Supplementary material

to the paper 'A remark on *ab initio* indexing of EBSD patterns' by A. Morawiec

This file contains results of indexing of the example EBSD pattern shown in Fig. 1. Input and output files of *DirAx*, *Ind_X* and *IndX_Laue* are in Tables 2–7. For convenience, the reflection indices listed in [1] are repeated in Table 1.

At the end, there is a derivation of the formula for determination of scattering vectors from positions of edges of EBSD bands.

Table 1: Reflection indices $\mathtt{h}_{Li}$ listed in [1].

	h	k	l
1	31	−20	−2
2	−12	7	1
3	−29	18	2
4	−43	28	3
5	6	−4	0
6	37	−24	−2
7	−25	16	2
8	6	−3	0
9	−24	16	2
10	−13	9	1
11	1	0	0
12	0	1	0
13	96	−61	−6
14	55	−36	−3
15	−6	4	1
16	0	0	1
17	−6	3	1
18	48	−31	−3
19	46	−29	−3
20	−44	28	3
21	−41	26	3
22	23	−14	−1
23	84	−54	−5
24	34	−22	−2
25	7	−4	0
26	12	−7	0

Table 2: *DirAx* input file. The parameters of the program are given in the first five commented lines. The wavelength (1.54056Å) is not used in computations. The following lines contain Cartesian components (in Å^{-1}) of the scattering vectors $\boldsymbol{H}_i$ ($i = 1, 2, \ldots, 26$).

```
!  LevelFit:   1/100 [1/A]
!  maximal D: 15A
!  IndexFitFactor:      3.00
!  Delta axes zero :    0.1A
!  Delta angles zero :  0.2deg
   1.54056
   -0.381613    0.245448   -0.040362
   -0.413404   -0.507353    0.056016
    0.444278    0.351223    0.001019
   -0.508321    0.399310    0.078563
   -0.317655   -0.161782    0.195319
   -0.027002   -0.373507    0.238714
    0.588358   -0.022478   -0.159996
    0.174490   -0.628767   -0.254487
   -0.578591    0.535110    0.240619
    0.199885   -0.604781   -0.115379
   -0.055426   -0.603809   -0.087438
    0.178921    0.911853    0.068243
    0.825259    0.142683    0.231164
   -0.068180   -0.788425    0.309236
   -0.610669    0.098132    0.320284
    0.908075    0.061048   -0.502669
    0.775171    0.699036   -0.265922
    0.331995   -0.301704    0.086418
    0.540518    0.253031    0.062502
    0.580123    0.047910   -0.021023
    0.577995    0.087090   -0.081528
    0.103485   -0.482924   -0.312692
    0.382132   -0.344033    0.269722
    0.251451   -0.502520    0.235751
   -0.262867    0.326993    0.256804
    0.476508   -0.461288   -0.440052
```

