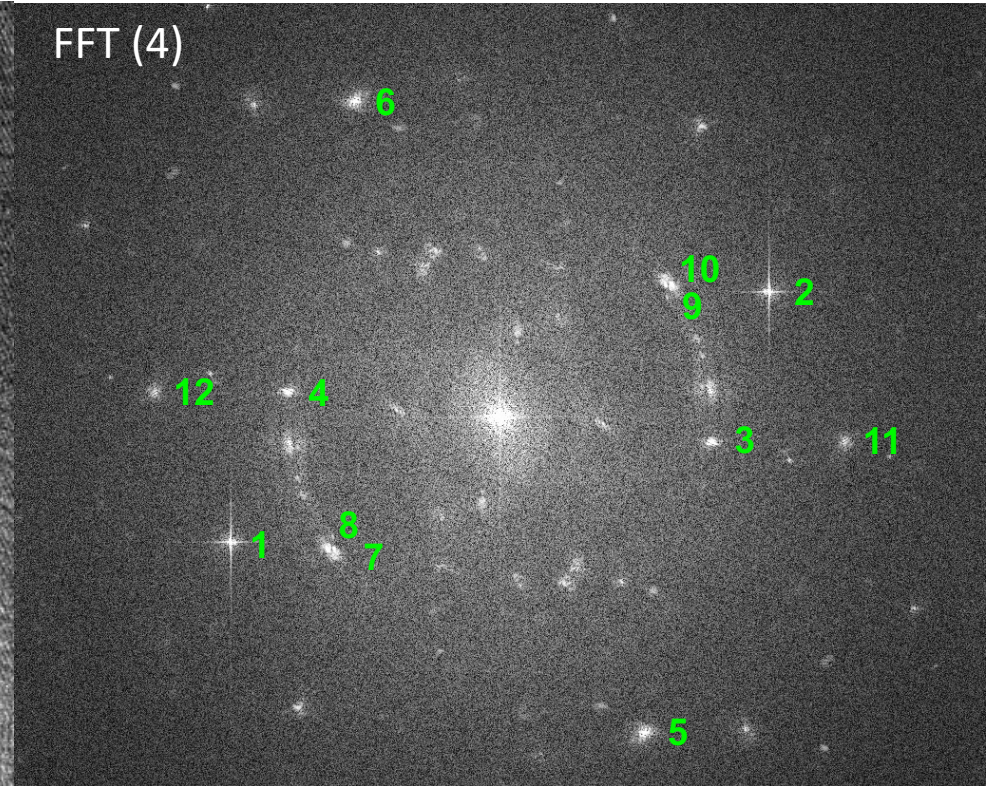
Spot#	d-Spacing (nm)	(hkl)	Ideal d-Spacing (Å)
1	0.222296	$(112)_{\text{Py}}/(211)_{\text{py}}$	2.2111
2	0.222769	$(112)_{\text{Py}}/(211)_{\text{py}}$	2.2111
3	0.309592	$(310)_{\text{Po(mon)}}$	3.1093-3.1264
4	0.309801	$(310)_{\text{Po(mon)}}$	3.1093-3.1264
5	0.576752	$(-111)_{\text{Po(mon)}}$	5.7478-6.7739
6	0.583142	$(111)_{\text{Po(romb)}}$	5.8439-5.8456

10 nm





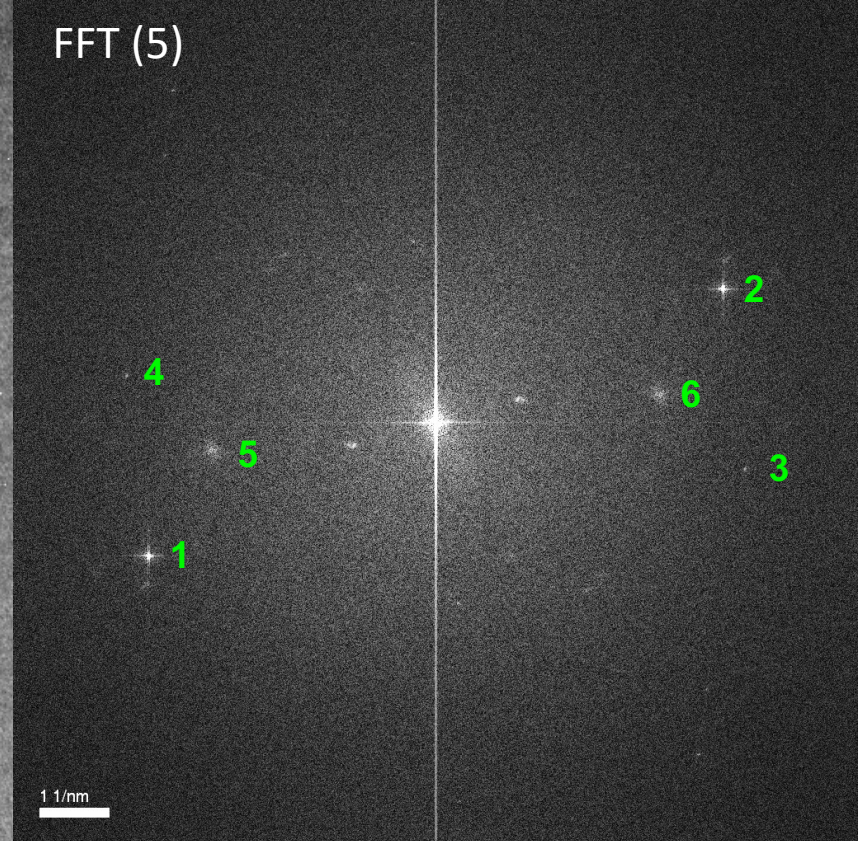
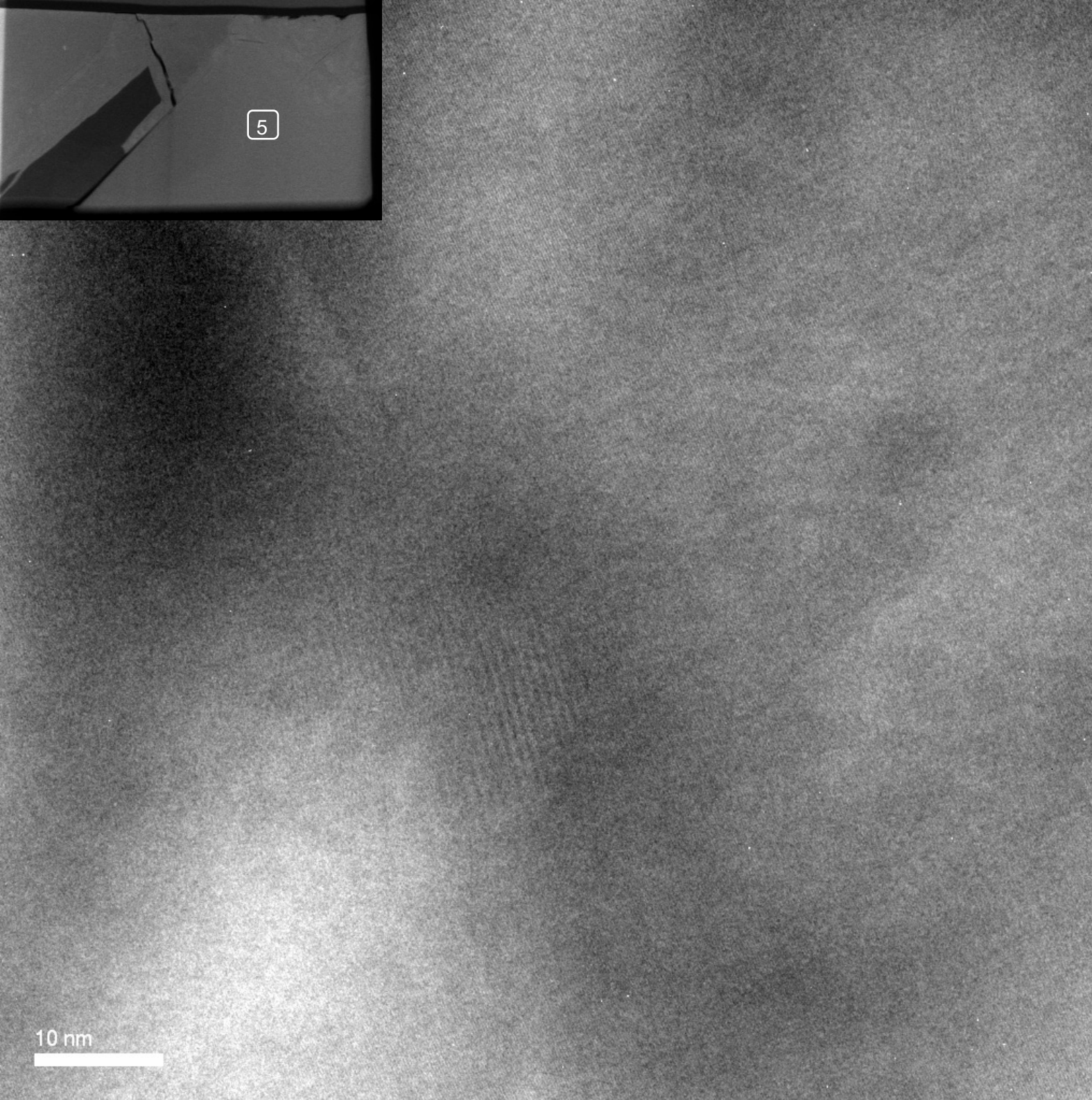
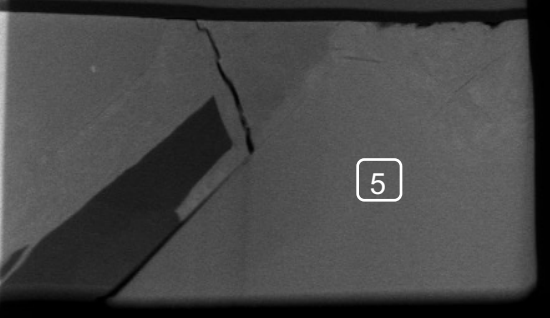
FFT (4)



Pyrite (FeS<sub>2</sub>) (cubic; P3a)  
Marcasite (FeS<sub>2</sub>) (orthorrombic; Pnnm)  
Pyrrhotite (FeS)( monoclinic; C2/c politype 4C  
& orthorrhombic; Cmca polytype 5C)

Spot#	d-Spacing (nm)	(hkl)	Ideal d-Spacing (Å)
1	0.222955	(112) <sub>Py</sub> /(211) <sub>py</sub>	2.2111
2	0.223701	(112) <sub>Py</sub> /(211) <sub>py</sub>	2.2111
3	0.310442	(301) <sub>Po(mon)</sub>	3.1264
4	0.309011	(028) <sub>Po(romb)</sub>	3.0698
5	0.190225	(121) <sub>Mc</sub> / (202) <sub>Py</sub>	1.9113/1.9151
6	0.191192	(121) <sub>Mc</sub> / (202) <sub>Py</sub>	1.9113/1.9151
7	0.311914	(301) <sub>Po(mon)</sub>	3.1264
8	0.303478	(028) <sub>Po(romb)</sub>	3.0698
9	0.313359	(310) <sub>Po(mon)</sub>	3.1093-3.1264
10	0.30508	(028) <sub>Po(romb)</sub>	3.0698
11	0.191999	(121) <sub>Mc</sub> / (202) <sub>Py</sub>	1.9113/1.9151
12	0.192012	(121) <sub>Mc</sub> / (202) <sub>Py</sub>	1.9113/1.9151

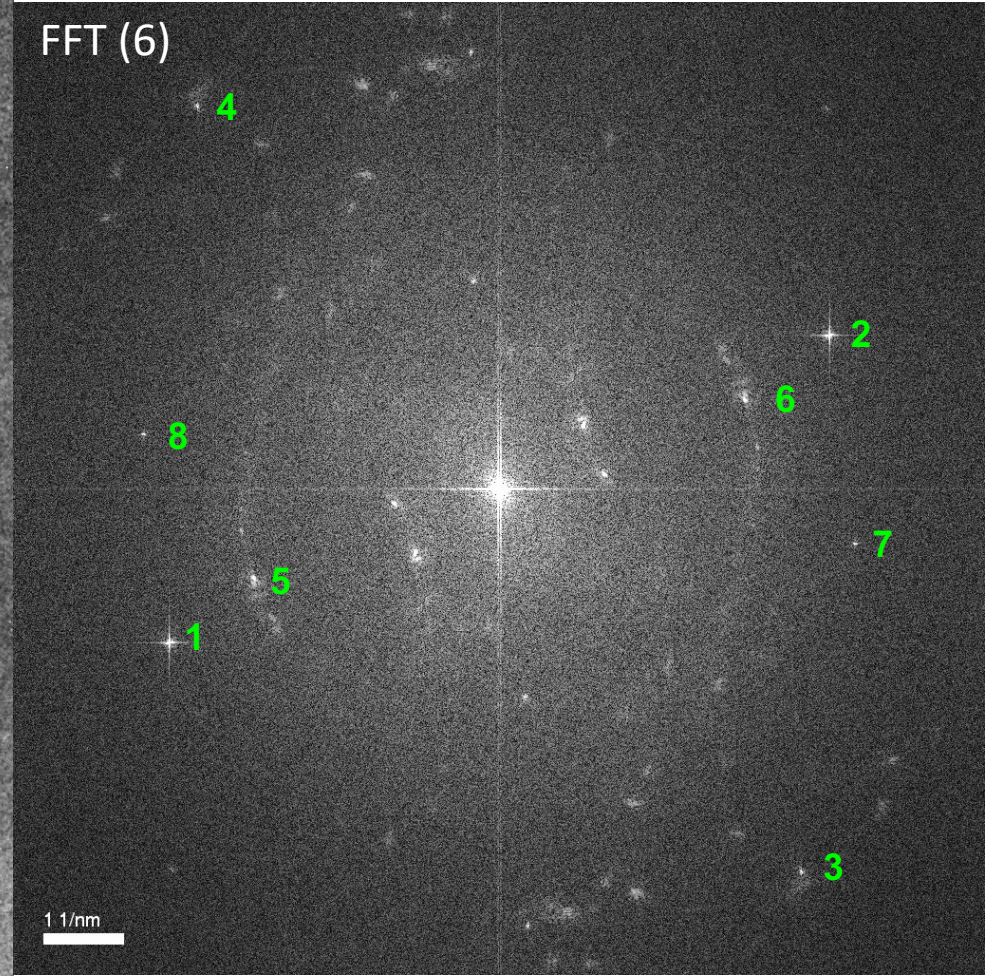
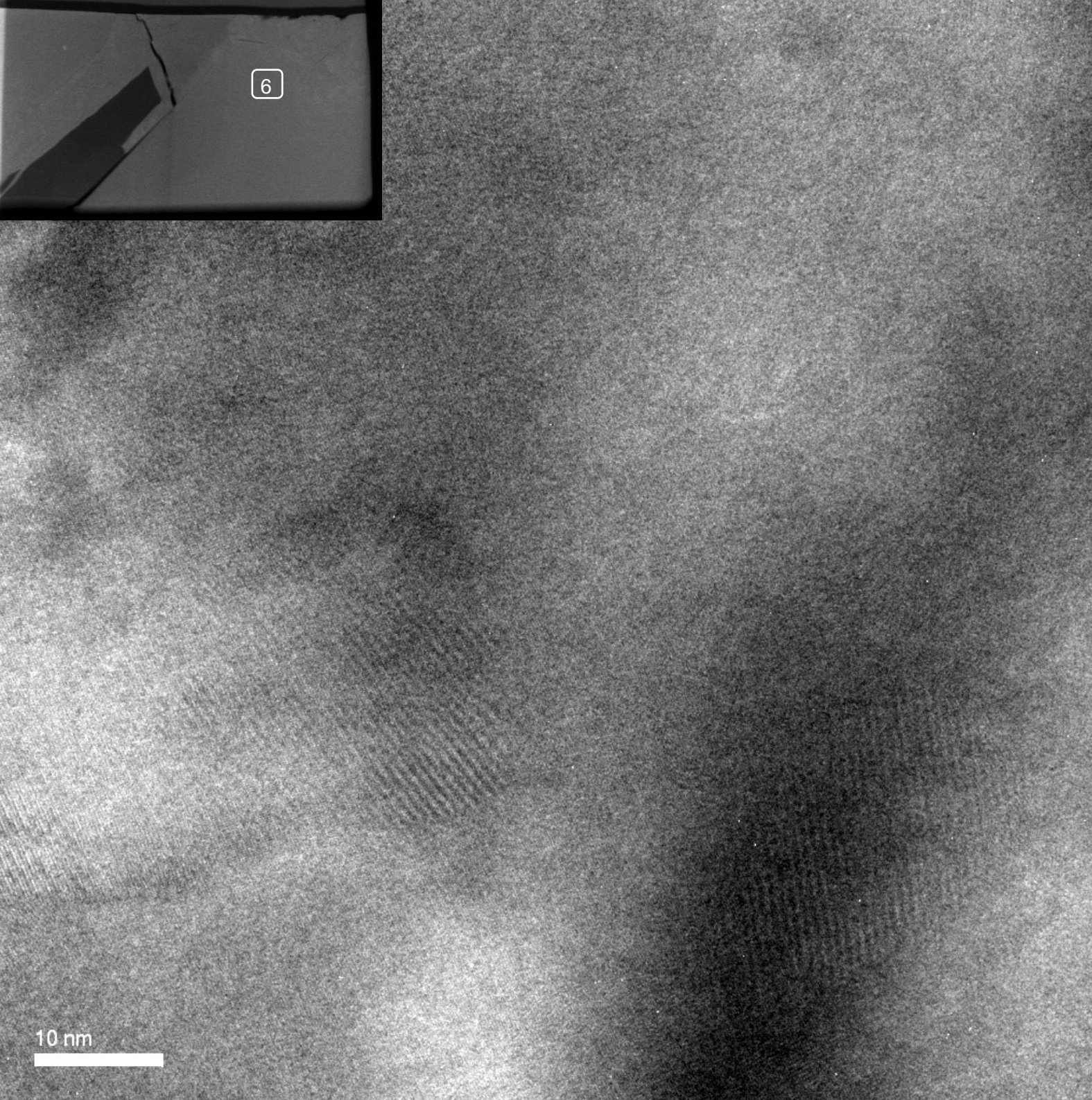
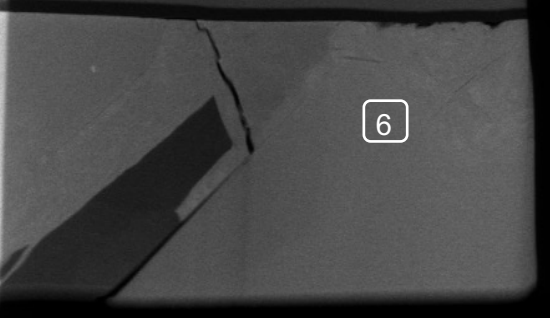




Pyrite (FeS<sub>2</sub>) (cubic; P3a)

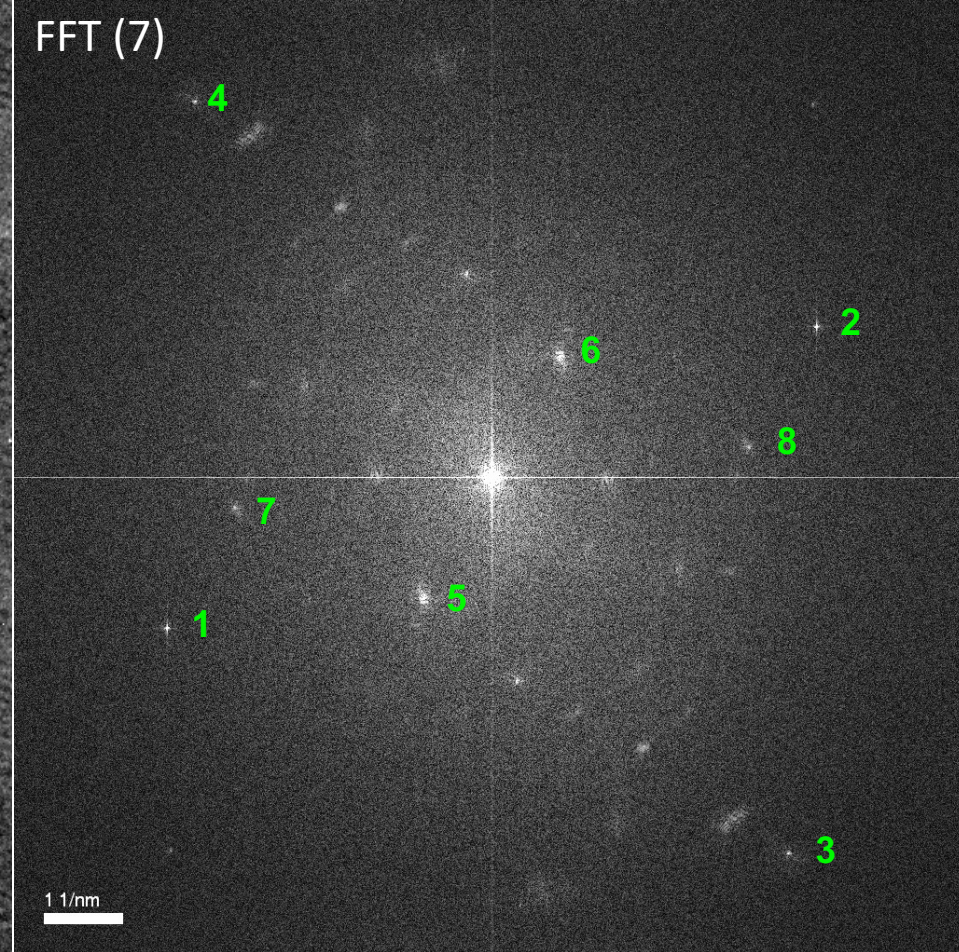
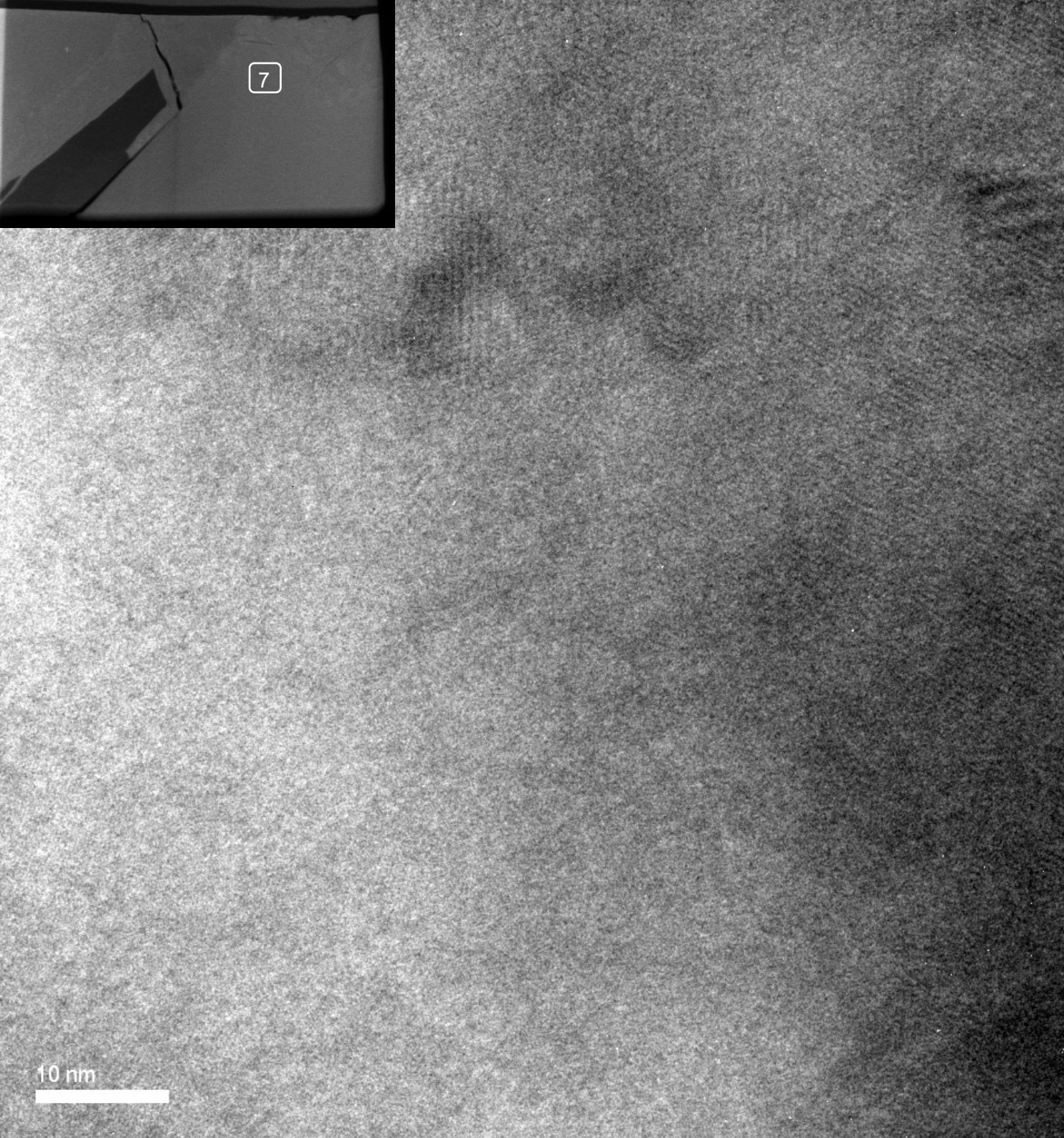
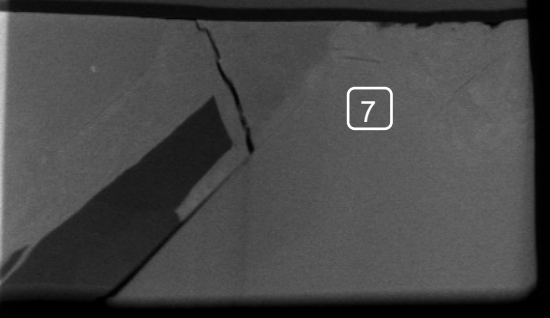
Spot#	d-Spacing (nm)	(hkl)	Ideal d-Spacing (Å)
1	0.222058	(112) <sub>Py</sub> /(211) <sub>Py</sub>	2.2113
2	0.222559	(112) <sub>Py</sub> /(211) <sub>Py</sub>	2.2113
3	0.225559	(112) <sub>Py</sub> /(211) <sub>Py</sub>	2.2113
4	0.225704	(112) <sub>Py</sub> /(211) <sub>Py</sub>	2.2113
7	0.310191	(111) <sub>py</sub>	3.1269-3.1273
6	0.310467	(111) <sub>py</sub>	3.1269-3.1273





