Summary Remarks: for how indexing the diffraction pattern from the Ultran CCD of the JEM-2010

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Hi, Maneesh

I write a short summary for how to indexing your digital diffraction pattern, which I would like to use for the other TEM user's future reference!

First we should calculate all the possible diffraction orientation data for all phases in your sample system. As I know you only have Si and Al phases which I calculated in the next page (now you mentioned there were also possible with Mn contained phases which can be added later!). As you see, there are several columns on the next page data, where **K** is just series calculation number; **U V W** is the zone axis; **H1 K1 L1** and **H2 K2 L2** are the closest and second closest diffracted spots relative to the transmitted spot (000) in diffraction (i.e. reciprocal) space; **R2/R1** and **R3/R1 (R3** the third closest spot) are the ratio among the spots as shown in the below Diff pattern example; **FAI** is the angle between **H1 K1 L1** and **H2 K2 L2**, and **D1** and **D2** are the lattice distances of **H1 K1 L1** and **H2 K2 L2** in the real space. (* now by using so called "parallelogram rule" with these **H1 K1 L1** and **H2 K2 L2** and **FAI,** you can reconstruct this whole **U V W** diffraction pattern).

Here I am using your TODAY diff pattern named "01 Diff300.dm3" (the original digital size as 14.3 x 14.3 mm) as indexing example. First we should find the closest and second closest diffracted spots relative to the transmitted spot (000)**,** which are the arrow-marked 1 and 2 in the below pattern. Then we measure the length of a symmetry diffracted spots around the (000), and further to calculate their lattice space in real space, by using the rule bar on the Diff pattern (here, used 2 symmetry spots around (000) for this measurement) and the equation for "**LINE 1**"should be as,

$$\textbf{(42/2)}_{\text{(mm, divided by 2 for 2 spots)}} : \textbf{(1/ d1)}_{(1/nm)} = \textbf{21.5}_{\text{(mm, the rule bare length)}} : \textbf{5}_{(1/nm)}$$

which were measured on the original picture (i.e. 14.3 x 14.3 mm in picture size)
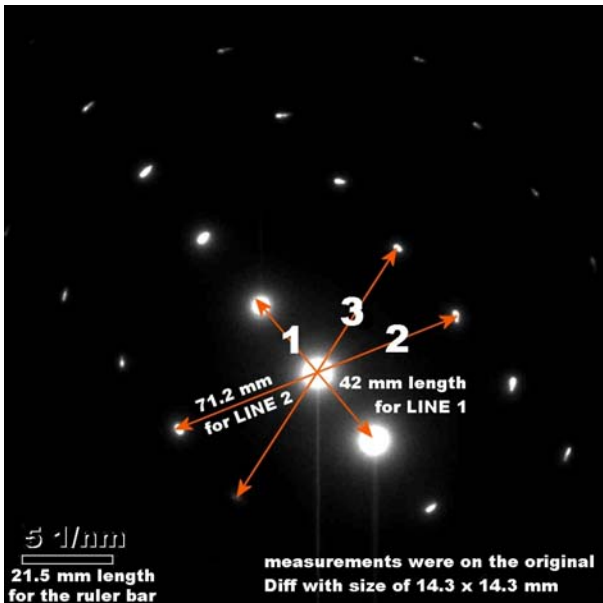
Then the resulted **d1** (i.e. **H1 K1 L1**) is as **0.204 nm**. With the same way, **d2** (i.e. "**LINE 2**" for **H2 K2 L2**) is as **0.121 nm**. The angle between d1 and d2 as **107.5** degree (could also be as 180-107.5 for the TEM diffraction 180 degree uncertain).

As comparing with all possible diffraction orientations from both Al and Si phases on next page, the only well fitted result should be indexed as Al [310] with d1 represents as (00-2) and d2 represents as (-131) planes, as with the squared marked in the next page data list.

The further confirmation could be done by comparing with d3, i.e. using **R2/R1** and **R3/R1**, which could be done both in real d space or reciprocal diffraction 1/d space.