Table 3: *DirAx* output file.

```
results from DIRAX for EBSD_DAT                    Friday 21 May 2021 - 10:17:09
================================================================================
Lambda: 1.54056  LevelFit: 1/100  IndexFitFactor: 3.00
IndexFit = LevelFit*IndexFitFactor = (1/100)*3.00 = 1/33
Dmax: 15  Acceptance Level (ACL): 19
--------------------------------------------------------------------------------
 nr      h       k       l     theta    phib    chib     dth      dom      dch
--------------------------------------------------------------------------------
 1=N  -1.379  -0.045  -2.662   20.54   57.25   -5.08
 2 H  -2.947  -1.981   0.904   30.39  140.83    4.89   -0.862   -0.843   -0.605
 3=N   2.767   1.834   0.058   25.86  -51.67    0.10
 4=N  -1.841   0.862  -3.590   30.10   51.85    6.93
 5 H  -2.015  -0.002  -0.025   18.25  116.99   28.72    0.094   -0.505   -0.222
 6 H  -1.020   0.020   2.145   20.00  175.87   32.52    1.116    0.987    0.200
 7 H   2.969   0.037   1.974   28.03  -92.19  -15.20   -0.403    0.309    0.449
 8 H  -0.006  -3.047   3.005   32.65 -164.49  -21.31    0.314   -0.160   -0.339
 9 H  -2.103   2.028  -4.128   39.40   47.24   16.98    1.450    0.589   -0.108
10=N   0.022  -2.202   3.294   29.91 -161.71  -10.27
11=N  -1.240  -2.463   2.387   28.16  174.76   -8.21
12=N   2.397   3.539  -3.385   45.87  -11.10    4.20
13 H   4.021   2.988   2.962   42.01  -80.19   15.43    0.006    0.384   -0.431
14 H  -2.016  -0.994   4.059   40.88  175.06   21.34    0.606    0.128    0.172
15 H  -3.102   1.006  -2.057   32.45   80.87   27.38    1.064    0.276   -0.204
16 H   5.002  -0.977   2.046   53.21  -86.15  -28.91   -0.031   -0.258    0.369
17=N   5.243   2.073  -0.883   56.07  -47.96  -14.29
18 H   0.995   0.028   2.835   20.60 -132.26   10.90   -1.186    1.238   -0.143
19 H   3.001   1.998   1.009   27.53  -64.91    5.98    0.004   -0.133    0.021
20 H   2.915   0.974   1.922   26.66  -85.28   -2.07   -0.890    0.308   -0.107
21=N   3.033   0.778   1.601   27.04  -81.43   -7.94
22 H  -0.037  -3.003   1.936   26.76 -167.91  -32.34   -0.292   -0.810   -0.455
23=N   0.983   0.933   3.620   26.57 -132.00   27.68
24=N   0.106   0.042   3.785   27.99 -153.42   22.76
25 H  -0.954   1.959  -1.940   22.27   38.80   31.47   -0.678   -0.440    0.092
26 H   1.934  -3.001   2.965   37.81 -134.07  -33.57   -0.526   -0.660   -0.089
--------------------------------------------------------------------------------
  reciprocal axes matrix [R] (columns)     direct axes matrix [D] (rows)
--------------------------------------------------------------------------------
    0.156885    0.003599    0.062021         4.8452      1.7522     -0.9847
    0.081896    0.072225   -0.135871         1.6062      3.1742      5.2314
   -0.097860    0.146226    0.063400         3.7742     -4.6165      2.1873
--------------------------------------------------------------------------------
c e l l  f o r  EBSD_DAT
--------------------------------------------------------------------------------
a, b, c :      5.2455      6.3264      6.3514
al,be,ga:      85.931      76.028      75.707
  volume:      198.19

Niggli values:     27.5157     40.0229     40.3409
                    2.8509      8.0440      8.1928
--------------------------------------------------------------------------------
results from DIRAX for EBSD_DAT                    Friday 21 May 2021 - 10:17:09
================================================================================
```

For each accepted (type H) reflection, indices h obtained by *DirAx* (Table 3) are related to indices $\mathtt{h}_{Li}$ listed in [1] and Table 1 above by $\pm T\,\mathtt{h} = \mathtt{h}_{Li}$, where

$$T = \begin{bmatrix} -3 & 19 & 17 \\ 2 & -12 & -11 \\ 0 & -1 & -1 \end{bmatrix} .$$

For instance, the reflection 13 has the indices

$$\mathtt{h}_{Li} = \begin{bmatrix} 96 \\ -61 \\ -6 \end{bmatrix} = +T\,\mathtt{h} = T \begin{bmatrix} 4 \\ 3 \\ 3 \end{bmatrix} \approx T \begin{bmatrix} 4.021 \\ 2.988 \\ 2.962 \end{bmatrix} .$$

The $\pm$ sign in front of T is related to the choice of the first edge of a band. The choice determines the direction of the scattering vector.

Table 4: *Ind_X* input file. The lines following the keyword `_Reflections` contain Cartesian components (in Å^{-1}) of the scattering vectors $\boldsymbol{H}_i$ ($i = 1, 2, \ldots, 26$).

```
_NumberOfReflections
        26
_Reflections
 -0.381613    0.245448   -0.040362
 -0.413404   -0.507353    0.056016
  0.444278    0.351223    0.001019
 -0.508321    0.399310    0.078563
 -0.317655   -0.161782    0.195319
 -0.027002   -0.373507    0.238714
  0.588358   -0.022478   -0.159996
  0.174490   -0.628767   -0.254487
 -0.578591    0.535110    0.240619
  0.199885   -0.604781   -0.115379
 -0.055426   -0.603809   -0.087438
  0.178921    0.911853    0.068243
  0.825259    0.142683    0.231164
 -0.068180   -0.788425    0.309236
 -0.610669    0.098132    0.320284
  0.908075    0.061048   -0.502669
  0.775171    0.699036   -0.265922
  0.331995   -0.301704    0.086418
  0.540518    0.253031    0.062502
  0.580123    0.047910   -0.021023
  0.577995    0.087090   -0.081528
  0.103485   -0.482924   -0.312692
  0.382132   -0.344033    0.269722
  0.251451   -0.502520    0.235751
 -0.262867    0.326993    0.256804
  0.476508   -0.461288   -0.440052

_MinMaxVolumeOfPrimitiveCell
    100.0  1000.0
_TheMainCriterion
     0.24
_MaxAllowedMillerIndex
      8
```