Pyrite (FeS <sub>2</sub> ) (cubic; P3a)			
Pyrrhotite (FeS)( monoclinic; C2/c polytype 4C)			
Spot#	d-Spacing (nm)	(hkl)	Ideal d-Spacing (Å)
1	0.222283	(112) <sub>Py</sub> /(211) <sub>Py</sub>	2.2113
2	0.222743	(112) <sub>Py</sub> /(211) <sub>Py</sub>	2.2113
3	0.166243	(222) <sub>py</sub> /(130) <sub>Mc</sub>	1.6526/1.6749
4	0.166481	(222) <sub>py</sub> /(130) <sub>Mc</sub>	1.6526/1.6749
5	0.309353	(310) <sub>Po(mon)</sub>	3.1093-3.1264
6	0.31022	(310) <sub>Po(mon)</sub>	3.1093-3.1264
7	0.224774	(112) <sub>Py</sub> /(211) <sub>Py</sub>	2.2113
8	0.22506	(112) <sub>Py</sub> /(211) <sub>Py</sub>	2.2113





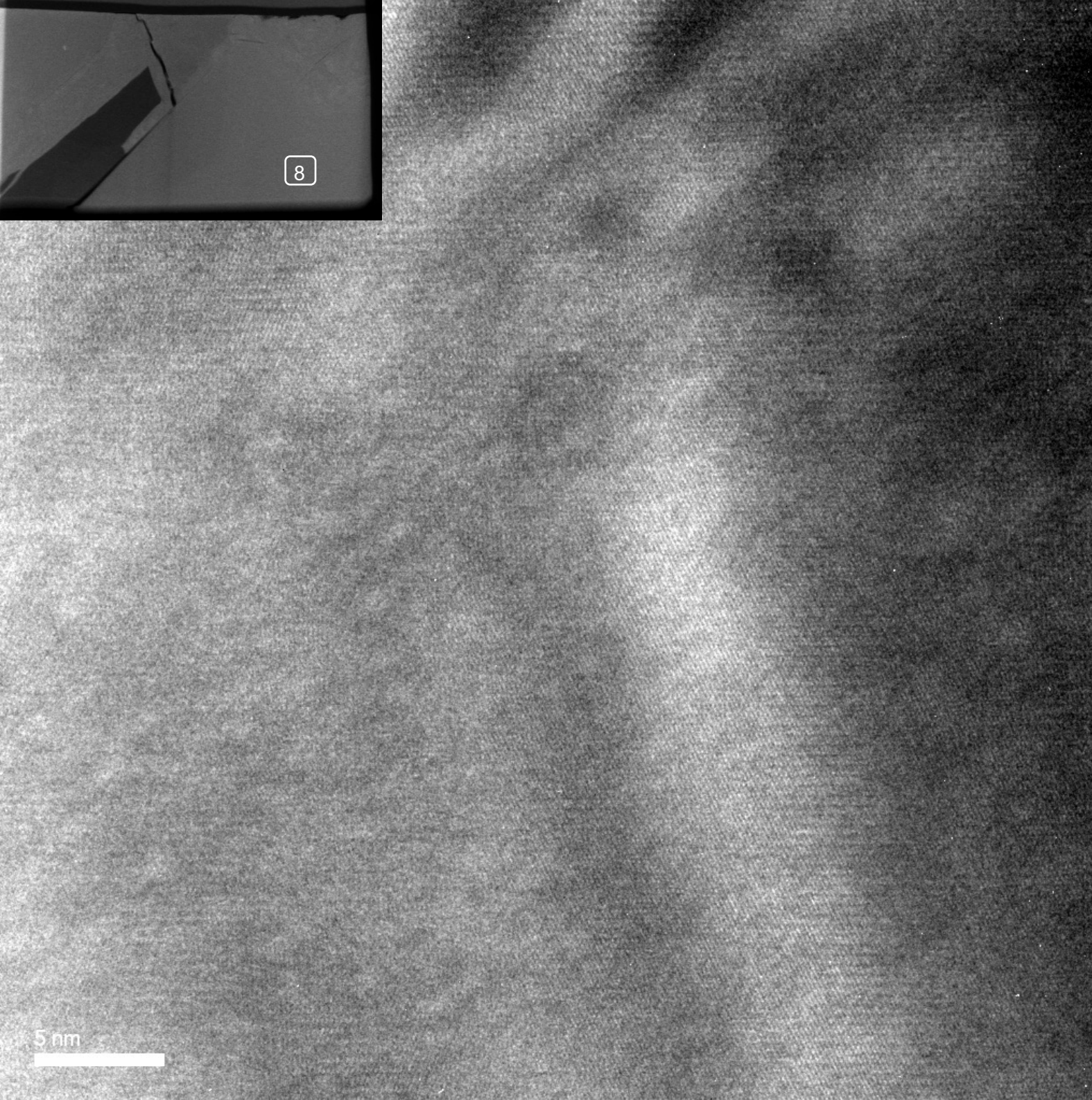
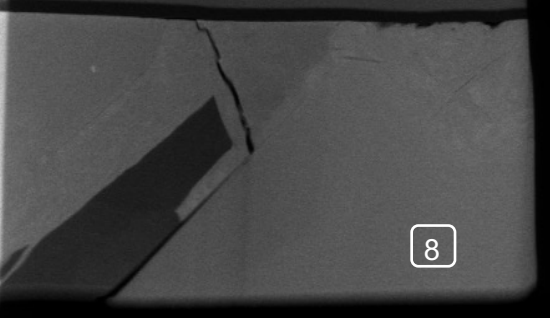
Pyrite ( $\text{FeS}_2$ ) (cubic; P3a)

Marcasite ( $\text{FeS}_2$ ) (orthorhombic; Pnnm)

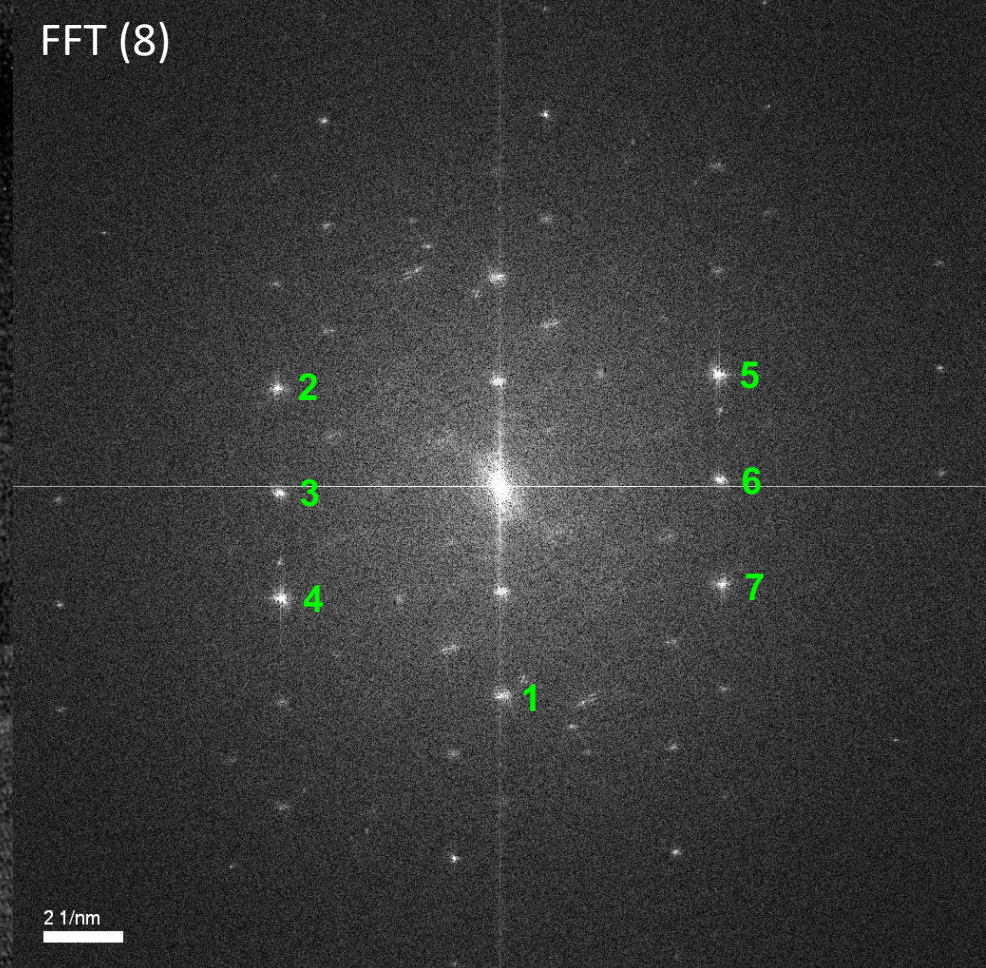
Pyrrhotite ( $\text{FeS}$ ) (monoclinic; C2/c politype 4c & rhombic; Cmca)

Spot#	d-Spacing (nm)	(hkl)	Ideal d-Spacing (Å)
1	0.222326	$(112)_{\text{Py}}/(211)_{\text{py}}$	2.2111
2	0.222821	$(112)_{\text{Py}}/(211)_{\text{py}}$	2.2111
3	0.165979	$(222)_{\text{py}}/(130)_{\text{mc}}$	1.6526
4	0.166465	$(222)_{\text{py}}/(130)_{\text{mc}}$	1.6526
5	0.572329	$\{101\}_{\text{py}}/(-111)_{\text{po}}$	5.7249/ 5.7478-5.7606
6	0.576488	$\{101\}_{\text{py}}/(-111)_{\text{po}}$	5.7249/ 5.7478-5.7606
7	0.30695	$(028)_{\text{Po(romb)}}$	3.0698
8	0.30743	$(028)_{\text{Po(romb)}}$	3.0698



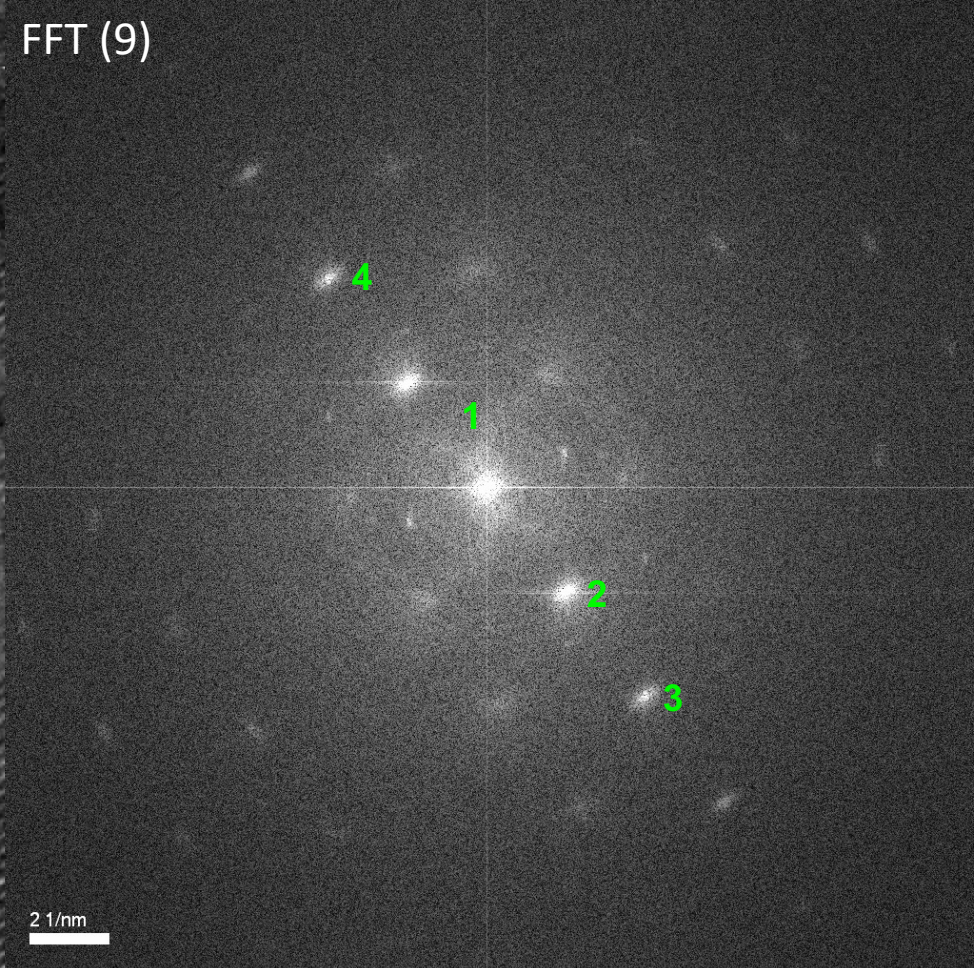
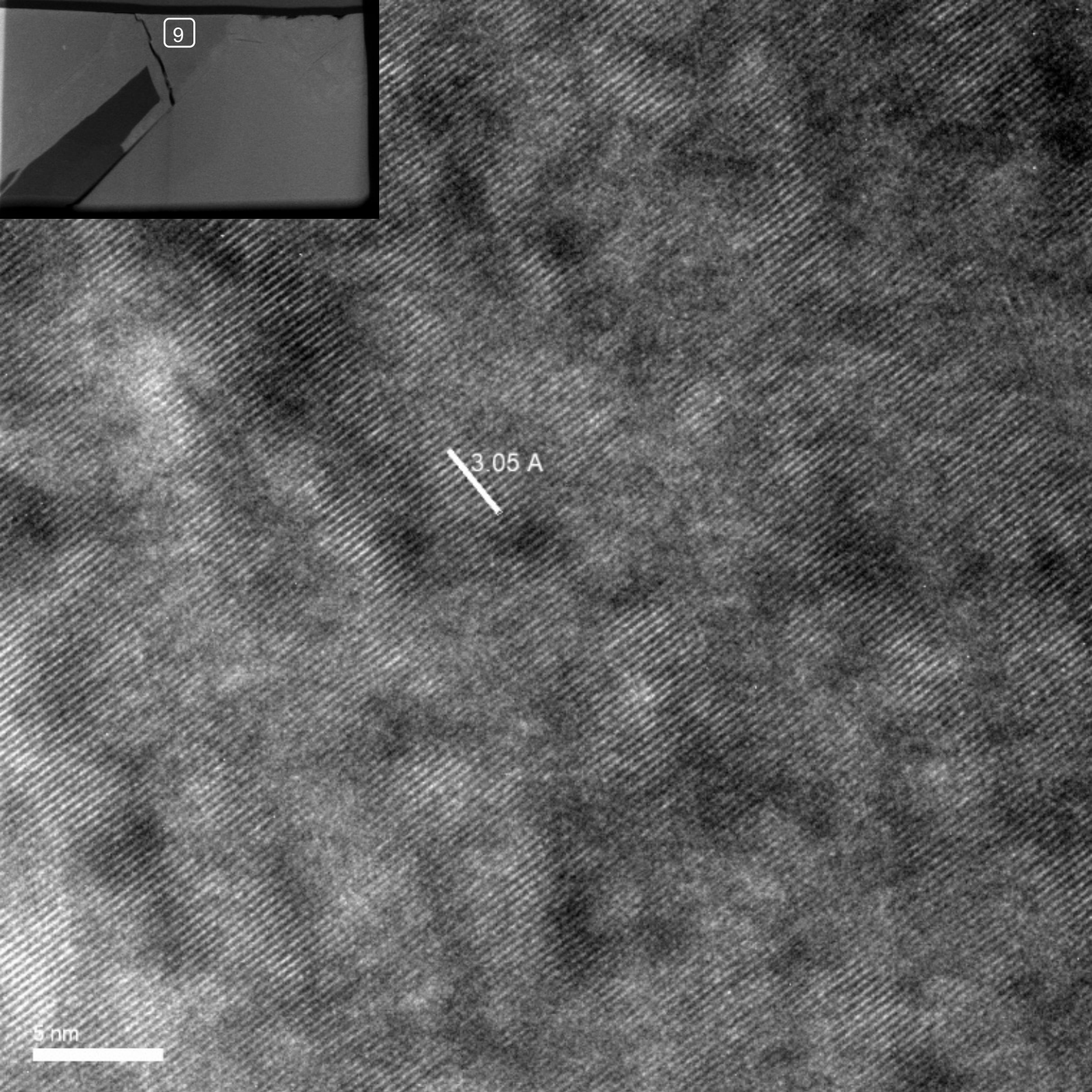
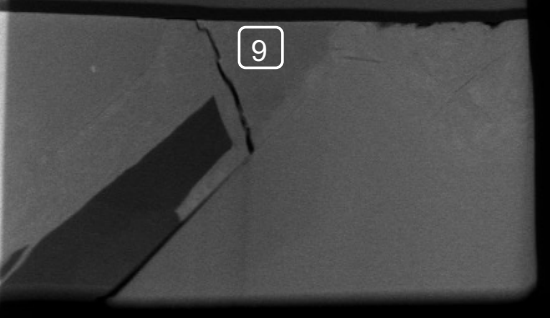


FFT (8)

Pyrite ( $\text{FeS}_2$ ) (cubic; P3a)Marcasite ( $\text{FeS}_2$ ) (orthorrombic; Pnnm)Pyrrhotite ( $\text{FeS}$ ) (monoclinic; C2/c politype 4c)

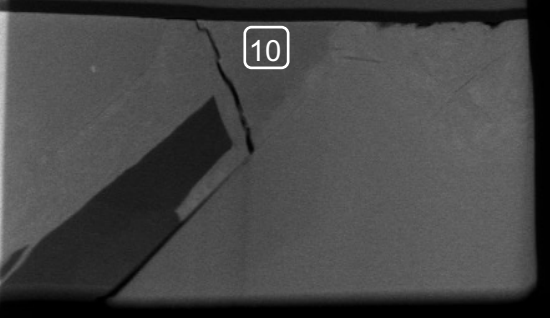
Spot#	d-Spacing (nm)	(hkl)	Ideal d-Spacing (Å)
1	0.191392	$(221)_{\text{py}}/(121)_{\text{Mc}}$	1.9083/1.9113
2	0.166191	$(222)_{\text{py}}/(130)_{\text{Mc}}$	1.6526/1.6749
3	0.182345	$(331)_{\text{po(mon)}}$	1.8186
4	0.16322	$(311)_{\text{py}}$	1.6330
5	0.163644	$(311)_{\text{py}}$	1.6330
6	0.182333	$(331)_{\text{po(mon)}}$	1.8186
7	0.165893	$(222)_{\text{py}}/(130)_{\text{Mc}}$	1.6526/1.6749





Chalcopyrite (tetragonal; $I\bar{4}2d$ )				
Spot#	d-Spacing (nm)	(hkl)	Ideal d-Spacing (Å)	
1	0.30841	(112)	3.0387	
2	0.304984	(112)	3.0387	
3	0.152778	(224)	1.519	
4	0.153576	(224)	1.519	





3.05 Å

5 nm

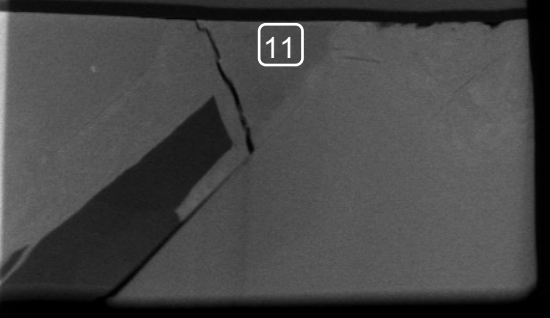
FFT (10)

2 1/nm

Chalcopyrite (tetragonal; I42d)