For the possible existed error in indexing Diff pattern, the measured angle should be more accurate than d values. For getting accurate SAED patterns from the TEM operation, please try to follow the diffraction alignment procedures as outlined in the JEM-2010 Handbook Operation, i.e. in the image mode, to focus the sample by using Z (sample height) control, and at the same time to keep the objective lens at the standard current (at DV +0). Then insert the SA aperture, change to the Diff mode and tilt DIFF around (000) as symmetry as possible, and sharpening the diffraction spots by adjusting Diff Focus knob. More information available at,
    http://folk.ntnu.no/yingday/NilsYD/TEMCCDbasic/Diff_Mag_Calibration.pdf

Note here, the calculation of lattice distance is in angstrom unit

********** Al **********

    PARAMETERS
          A= 4.0500   B= 4.0500   C= 4.0500
          AF= 90.000   BT= 90.000   GM= 90.000
          NUVW= 8   NSY= 1   NL= 1
          SY: 1-CUBIC; 2-TETRA; 3-ORTH; 4-HEX; 5-MONO; 6-TRIC
          LT: 1-F; 2-I; 3-C; 4-B; 5-A; 6-P; 7-R;

K	U V W	H1 K1 L1	H2 K2 L2	R2/R1	R3/R1	FAI	D1	D2
1	1 1 1	0 2 -2	-2 0 2	1.000	1.000	120.00	1.432	1.432
2	1 1 0	-1 1 -1	-1 1 1	1.000	1.155	70.53	2.338	2.338
3	1 0 0	0 -2 0	0 0 -2	1.000	1.414	90.00	2.025	2.025
4	5 2 1	1 -3 1	1 -1 -3	1.000	1.348	84.78	1.221	1.221
5	4 1 1	0 -2 2	1 -3 -1	1.173	1.173	64.76	1.432	1.221
6	3 3 2	2 -2 0	1 1 -3	1.173	1.541	90.00	1.432	1.221
7	2 1 1	1 -1 -1	0 2 -2	1.633	1.915	90.00	2.338	1.432
8	3 1 0	0 0 -2	-1 3 1	1.658	1.658	107.55	2.025	1.221

********** si **********

    PARAMETERS
          A= 5.4300   B= 5.4300   C= 5.4300
          AF= 90.000   BT= 90.000   GM= 90.000
          NUVW= 6   NSY= 1   NL= 1
          SY: 1-CUBIC; 2-TETRA; 3-ORTH; 4-HEX; 5-MONO; 6-TRIC
          LT: 1-F; 2-I; 3-C; 4-B; 5-A; 6-P; 7-R;

K	U V W	H1 K1 L1	H2 K2 L2	R2/R1	R3/R1	FAI	D1	D2
1	1 1 1	0 2 -2	-2 0 2	1.000	1.000	120.00	1.920	1.920
2	6 5 3	-1 3 -3	-3 3 1	1.000	1.026	61.73	1.246	1.246
3	4 2 1	0 2 -4	-2 4 0	1.000	1.095	66.42	1.214	1.214
4	1 1 0	-1 1 -1	-1 1 1	1.000	1.155	70.53	3.135	3.135
5	5 2 1	1 -3 1	1 -1 -3	1.000	1.348	84.78	1.637	1.637
6	1 0 0	0 -2 0	0 0 -2	1.000	1.414	90.00	2.715	2.715
7	5 3 1	2 -2 -4	-2 4 -2	1.000	1.291	99.59	1.108	1.108
8	4 3 2	2 0 -4	-2 4 -2	1.095	1.342	79.48	1.214	1.108
9	4 1 1	0 -2 2	1 -3 -1	1.173	1.173	64.76	1.920	1.637
10	3 3 2	2 -2 0	1 1 -3	1.173	1.541	90.00	1.920	1.637
11	6 3 1	1 -1 -3	-1 3 -3	1.314	1.348	69.77	1.637	1.246
12	5 4 3	1 1 -3	-3 3 1	1.314	1.477	101.98	1.637	1.246
13	6 1 1	0 2 -2	-1 3 3	1.541	1.837	90.00	1.920	1.246
14	4 3 3	0 2 -2	-3 1 3	1.541	1.541	108.93	1.920	1.246
15	2 2 1	2 -2 0	0 2 -4	1.581	1.581	108.43	1.920	1.214
16	2 1 1	1 -1 -1	0 2 -2	1.633	1.915	90.00	3.135	1.920
17	3 1 0	0 0 -2	-1 3 1	1.658	1.658	107.55	2.715	1.637
18	3 1 1	0 -2 2	2 -4 -2	1.732	1.732	73.22	1.920	1.108
19	5 5 2	2 -2 0	1 1 -5	1.837	2.092	90.00	1.920	1.045
20	2 1 0	0 0 -2	-2 4 0	2.236	2.449	90.00	2.715	1.214
21	3 2 1	1 -1 -1	-1 3 -3	2.517	2.582	97.61	3.135	1.246
22	5 1 0	0 0 -2	-1 5 1	2.598	2.598	101.10	2.715	1.045