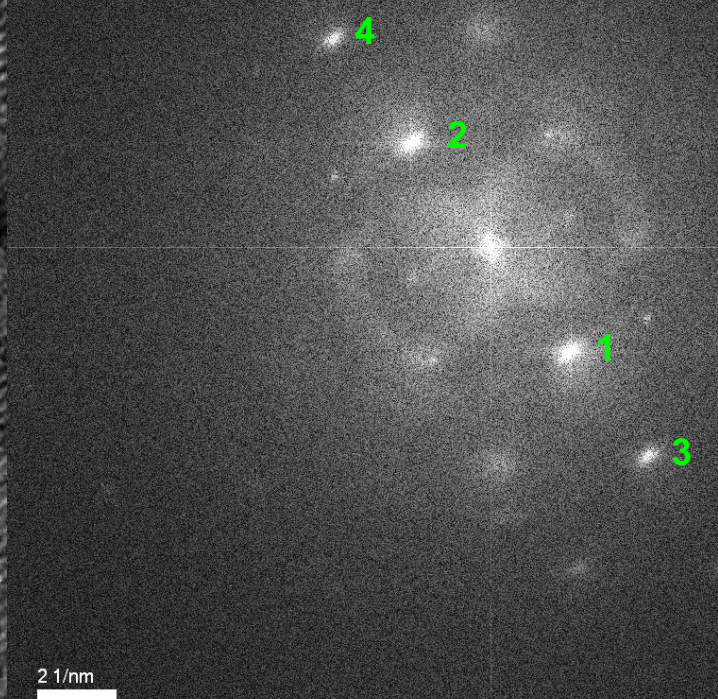
Spot#	d-Spacing (nm)	(hkl)	Ideal d-Spacing (Å)
1	0.305258	(112)	3.0387
2	0.305802	(112)	3.0387
3	0.154459	(224)	1.519
4	0.153537	(224)	1.519





3.05 Å - 3.06 Å

FFT (11)

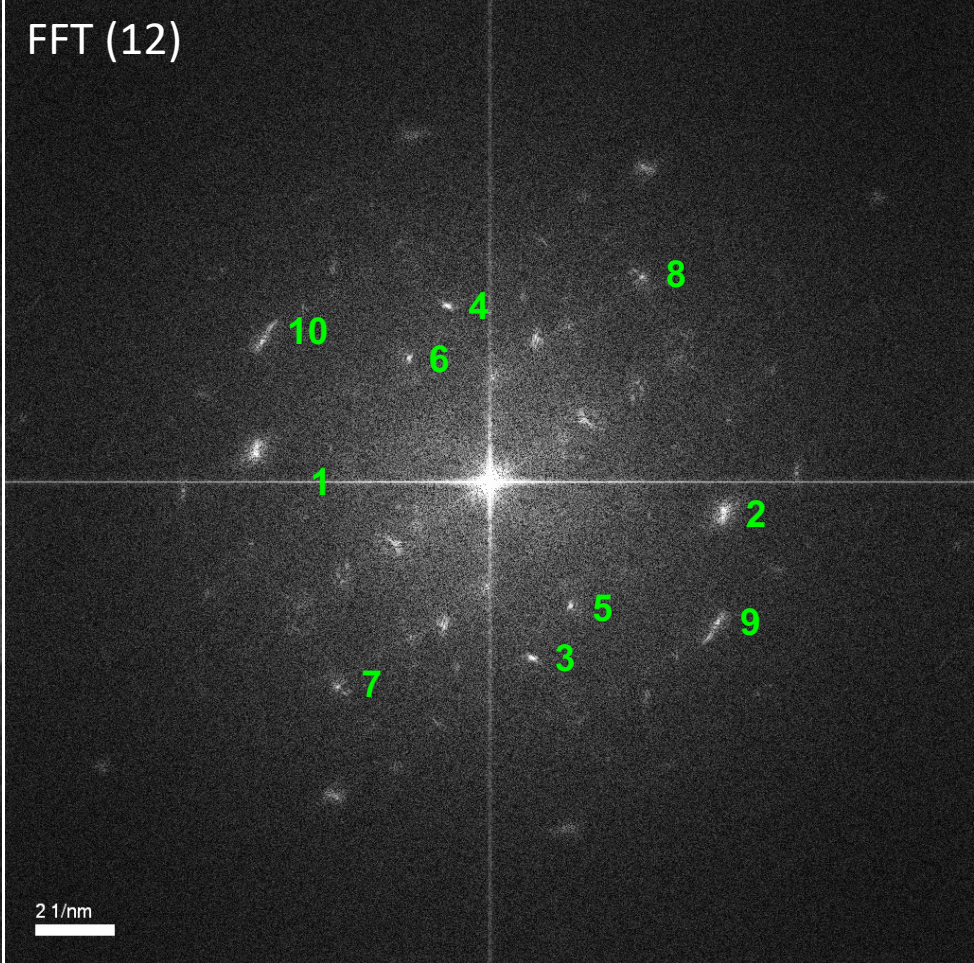
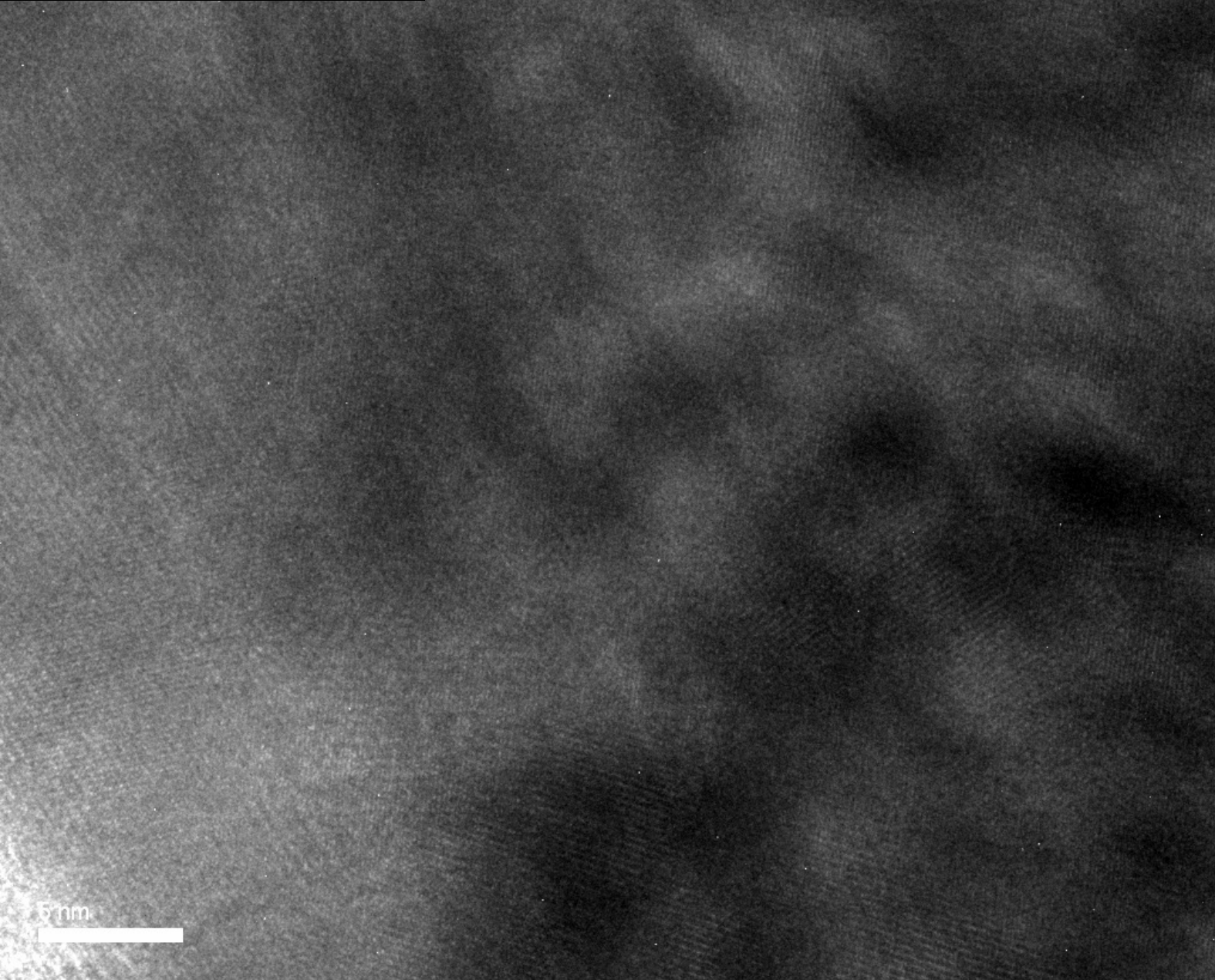
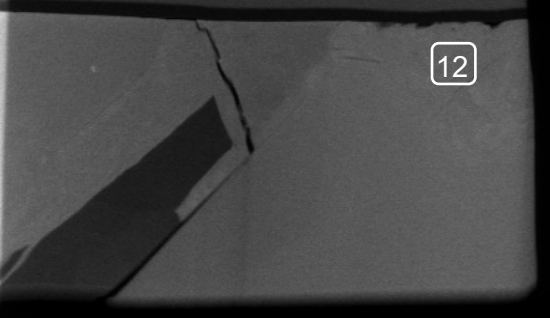


2 1/nm

5 nm

Chalcopyrite (tetragonal; $I4_2d$ )				
Spot#	d-Spacing (nm)	(hkl)	Ideal d-Spacing (Å)	
1	0.303757	(112)	3.0387	
2	0.306955	(112)	3.0387	
3	0.153533	(224)	1.519	
4	0.154323	(224)	1.519	





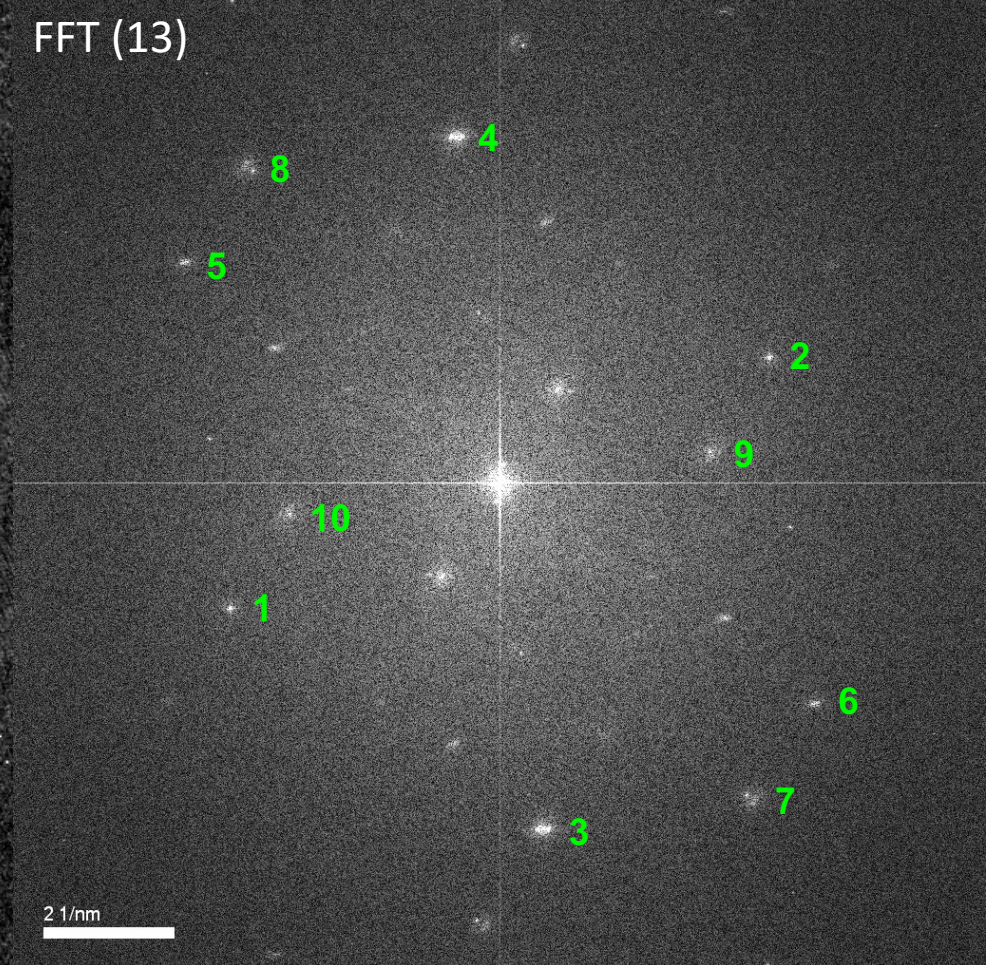
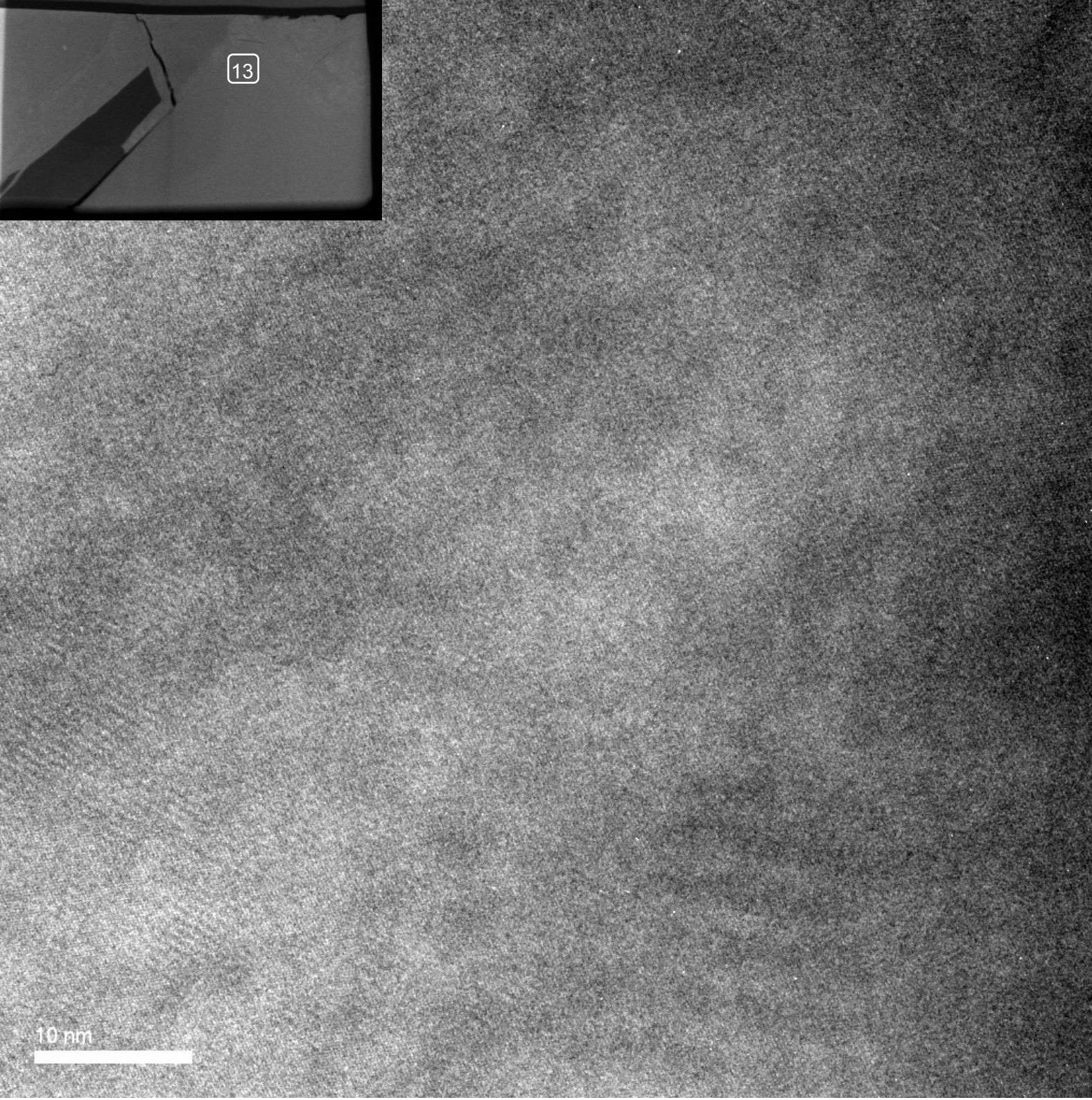
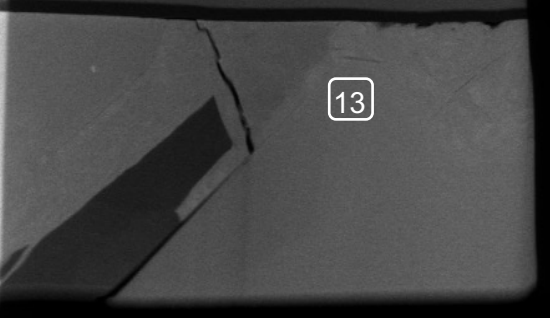
Pyrite ( $\text{FeS}_2$ ) (cubic; P3a)

Marcasite ( $\text{FeS}_2$ ) (orthorrombic; Pnnm)

Goethite ( $\text{FeOOH}$ ) (orthorrombic; Pbnm)

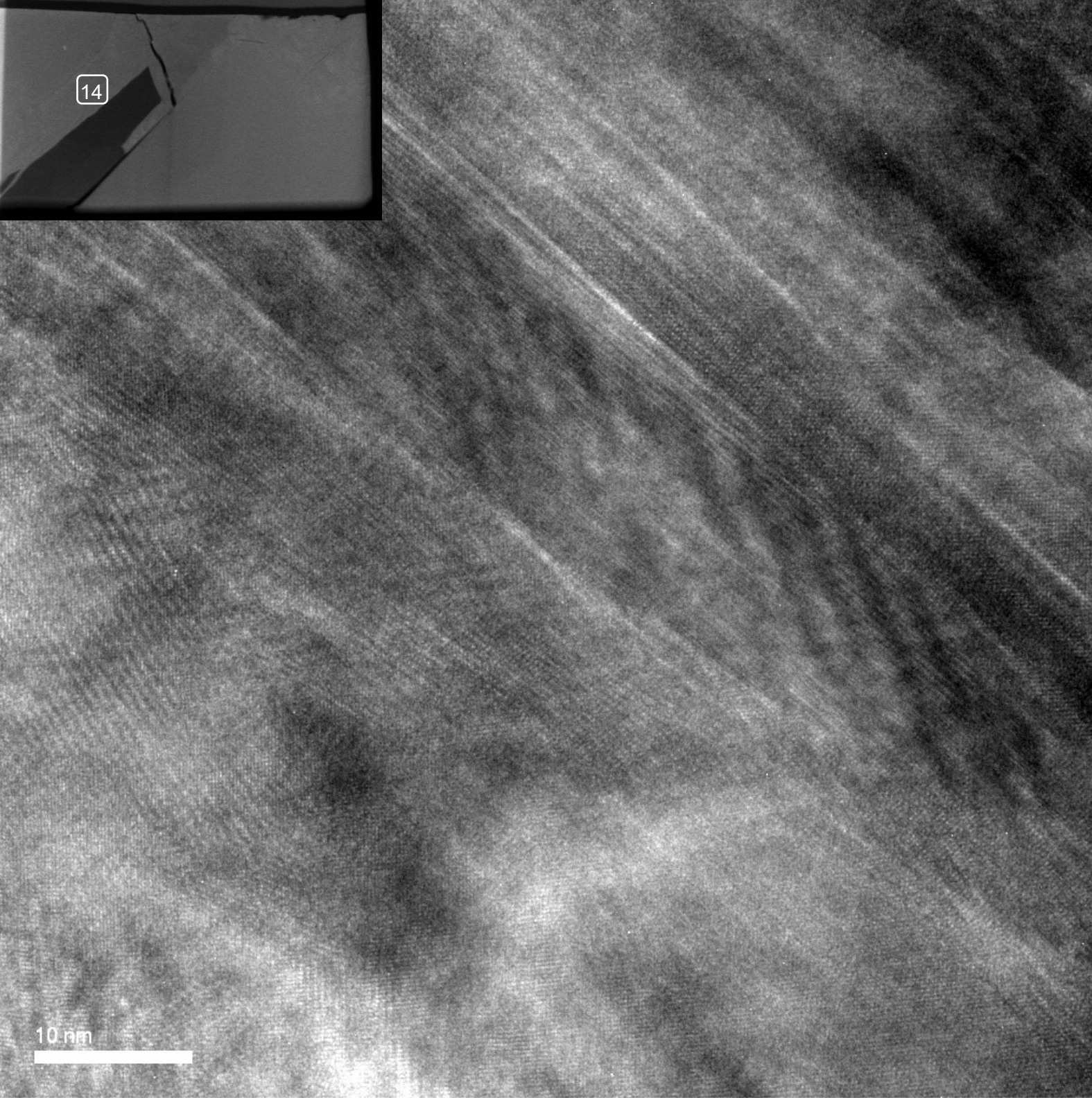
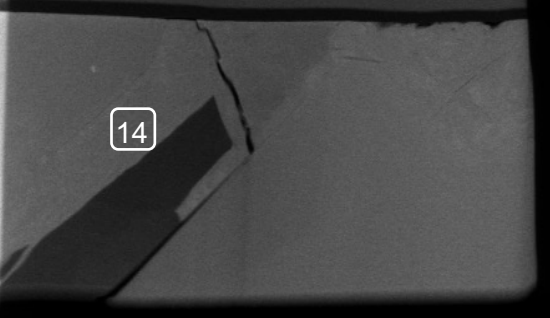
Spot#	d-Spacing (nm)	(hkl)	Ideal d-Spacing (Å)
1	0.170873	(212) <sub>Ght</sub>	1.7111
2	0.170595	(212) <sub>Ght</sub>	1.7111
3	0.219867	(112) <sub>Py</sub> /(211) <sub>py</sub>	2.2111
4	0.221872	(112) <sub>Py</sub> /(211) <sub>py</sub>	2.2111
5	0.2686	(130) <sub>Ght</sub>	2.7024
6	0.272061	(130) <sub>Ght</sub>	2.7024
7	0.156059	(222) <sub>py</sub>	1.5635
8	0.157067	(222) <sub>py</sub>	1.5635
9	0.149724	(302) <sub>py</sub> /(131) <sub>mc.</sub>	1.5021 /1.5033
10	0.150079	(302) <sub>py</sub> /(131) <sub>mc.</sub>	1.5021 /1.5033



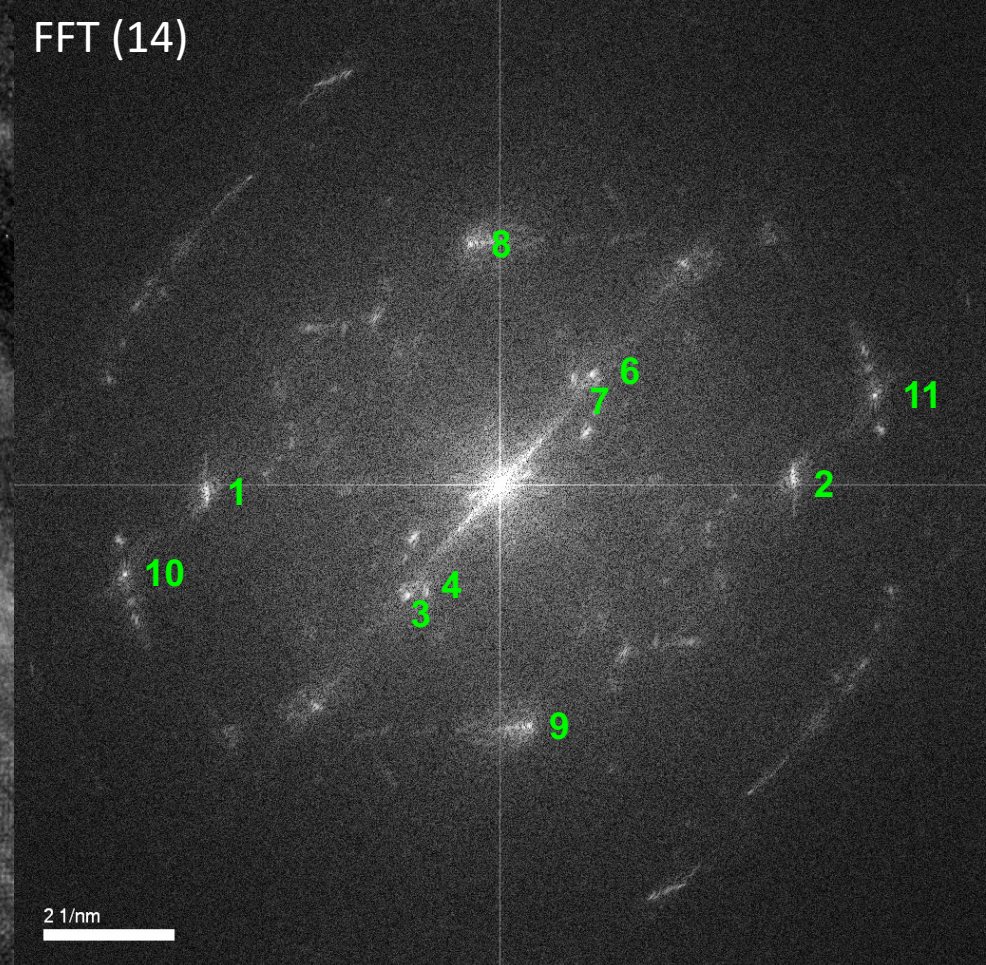


Pyrite (FeS <sub>2</sub> ) (cubic; P3a)			
Marcasite (FeS <sub>2</sub> ) (orthorrombic; Pnnm)			
Spot#	d-Spacing (nm)	(hkl)	Ideal d-Spacing (Å)
1	0.222183	(112) <sub>Py</sub> /(211) <sub>Py</sub>	2.2113
2	0.222745	(112) <sub>Py</sub> /(211) <sub>Py</sub>	2.2113
3	0.189415	(221) <sub>Py</sub>	1.9083
4	0.190405	(221) <sub>Py</sub>	1.9083
5	0.172968	(311) <sub>Py</sub>	1.7261
6	0.172563	(311) <sub>Py</sub>	1.7261
7	0.16583	(222) <sub>py</sub> /(130) <sub>Mc</sub>	1.6526/1.6749
8	0.166377	(222) <sub>py</sub> /(130) <sub>Mc</sub>	1.6526/1.6749
9	0.310671	(310) <sub>Po(mon)</sub>	3.1093-3.1264
10	0.310298	(310) <sub>Po(mon)</sub>	3.1093-3.1264





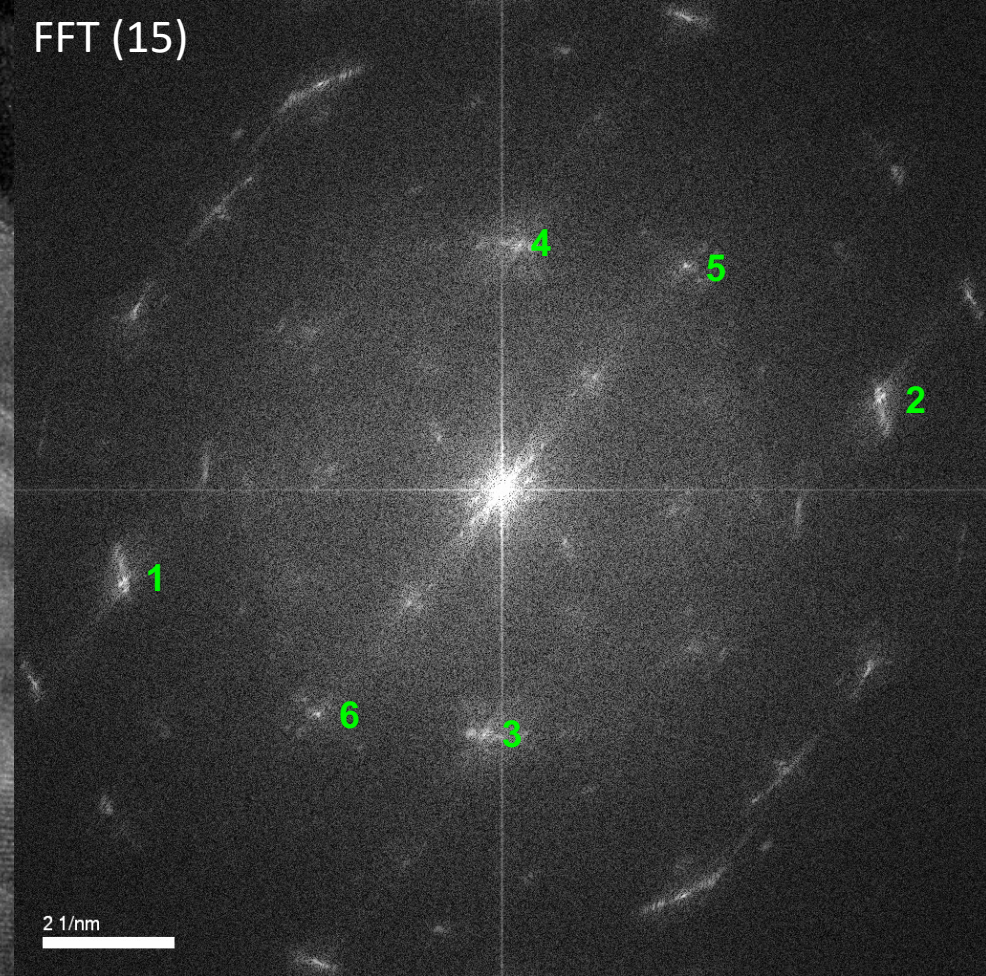
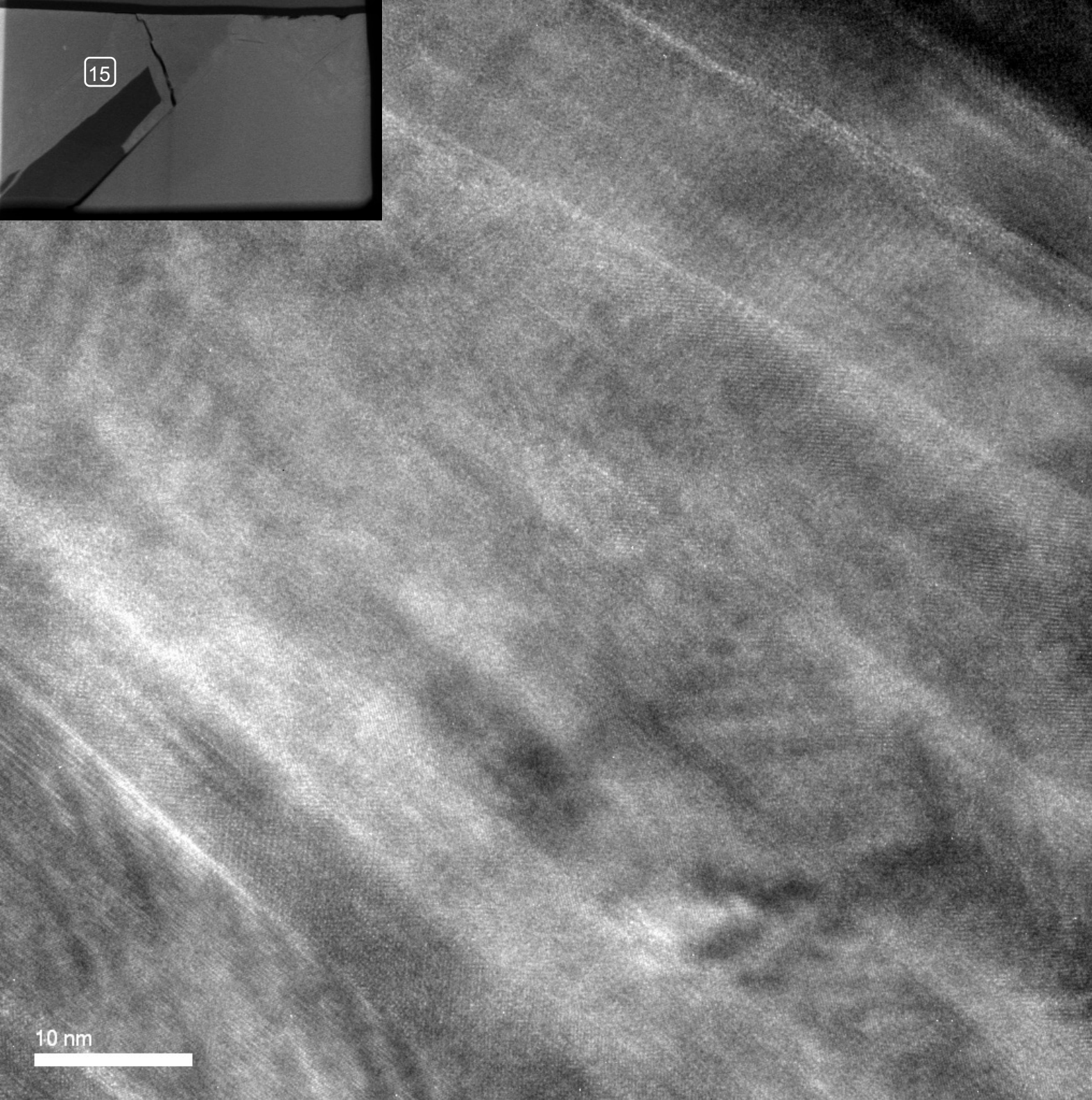
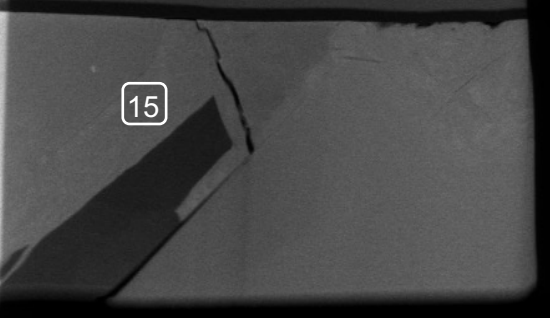
FFT (14)



Goethite (FeOOH) (orthorrombic; Pbnm)

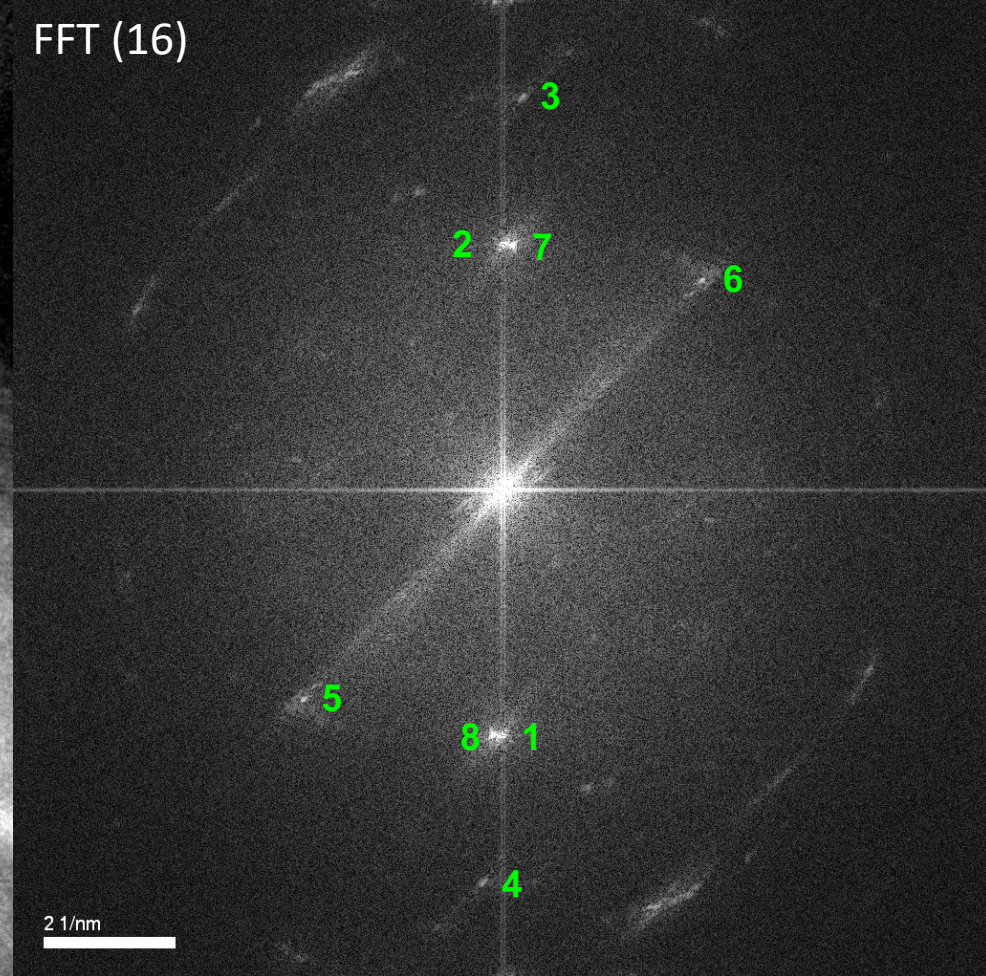
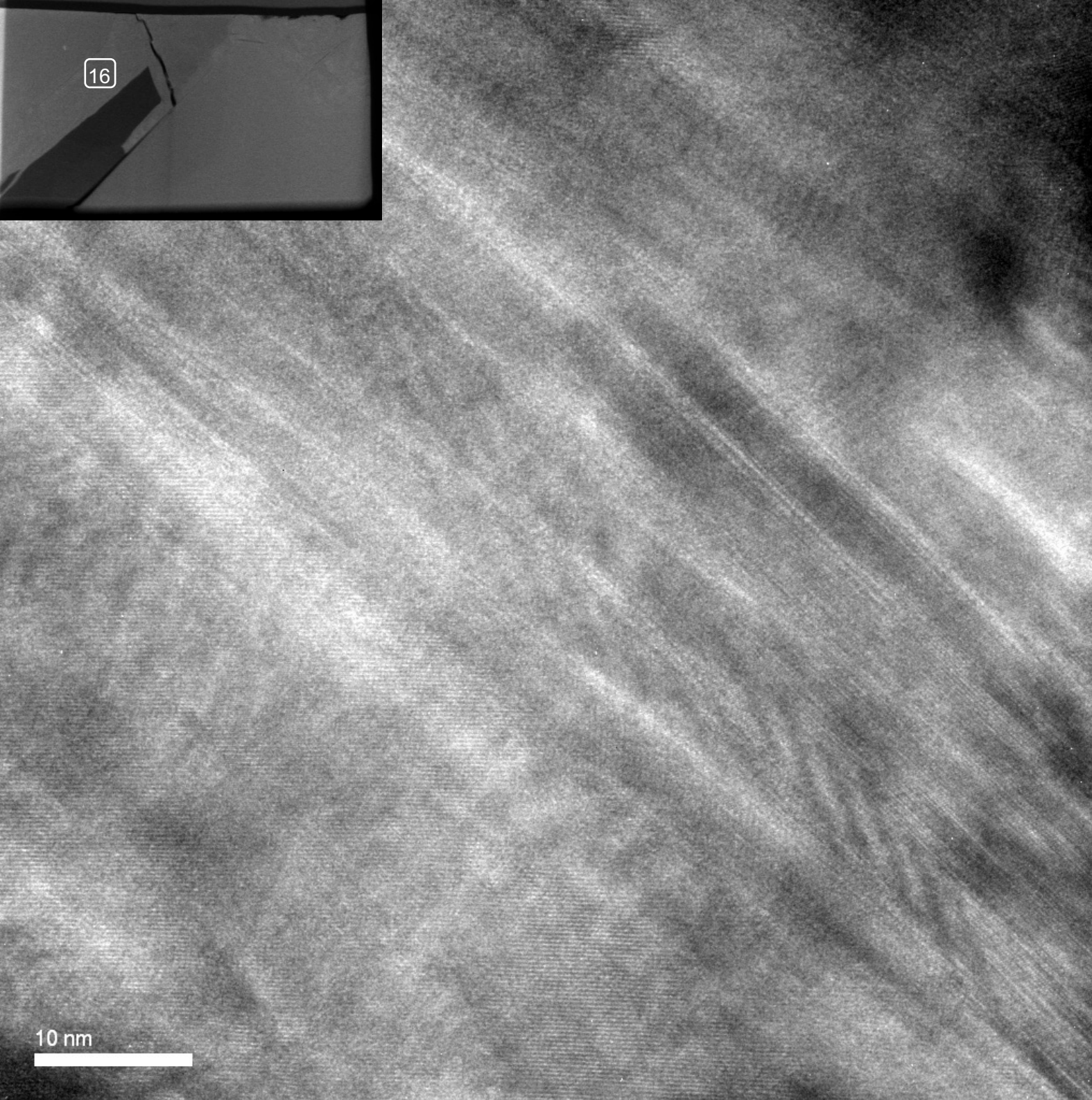
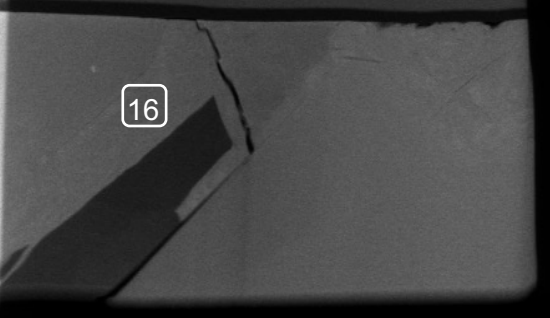
Spot#	d-Spacing (nm)	(hkl)	Ideal d-Spacing (Å)
1	0.225386	(210)	2.2529
2	0.224706	(210)	2.2529
3	0.453354	{101}	4.5800
4	0.503457	{101}	4.5800
6	0.458735	{101}	4.5800
7	0.509174	{101}	4.5800
8	0.272951	(130)	2.7024
9	0.271005	(130)	2.7024
10	0.171888	(212)	1.7111
11	0.171518	(212)	1.7111





Goethite (FeOOH) (orthorrombic; Pbnm)			
Spot#	d-Spacing (nm)	(hkl)	Ideal d-Spacing (Å)
1	0.170351	(212)	1.7111
2	0.169898	(212)	1.7111
3	0.27026	(130)	2.7024
4	0.272051	(130)	2.7024
5	0.230762	(200)	2.2900-2.3125
6	0.229574	(200)	2.2900-2.3125

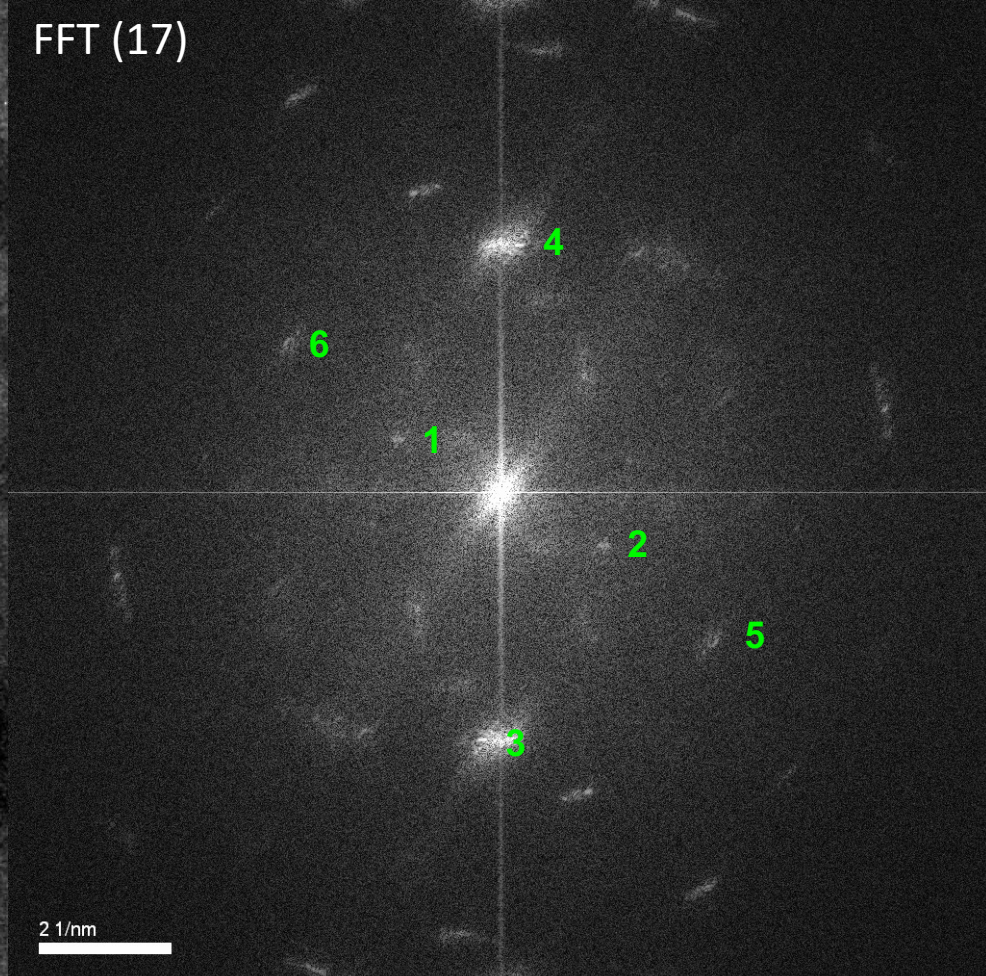
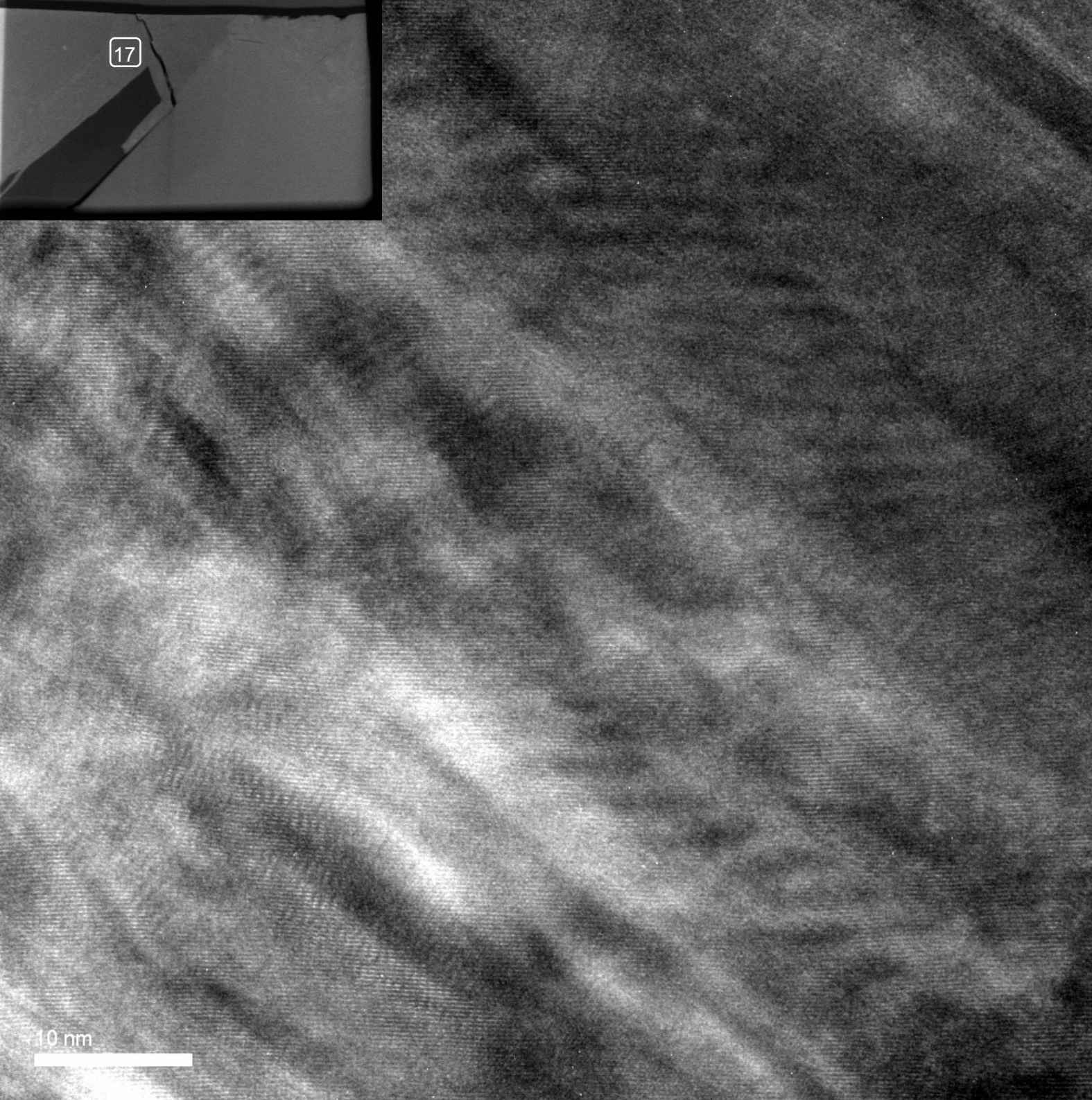
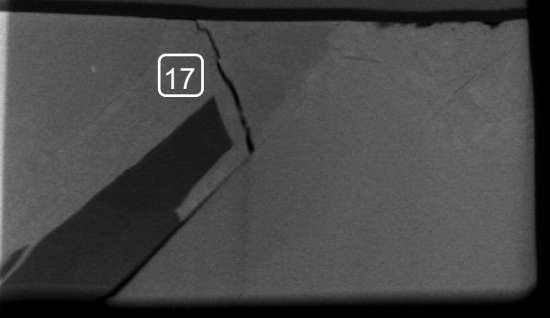




Goethite (FeOOH) (orthorrombic; Pbnm)

Spot#	d-Spacing (nm)	(hkl)	Ideal d-Spacing (Å)
1	0.268943	(130)	2.7024
2	0.271126	(130)	2.7024
3	0.169298	(240)	1.6968
4	0.168359	(240)	1.6968
5	0.229013	(200)	2.2900-2.3125
6	0.230013	(200)	2.2900-2.3125
7	0.272211	(212)	1.7111
8	0.270066	(212)	1.7111

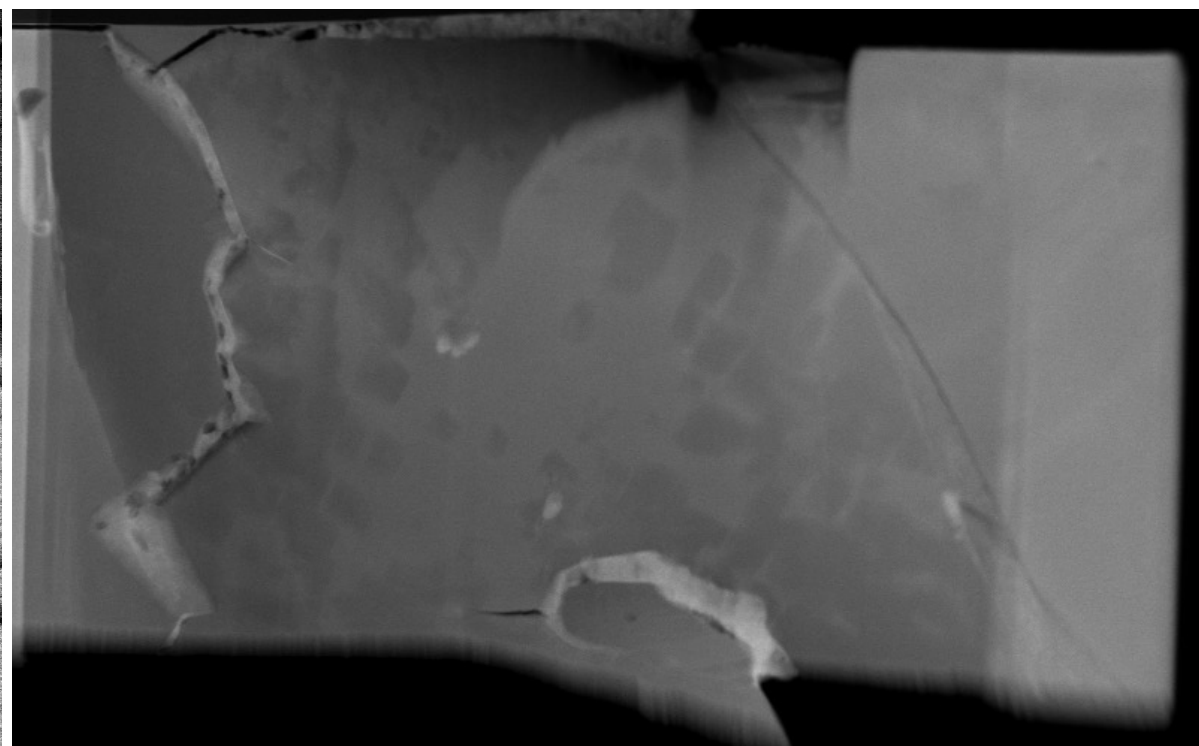
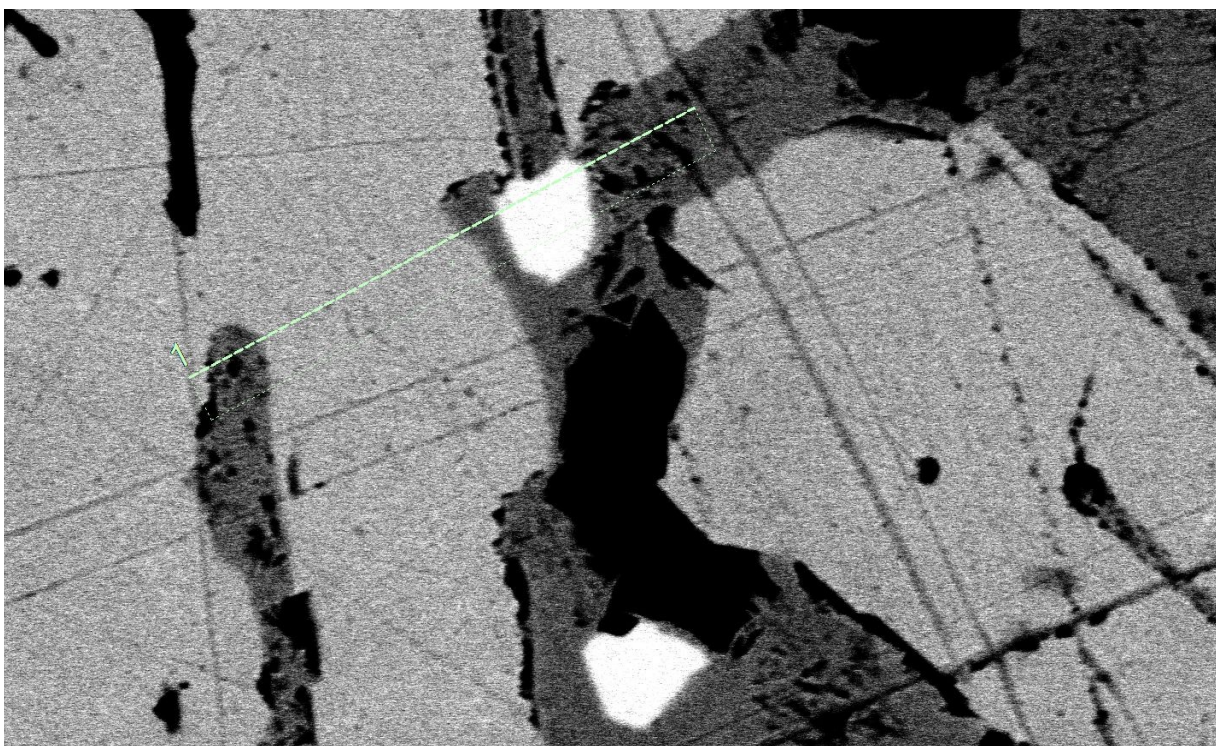




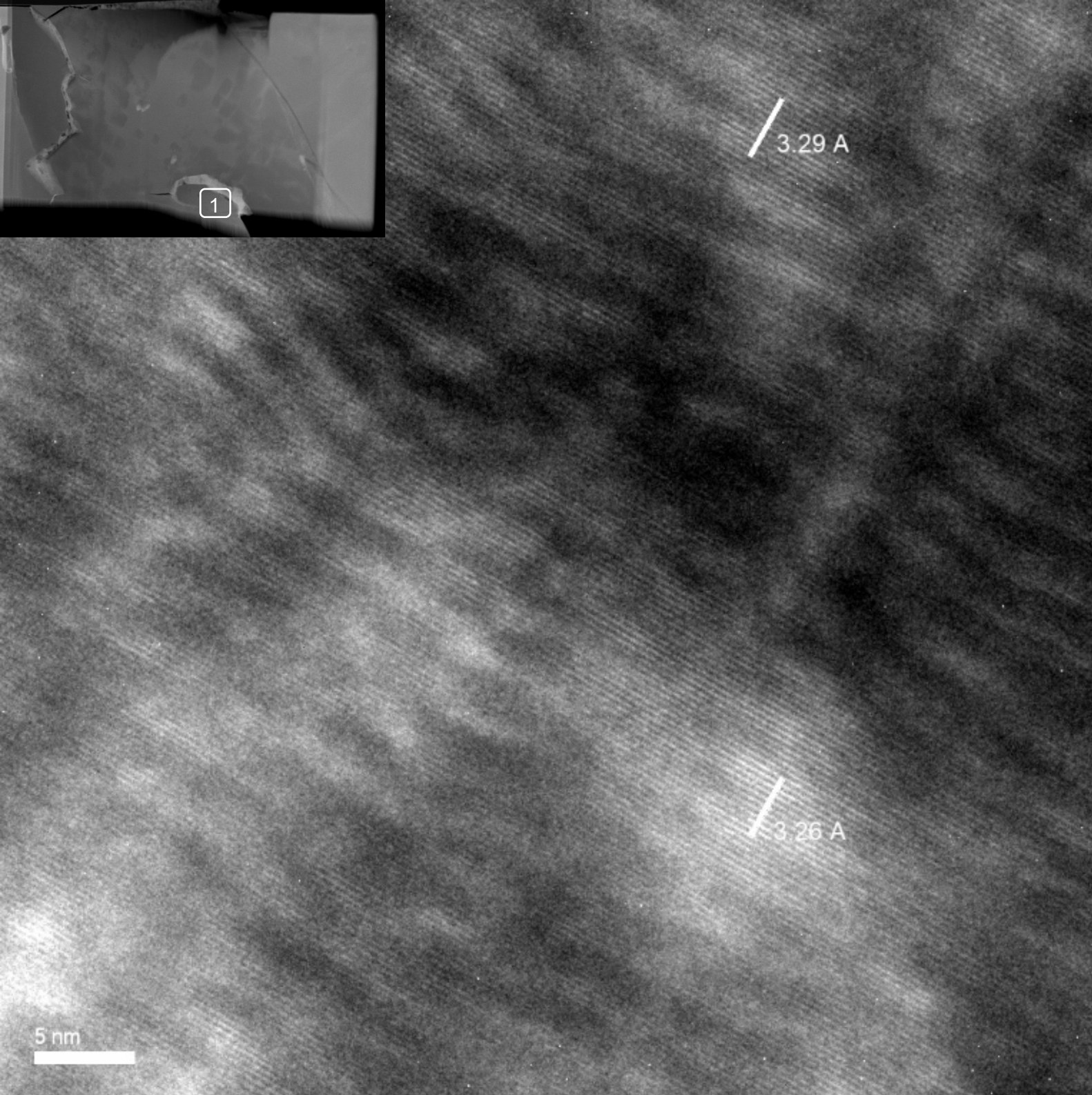
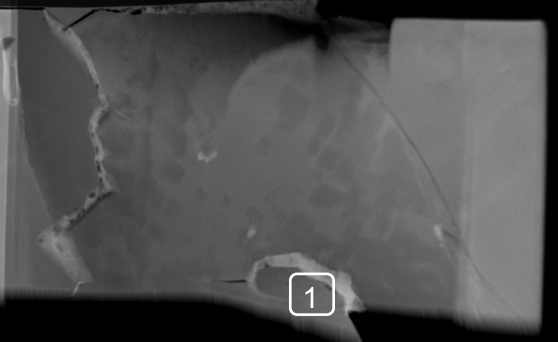
Goethite (FeOOH) (orthorrombic; Pbnm)			
Spot#	d-Spacing (nm)	(hkl)	Ideal d-Spacing (Å)
1	0.577073	$(-111)_{po}$	5.7478-5.760
2	0.572506	$(-111)_{po}$	5.7478-5.760
3	0.269435	(130)	2.7024
4	0.271848	(130)	2.7024
5	0.254559	(101)	2.5386
6	0.256408	(101)	2.5386



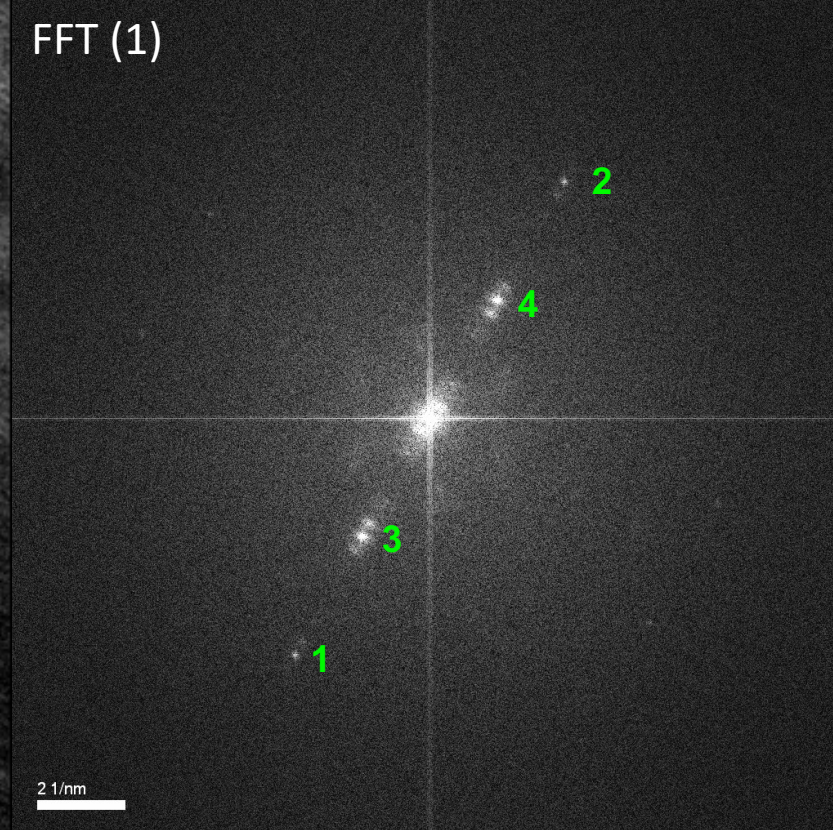
# PEÑA ARPADA (PA-21-3) THIN-FOIL #2







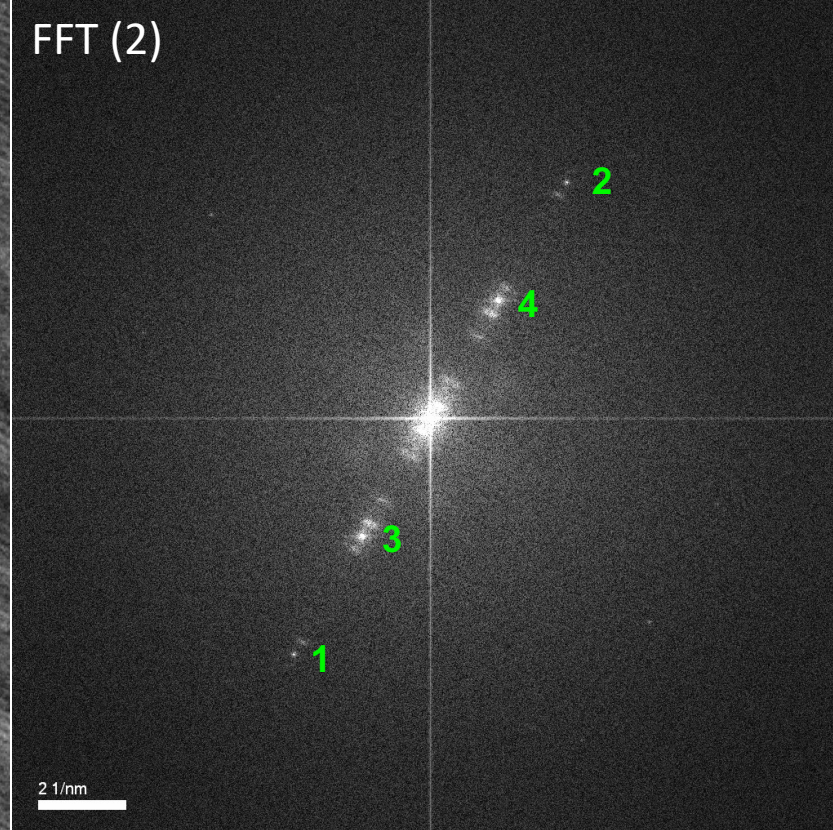
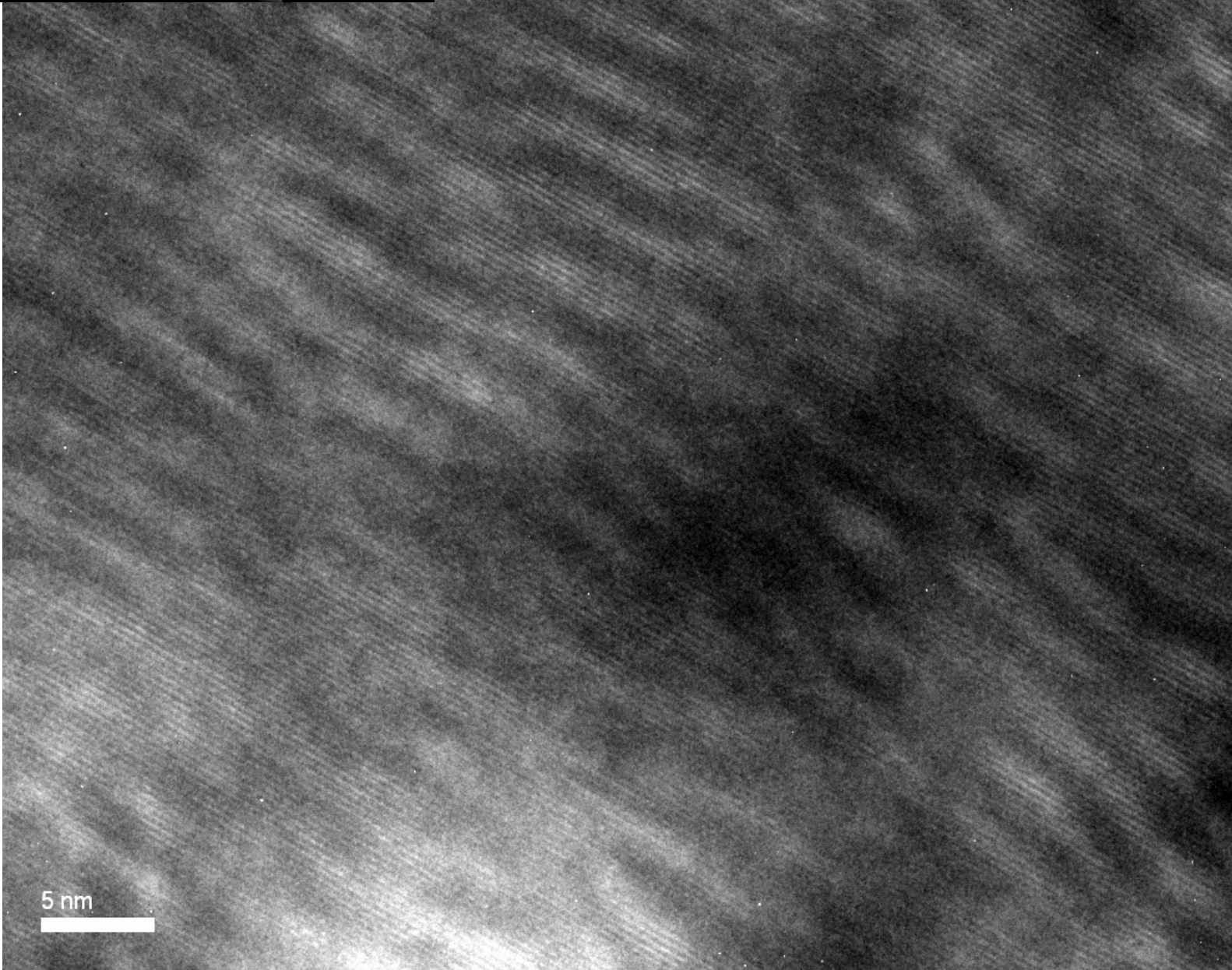
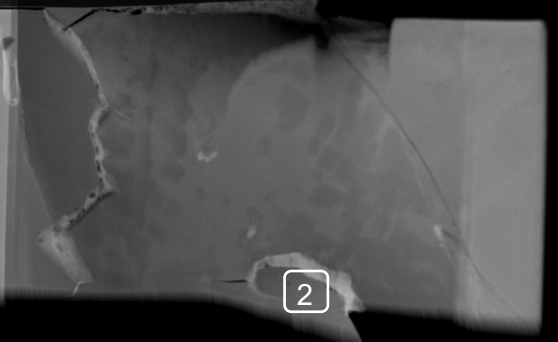
FFT (1)



Vaesite (NiS<sub>2</sub>) (cubic; P3a)

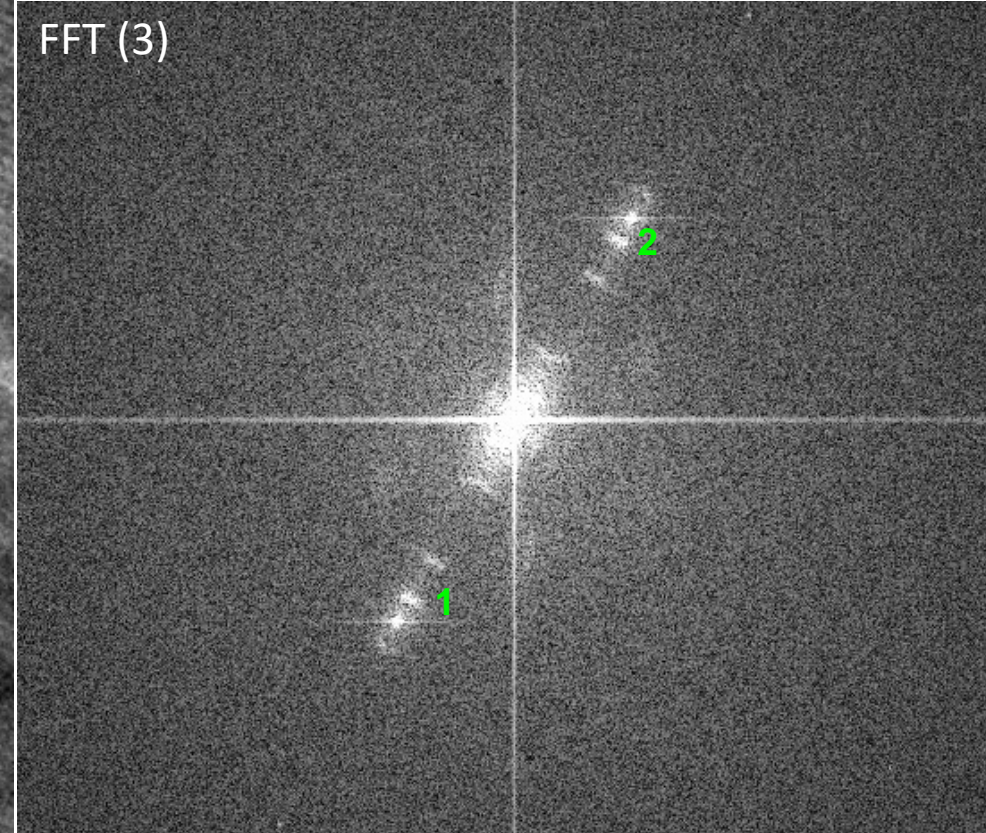
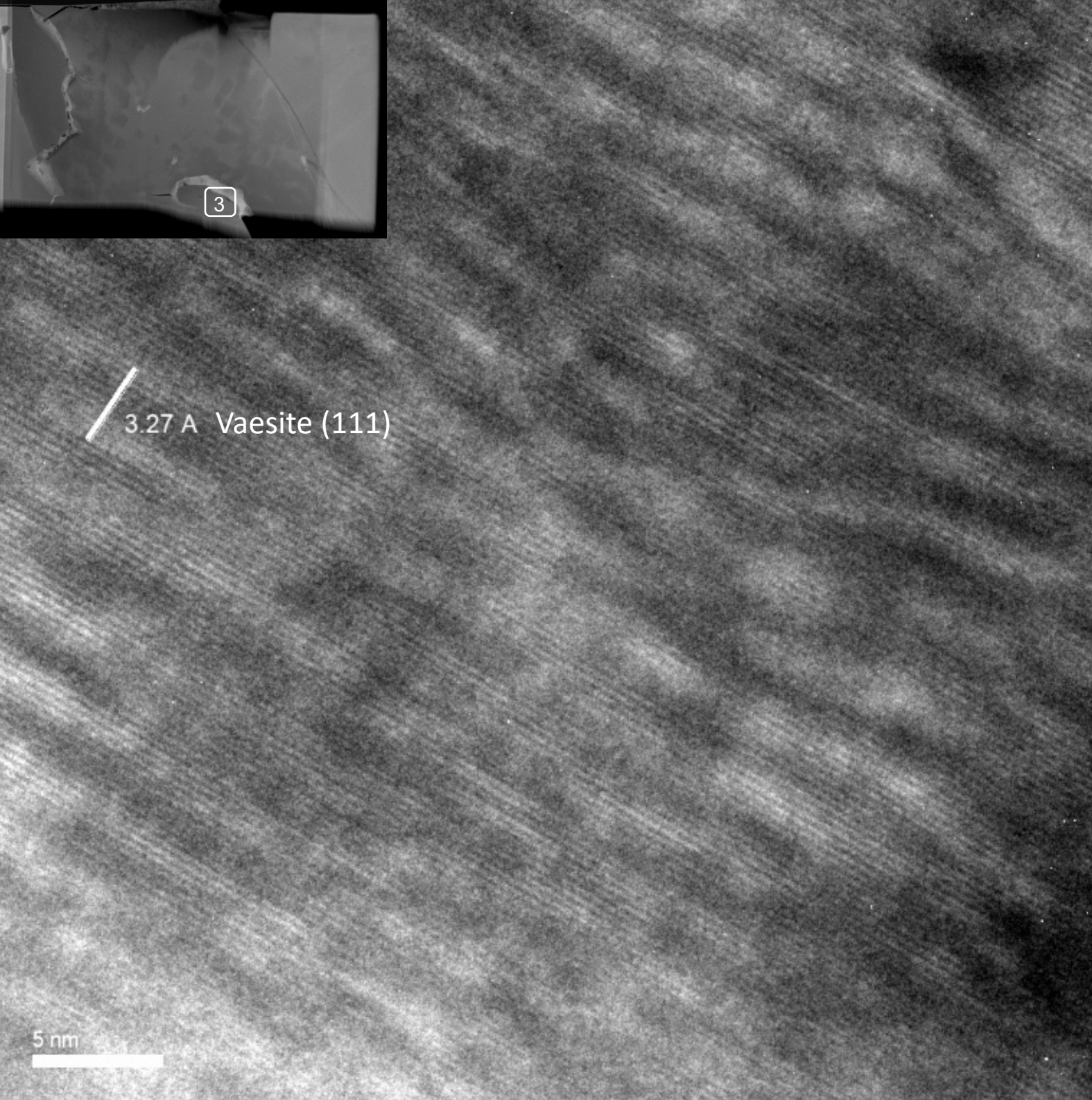
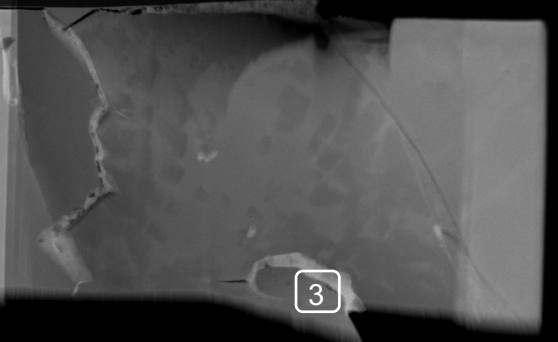
Spot#	d-Spacing (nm)	(hkl)	Ideal d-Spacing (Å)
1	0.163274	(222)	1.6387
2	0.163442	(222)	1.6387
3	0.322598	(111)	3.2773
4	0.326008	(111)	3.2773





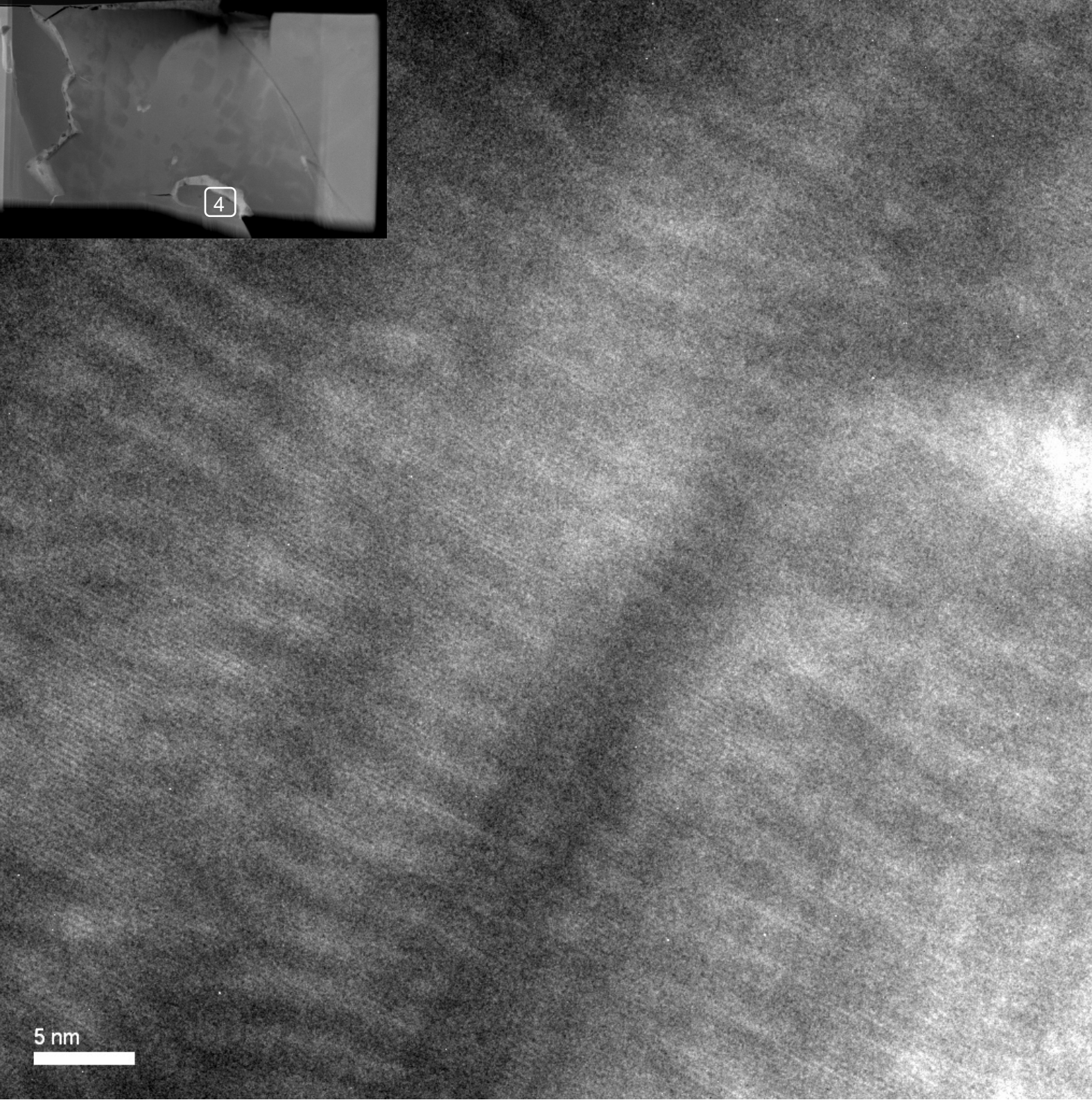
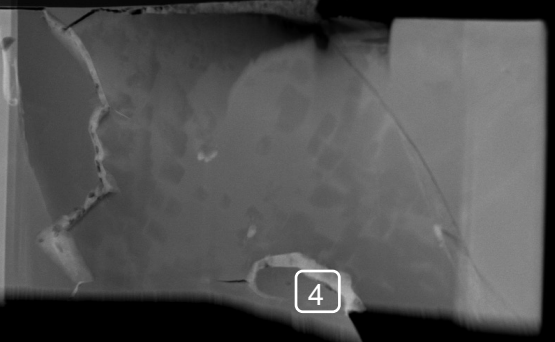
Vaesite (NiS <sub>2</sub> ) (cubic; P3a)			
Spot#	d-Spacing (nm)	(hkl)	Ideal d-Spacing (Å)
1	0.162741	(222)	1.6387
2	0.163621	(222)	1.6387
3	0.325978	(111)	3.2773
4	0.326785	(111)	3.2773





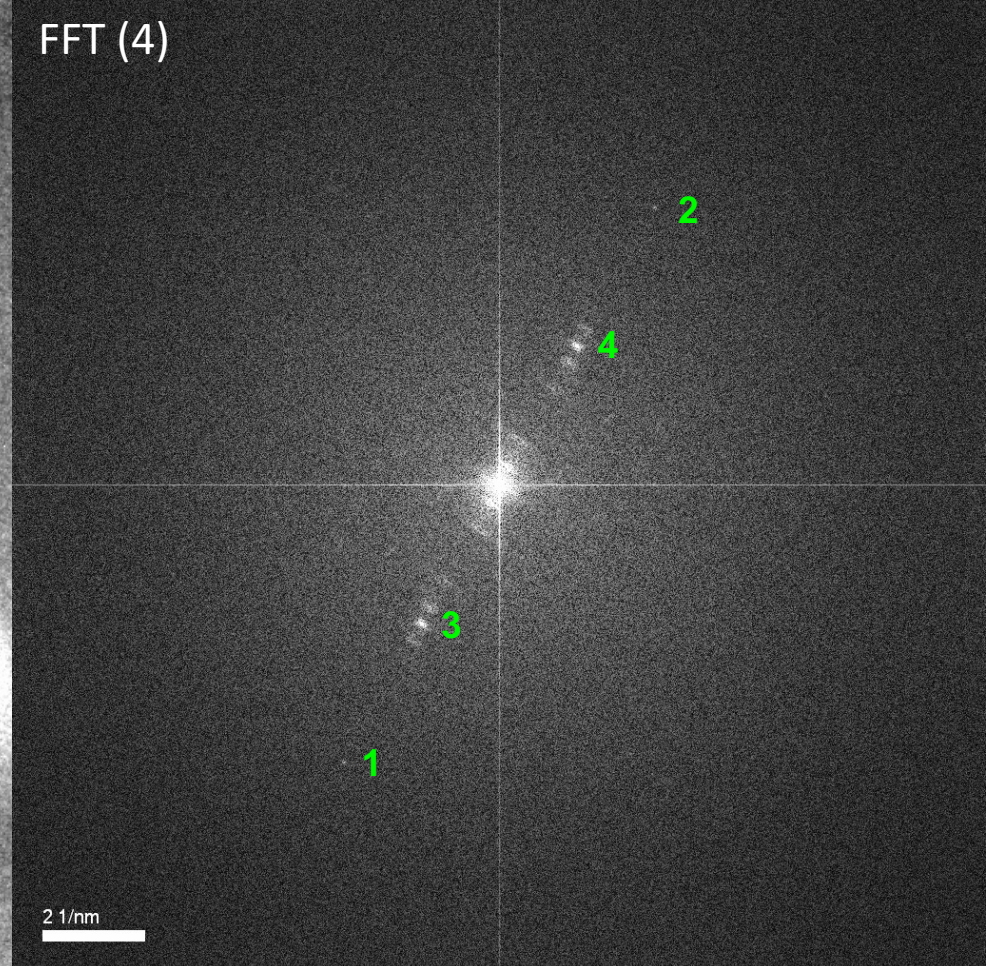
Vaesite (NiS <sub>2</sub> ) (cubic; P3a)			
Spot#	d-Spacing (nm)	(hkl)	Ideal d-Spacing (Å)
1	0.321747	(111)	3.2773
2	0.326074	(111)	3.2773





5 nm

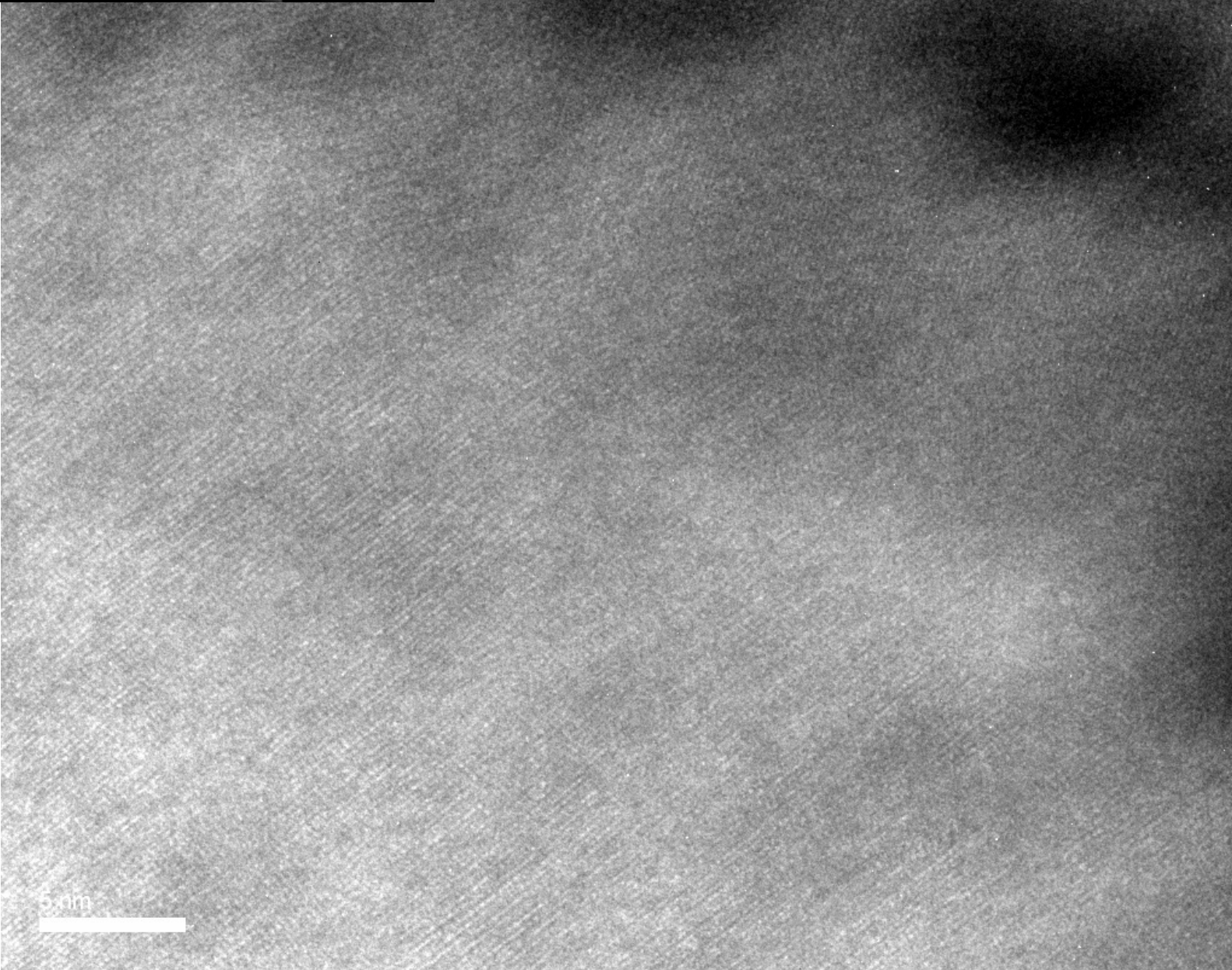
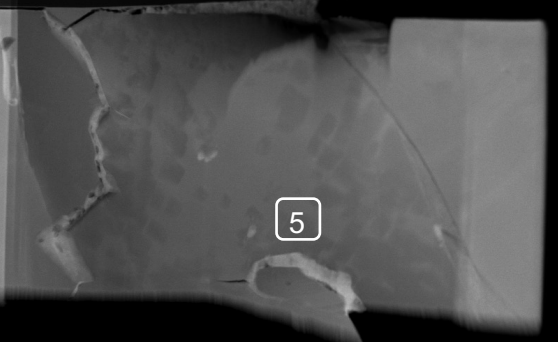
FFT (4)



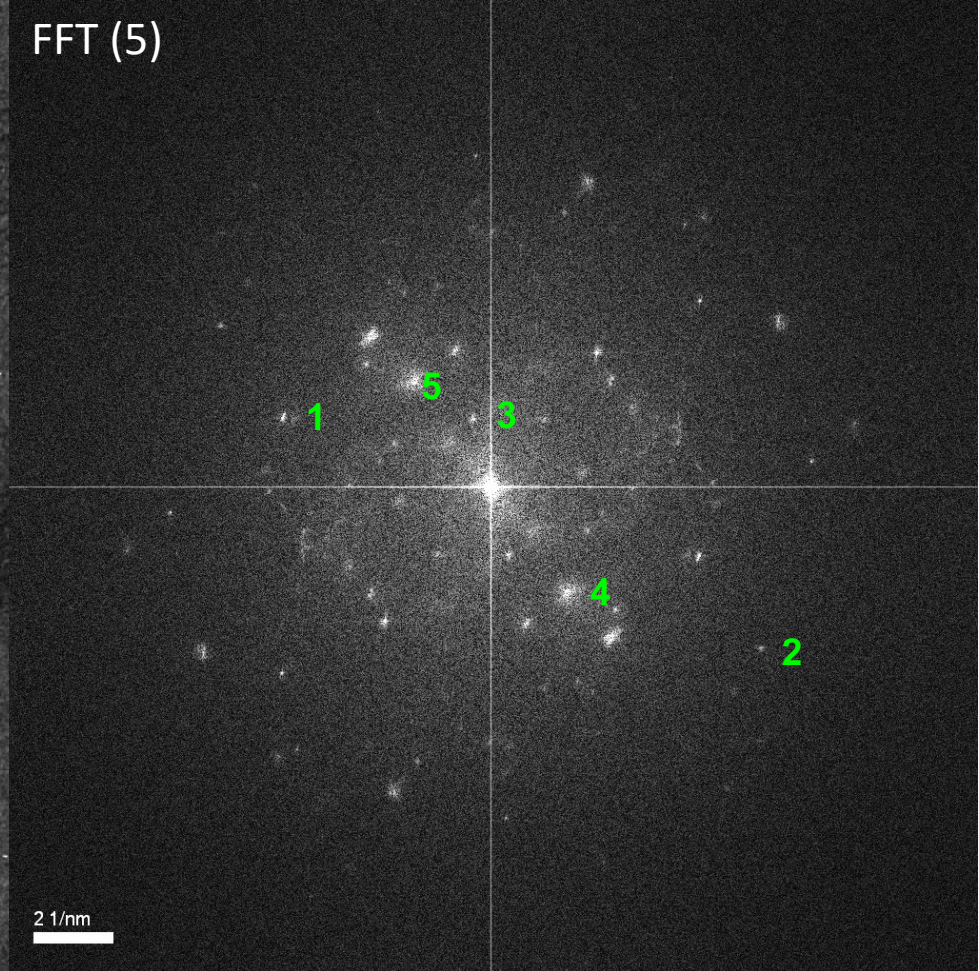
Vaesite (NiS<sub>2</sub>) (cubic; P3a)

Spot#	d-Spacing (nm)	(hkl)	Ideal d-Spacing (Å)
1	0.162476	(222)	1.6387
2	0.163353	(222)	1.6387
3	0.323547	(111)	3.2773
4	0.328269	(111)	3.2773



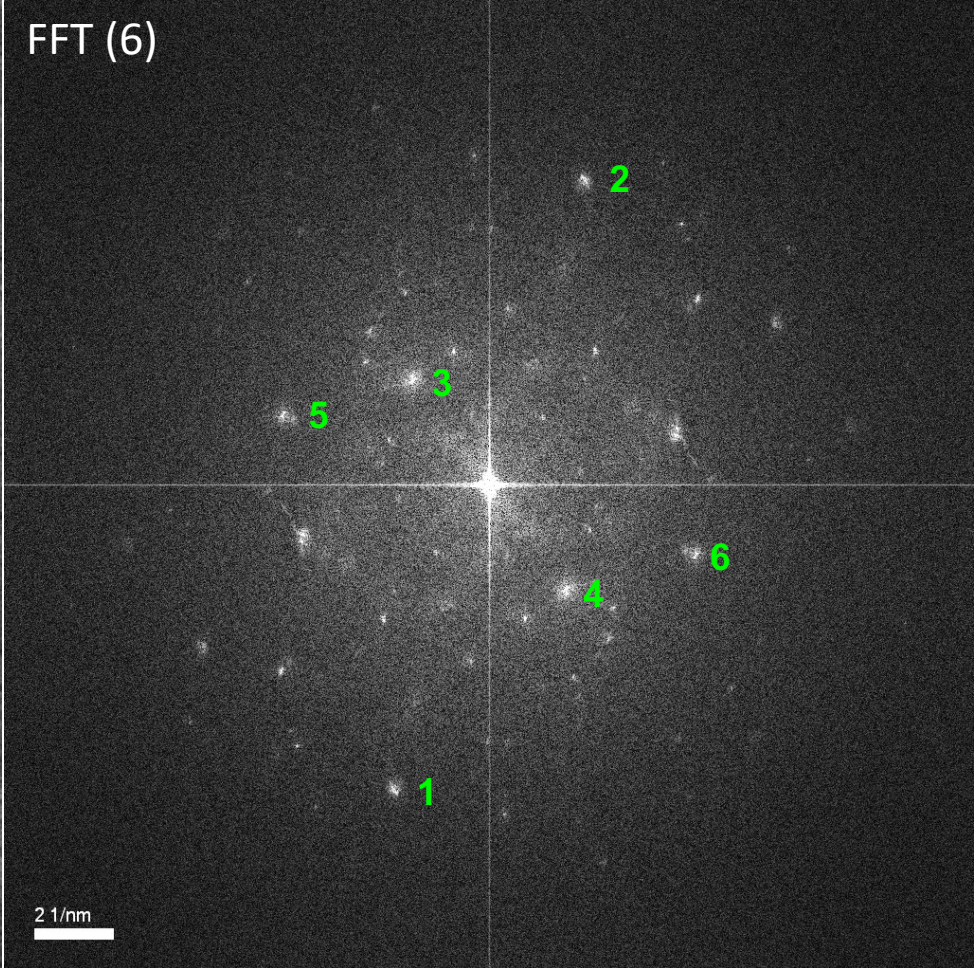
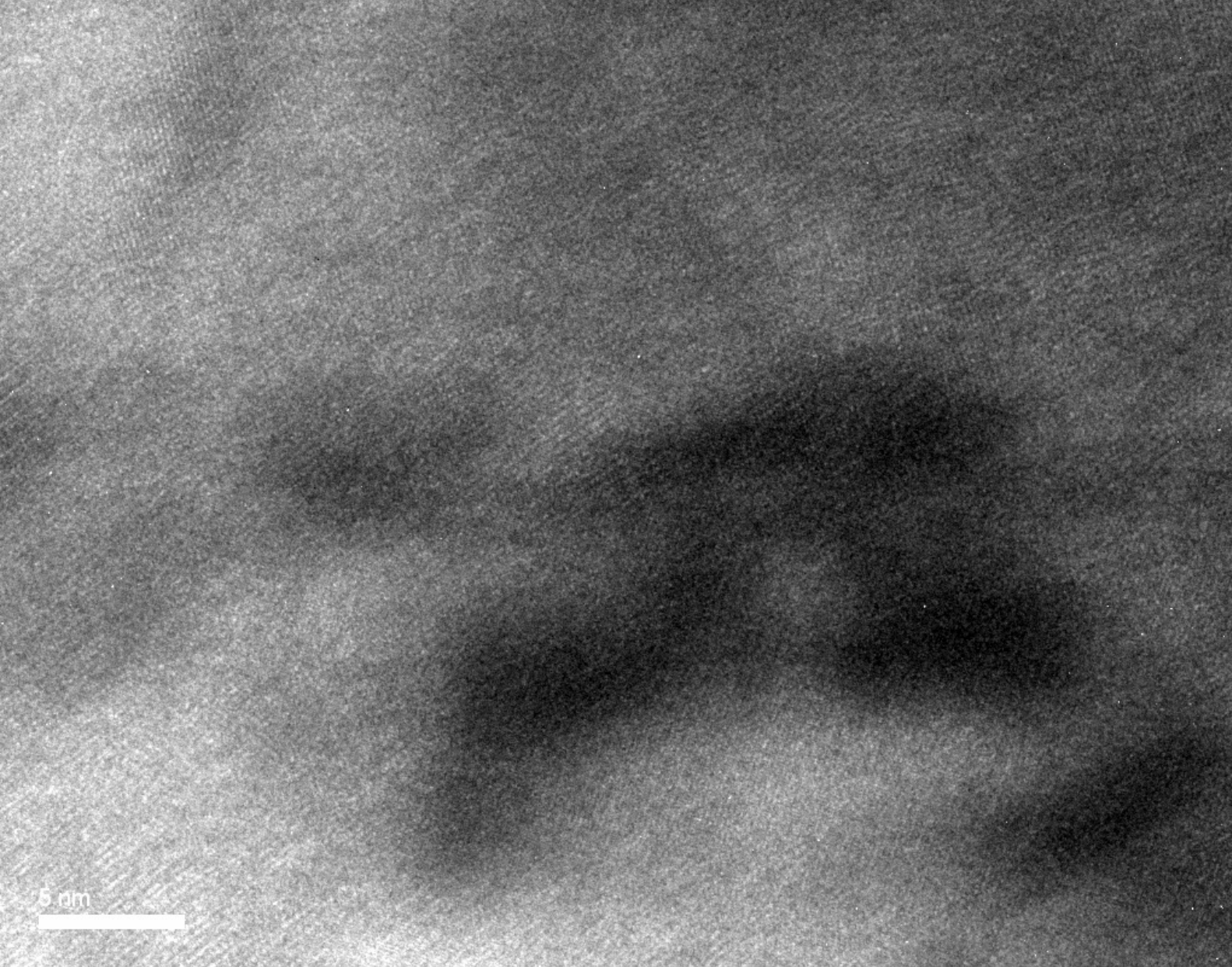
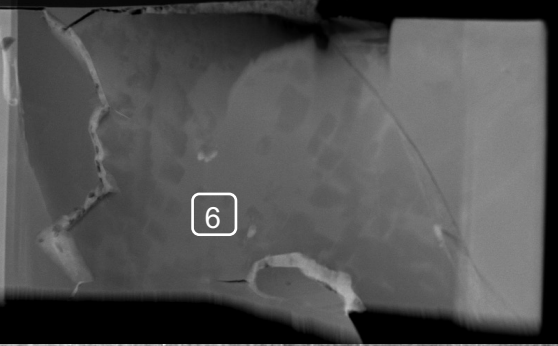


FFT (5)

Chalcopyrite (cubic;  $I\bar{4}2d/F\bar{4}3m$ )Pyrrhotite (FeS)(orthorhombic;  $Cmca$  polytype 5c)

Spot#	d-Spacing (nm)	(hkl)	Ideal d-Spacing (Å)
1	0.184549	$(220)_{cp}$	1.8484
2	0.184048	$(220)_{cp}$	1.8484
3	0.576661	$(110)_{Po}$	5.7606
4	0.303795	$(112)_{cp}$	3.0387
5	0.30705	$(112)_{cp}$	3.0387



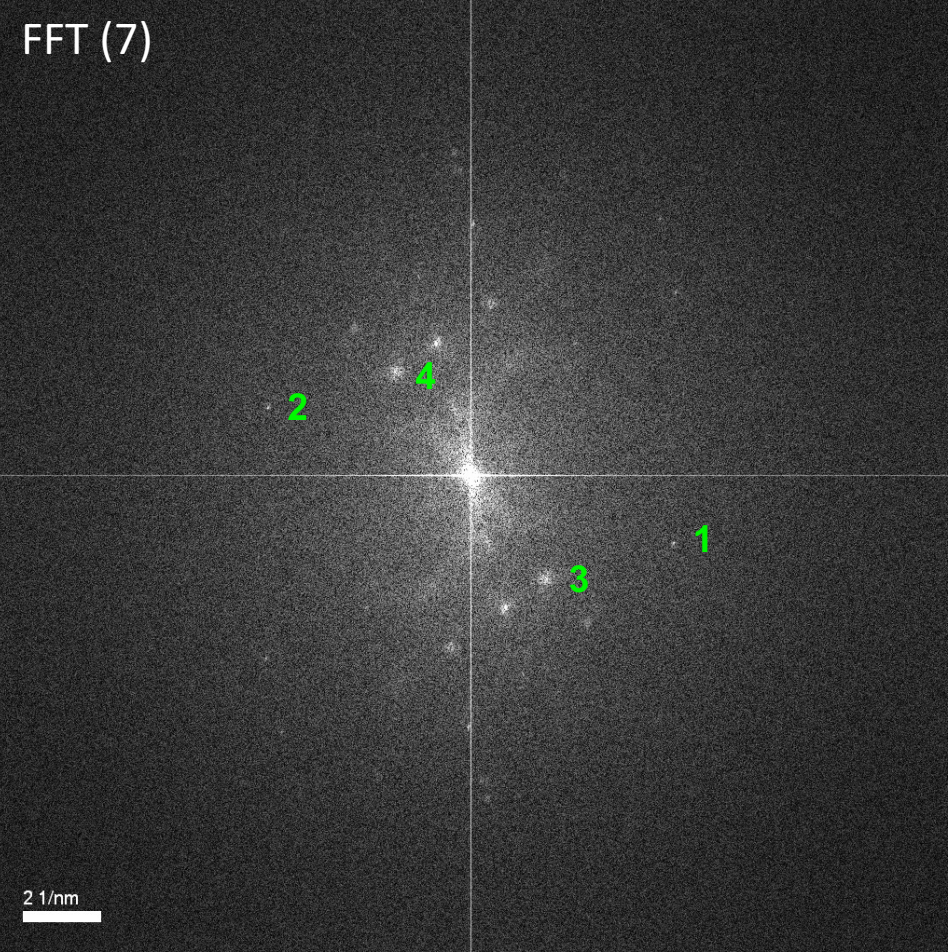
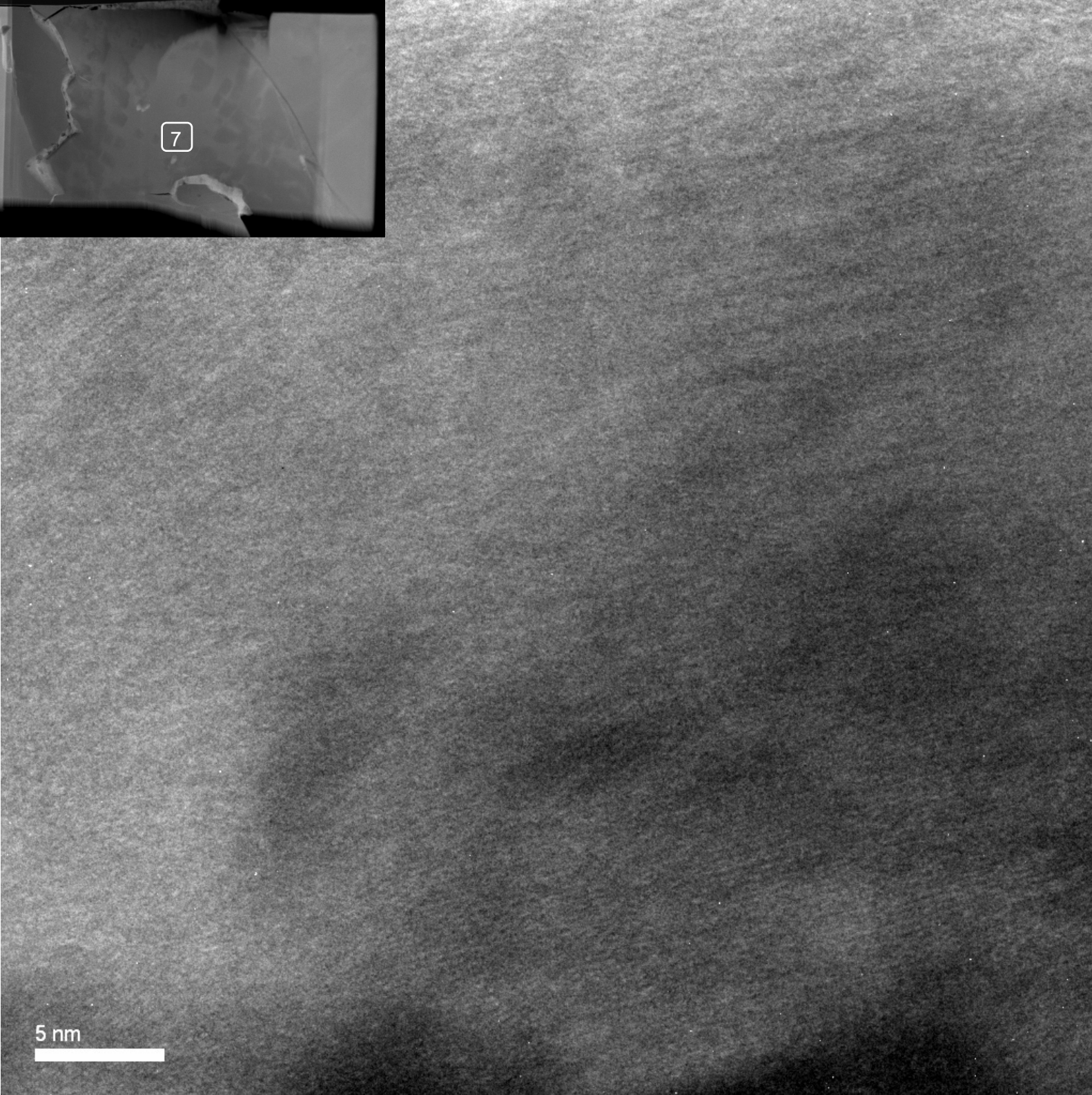
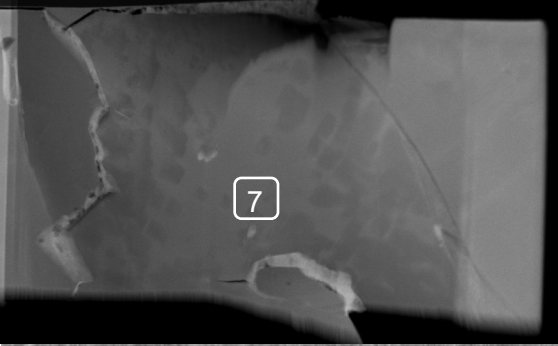


Chalcopyrite (cubic;  $I\bar{4}2d/F\bar{4}3m$ )

Pyrite ( $\text{FeS}_2$ ) (cubic;  $P3a$ )

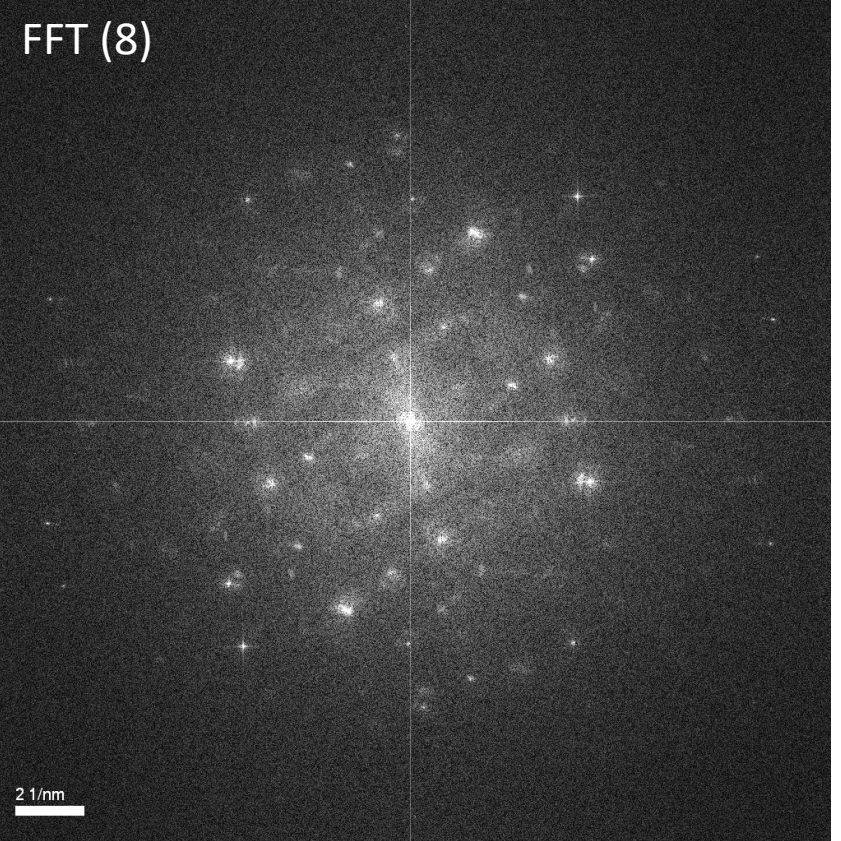
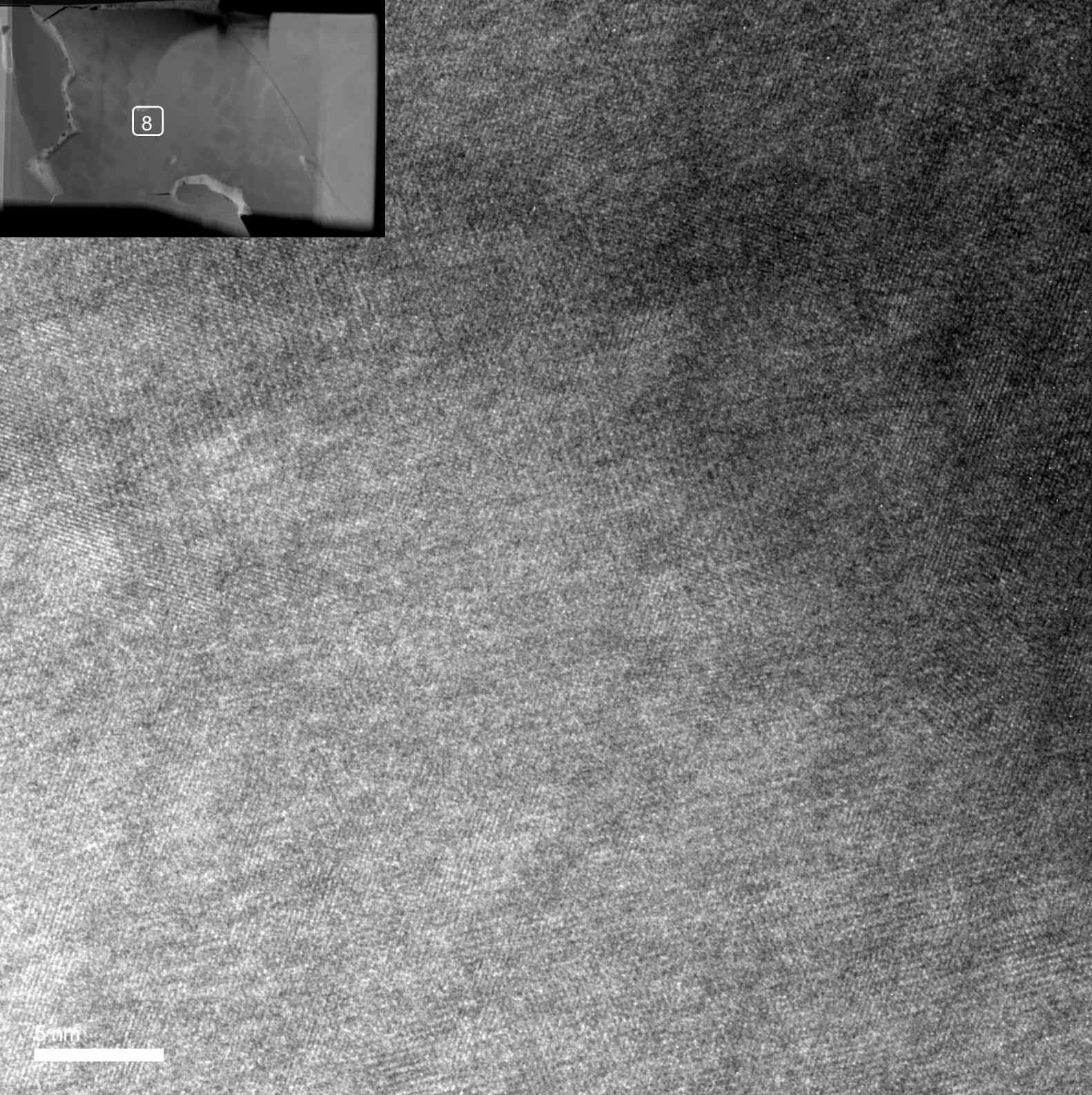
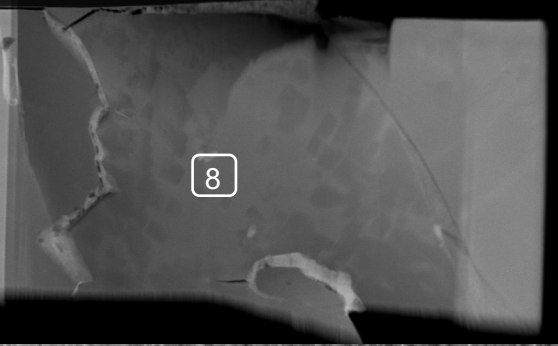
Spot#	d-Spacing (nm)	(hkl)	Ideal d-Spacing (Å)
1	0.125447	(331) <sub>py</sub>	1.2425
2	0.125212	(331) <sub>py</sub>	1.2425
3	0.311431	(112) <sub>cp</sub>	3.0387
4	0.308141	(112) <sub>cp</sub>	3.0387
5	0.184527	(220) <sub>cp</sub>	1.8484
6	0.183992	(220) <sub>cp</sub>	1.8484





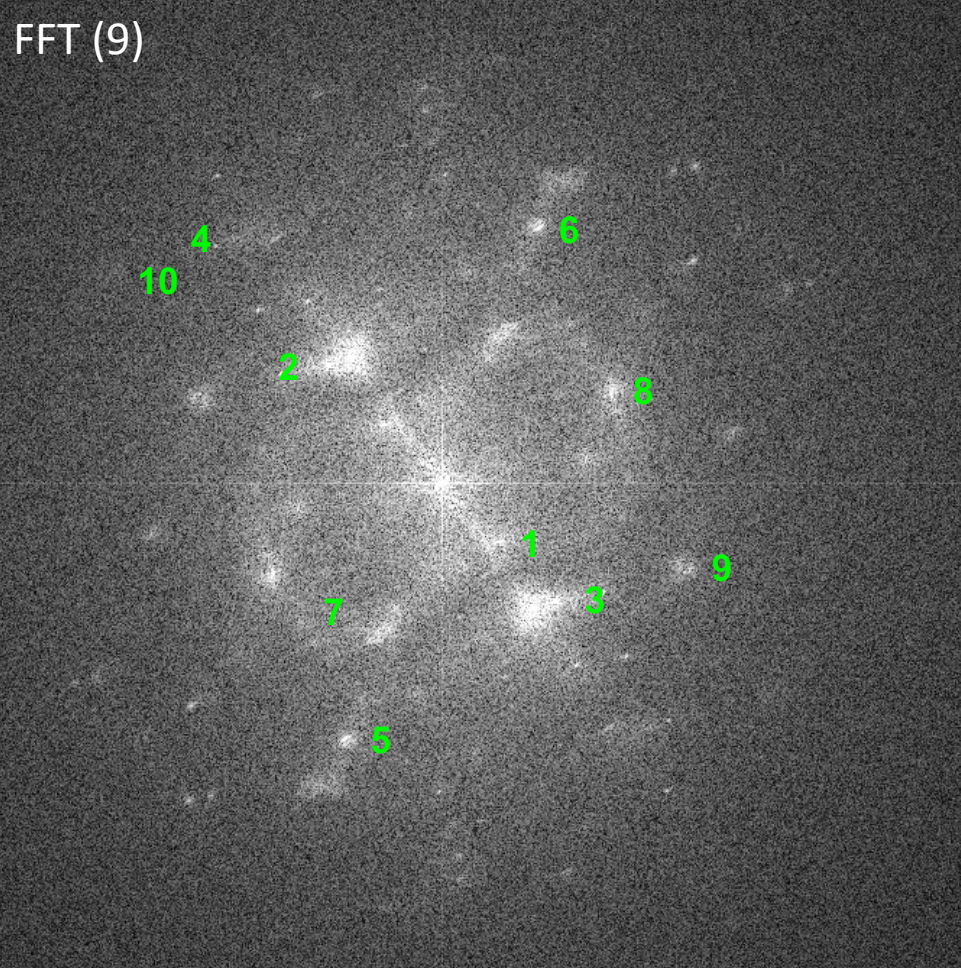
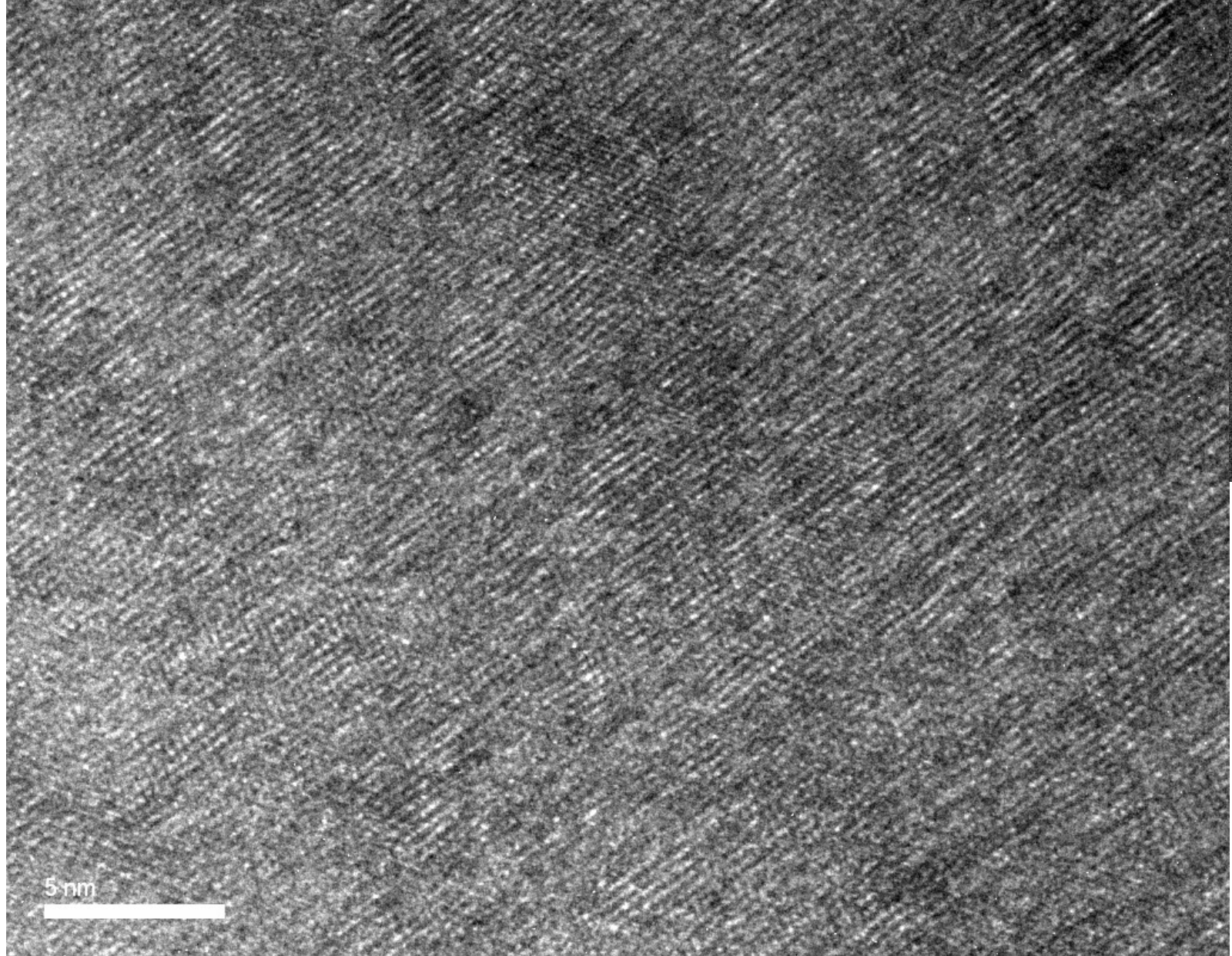
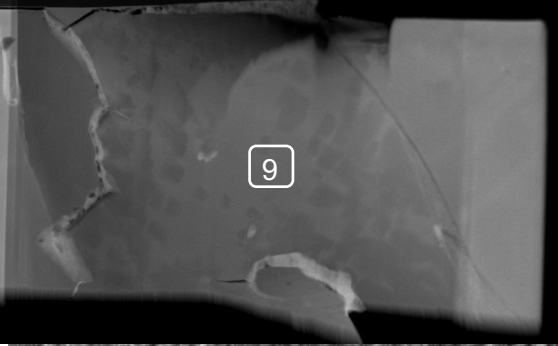
Chalcopyrite (cubic; $I\bar{4}2d$ )			
Pyrite ( $\text{FeS}_2$ ) (cubic; $P3a$ )			
Spot#	d-Spacing (nm)	(hkl)	Ideal d-Spacing (Å)
1	0.184103	$(204)_{\text{cp}}$	1.8365
2	0.184623	$(204)_{\text{cp}}$	1.8365
3	0.310144	$(204)_{\text{py}}$	3.1269
4	0.314008	$(204)_{\text{py}}$	3.1269





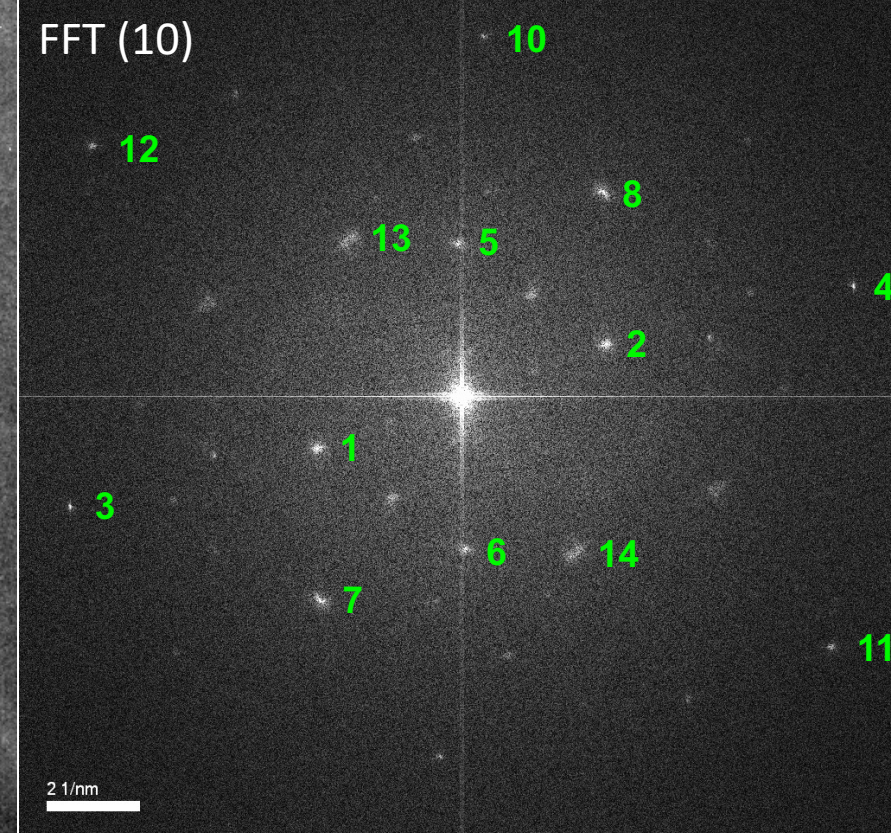
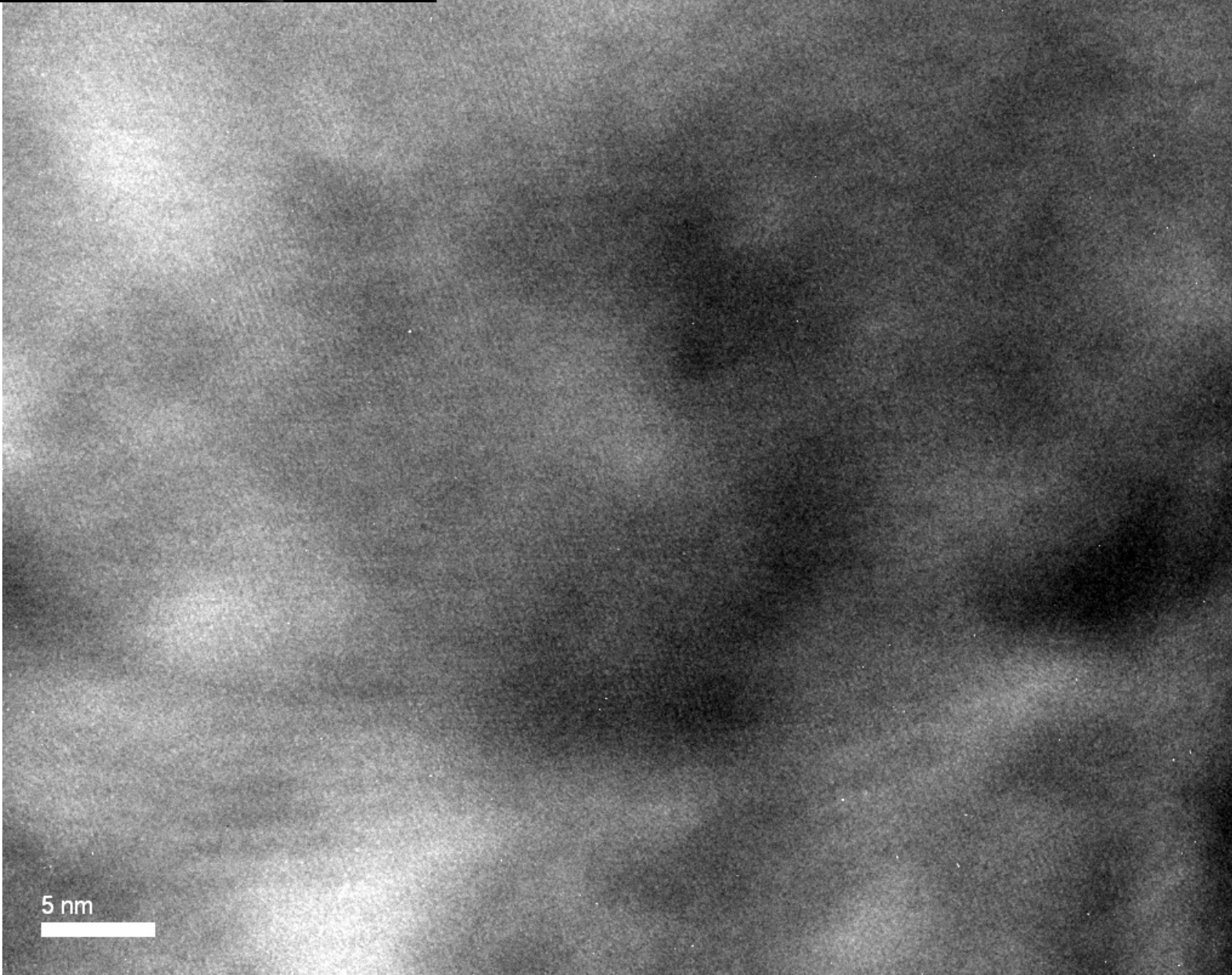
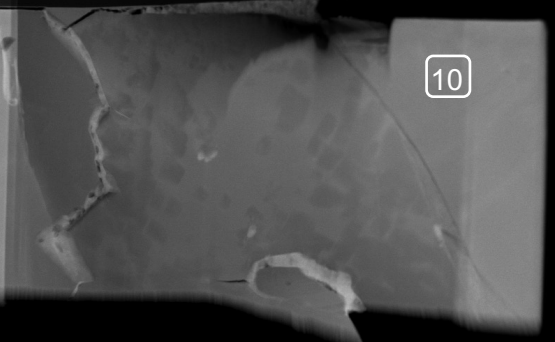
Chalcopyrite (cubic; $I\bar{4}2d/F-43m$ )			
Pyrite ( $\text{FeS}_2$ ) (cubic; $P3a$ )			
Spot#	d-Spacing (nm)	(hkl)	Ideal d-Spacing (Å)
1	0.123584	$(331)_{\text{py}}$	1.2425
2	0.124185	$(331)_{\text{py}}$	1.2425
5	0.183521	$(220)_{\text{cp}}$	1.8484
6	0.184056	$(220)_{\text{cp}}$	1.8484
15	0.132009	$(400)_{\text{cp}}$	1.3100-1.3223
16	0.131226	$(400)_{\text{cp}}$	1.3100-1.3223
17	0.544573	$(001)_{\text{mc}}$	5.4320





Chalcopyrite (cubic; I42d)			
Pyrrhotite (FeS)(orthorhombic; Cmca polytype 5c)			
Spot#	d-Spacing (nm)	(hkl)	Ideal d-Spacing (Å)
1	0.584782	(001) <sub>Po</sub>	5.8439-5.8456
2	0.597333	(001) <sub>Po</sub>	5.8439-5.8456
3	0.29552	(220) <sub>Po</sub>	2.9848
4	0.297605	(220) <sub>Po</sub>	2.9848
7	0.250115	(004) <sub>Cp</sub>	2.5750
8	0.257426	(004) <sub>Cp</sub>	2.5750
9	0.18631	(220) <sub>Cp</sub>	1.8699
10	0.187105	(220) <sub>Cp</sub>	1.8699





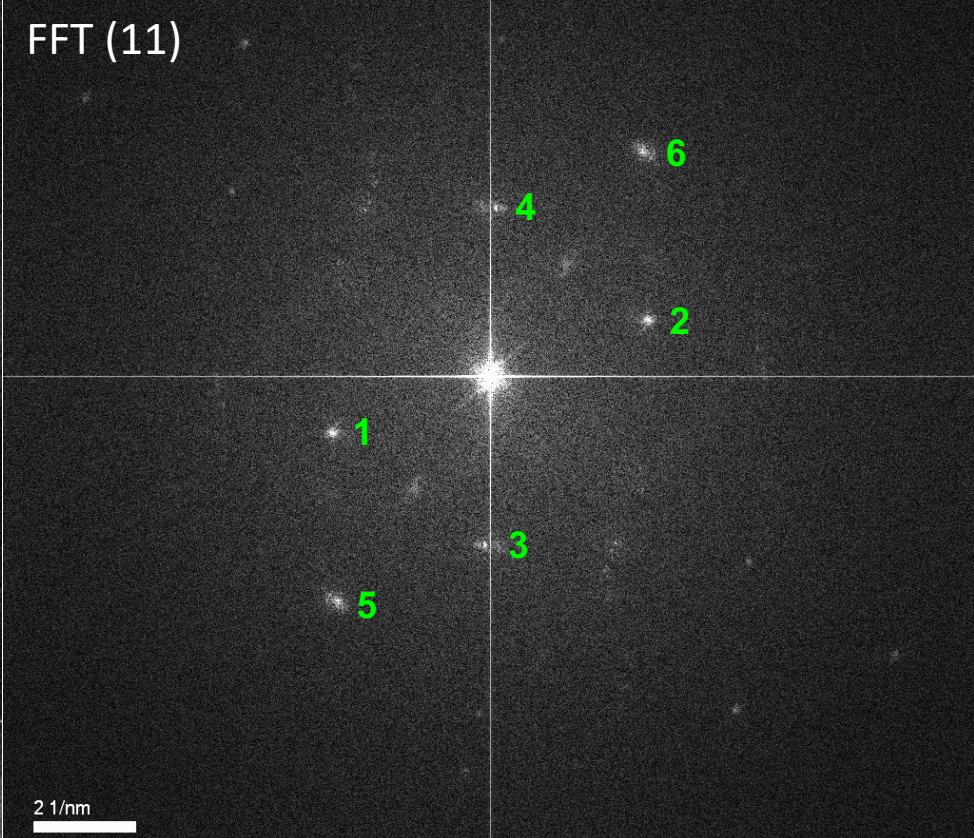
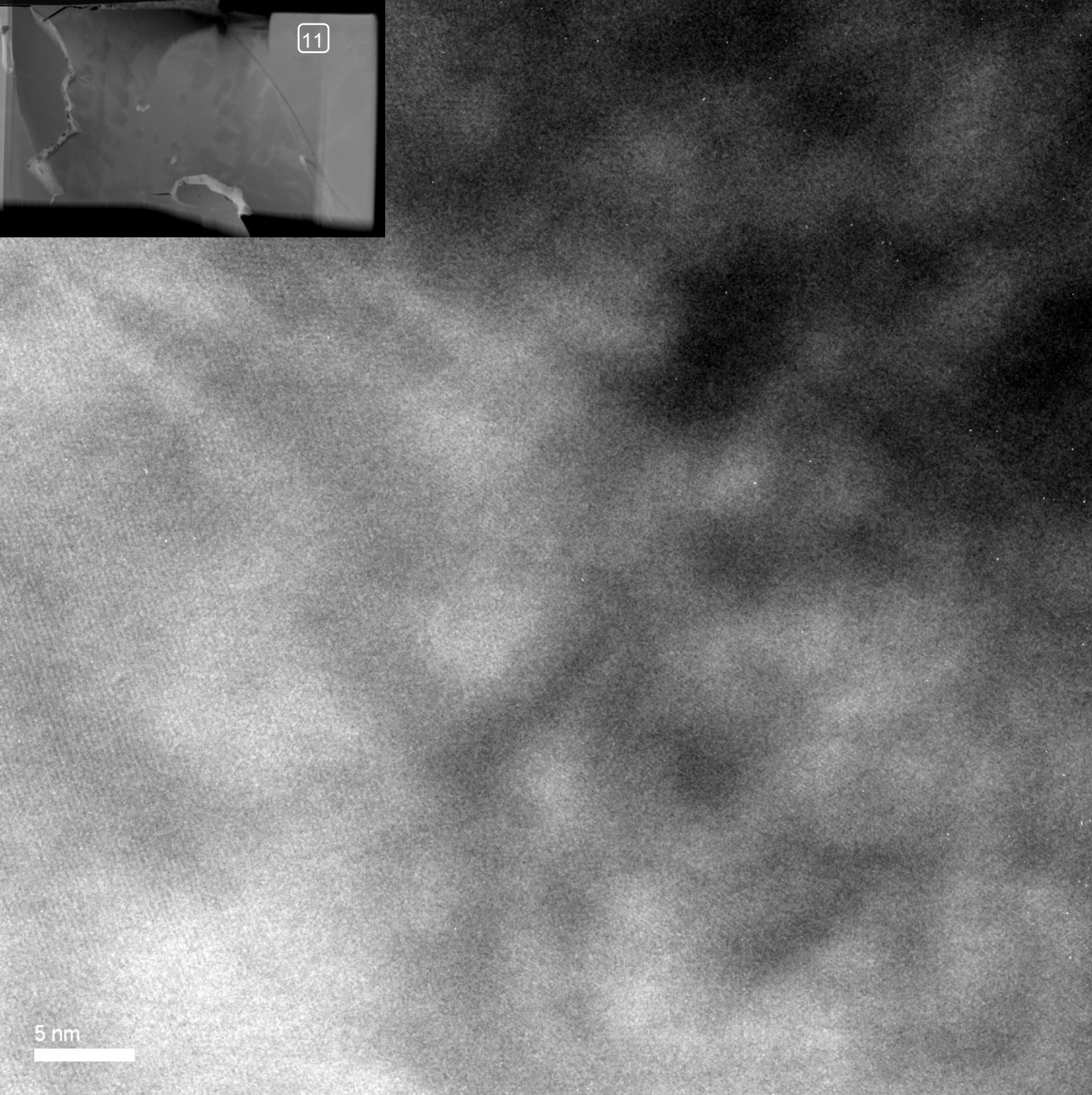
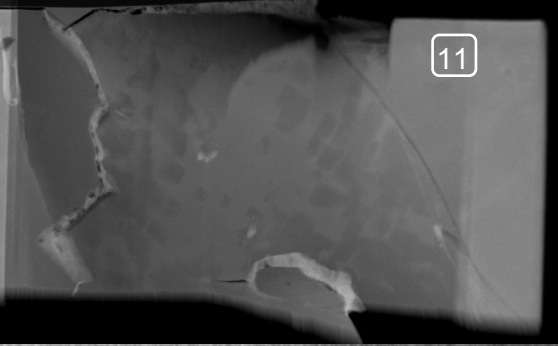
Pyrite (FeS<sub>2</sub>) (cubic; P3a)

Marcasite (FeS<sub>2</sub>) (orthorrombic; Pnnm)

Pyrrhotite (FeS)(orthorrombic; Cmca polytype 5c)

Spot#	d-Spacing (nm)	(hkl)	Ideal d-Spacing (Å)
1	0.3056	(028) <sub>Po</sub>	3.0698
2	0.306897	(028) <sub>Po</sub>	3.0698
3	0.115714	(240) <sub>Mc</sub>	1.15576
4	0.115841	(240) <sub>Mc</sub>	1.15576
5	0.309349	(028) <sub>Po</sub>	3.0698
6	0.305667	(028) <sub>Po</sub>	3.0698
7	0.189293	(121) <sub>Mc</sub> / (202) <sub>Py</sub>	1.9113/1.9151
8	0.189881	(121) <sub>Mc</sub> / (202) <sub>Py</sub>	1.9113/1.9151
9	0.130366	(212) <sub>Mc</sub>	1.3071
10	0.130734	(212) <sub>Mc</sub>	1.3071
11	0.105281	(312) <sub>Mc</sub>	1.0921
12	0.106091	(312) <sub>Mc</sub>	1.0921
13	0.243217	(111) <sub>Mc</sub> / (210) <sub>Py</sub>	2.4126/2.4224
14	0.241413	(111) <sub>Mc</sub> / (210) <sub>Py</sub>	2.4126/2.4224





Pyrite (FeS <sub>2</sub> ) (cubic; P3a)			
Marcasite (FeS <sub>2</sub> ) (orthorrombic; Pnnm)			
Pyrrhotite (FeS)(orthorrombic; Cmca polytype 5c)			
Spot#	d-Spacing (nm)	(hkl)	Ideal d-Spacing (Å)
1	0.307257	(028) <sub>Po</sub>	3.0698
2	0.308719	(028) <sub>Po</sub>	3.0698
3	0.305617	(028) <sub>Po</sub>	3.0698
4	0.309521	(028) <sub>Po</sub>	3.0698
5	0.189486	(121) <sub>Mc</sub> / (202) <sub>Py</sub>	1.9113/1.9151
6	0.190879	(121) <sub>Mc</sub> / (202) <sub>Py</sub>	1.9113/1.9151