Table 5: The best solution from the *Ind_X* output file.

```
  Direct basis vectors (in rows) = inverse of UB matrix;
  transforms RL vectors to Miller indices :
             4.84988326    1.72853023   -0.92048409
             3.74058721   -4.59675207    2.19643448
             1.63027287    3.14144189    5.26309708

       |   h   k   l |      Real (hkl)       |  Error
-------------------------------------------------------
  1    |             |  -1.39  -2.64  -0.06  |  0.531
  2  H- |  -3   1  -2 |  -2.93   0.91  -1.97  |  0.116
  3  -h |   3   0   2 |   2.76   0.05   1.83  |  0.296
  4    |             |  -1.85  -3.56   0.84  |  0.489
  5  H- |  -2   0   0 |  -2.00  -0.02   0.00  |  0.016
  6  -h |  -1   2   0 |  -1.00   2.14   0.04  |  0.146
  7  H- |   3   2   0 |   2.96   1.95   0.05  |  0.076
  8  H- |   0   3  -3 |  -0.01   2.98  -3.03  |  0.035
  9  H- |  -2  -4   2 |  -2.10  -4.10   2.00  |  0.140
 10    |             |   0.03   3.27  -2.18  |  0.330
 11    |             |  -1.23   2.38  -2.45  |  0.629
 12
 13  H- |   4   3   3 |   4.04   2.94   3.01  |  0.072
 14  H- |  -2   4  -1 |  -1.98   4.05  -0.96  |  0.066
 15  H- |  -3  -2   1 |  -3.09  -2.03   1.00  |  0.093
 16  H- |   5   2  -1 |   4.97   2.01  -0.97  |  0.040
 17  -h |   5  -1   2 |   5.21  -0.90   2.06  |  0.243
 18  -h |   1   3   0 |   1.01   2.82   0.05  |  0.188
 19  H- |   3   1   2 |   3.00   1.00   2.01  |  0.007
 20  H- |   3   2   1 |   2.92   1.90   0.99  |  0.129
 21    |             |   3.03   1.58   0.79  |  0.470
 22  H- |   0   2  -3 |  -0.05   1.92  -2.99  |  0.092
 23    |             |   1.01   3.60   0.96  |  0.399
 24  -h |   0   4   0 |   0.13   3.77   0.07  |  0.277
 25  H- |  -1  -2   2 |  -0.95  -1.92   1.95  |  0.107
 26  H- |   2   3  -3 |   1.92   2.94  -2.99  |  0.104
-------------------------------------------------------
  19h and  14H vectors out of  26.    Quality : 0.673

 Primitive cell :
                         5.230    6.320    6.342
                        85.40    75.17    75.68

 Volume of the cell  :      196.35

 -------------------------------------------------------
```

For an individual (type `H-` or `-h`) reflection, indices `h` listed in Table 5 are related to the indices $\mathtt{h}_{Li}$ by $\pm T\,\mathtt{h} = \mathtt{h}_{Li}$, where

$$T = \begin{bmatrix} -3 & 17 & 19 \\ 2 & -11 & -12 \\ 0 & -1 & -1 \end{bmatrix} .$$

The only exception is the reflection 24 with the indices related via $+T\,\mathtt{h} = 2\,\mathtt{h}_{Li}$.

Table 6: *IndX_Laue* input file. The lines following the keyword `_Reflections` contain Cartesian components of normalized scattering vectors $\boldsymbol{H}_i/|\boldsymbol{H}_i|$ $(i = 1, 2, \ldots, 26)$.

```
_NumberOfReflections
        26
_Reflections
 -0.837745    0.538825   -0.088605
 -0.629377   -0.772406    0.085280
  0.784472    0.620162    0.001799
 -0.780638    0.613227    0.120650
 -0.781473   -0.398006    0.480511
 -0.060801   -0.841051    0.537529
  0.964302   -0.036841   -0.262229
  0.249130   -0.897727   -0.363346
 -0.702157    0.649390    0.292006
  0.308787   -0.934281   -0.178241
 -0.090473   -0.985618   -0.142729
  0.192028    0.978652    0.073242
  0.949862    0.164226    0.266067
 -0.080245   -0.927951    0.363962
 -0.876754    0.140890    0.459840
  0.873390    0.058716   -0.483469
  0.719649    0.648967   -0.246875
  0.726702   -0.660396    0.189160
  0.900750    0.421665    0.104157
  0.995958    0.082252   -0.036092
  0.979358    0.147565   -0.138142
  0.177033   -0.826144   -0.534925
  0.658131   -0.592515    0.464532
  0.412641   -0.824654    0.386876
 -0.534384    0.664747    0.522059
  0.598686   -0.579564   -0.552884

_ExtentOfTheSearch
   9
_AngularDeviationCriterion
   2.0
_MaxAllowedMillerIndex
   8
```

Table 7: The best solution from the *IndX_Laue* output file.

```
  Direct basis vectors (in rows) = inverse of UB matrix;
  transforms RL vectors to Miller indices :
           -0.81431575   -0.30540891    0.19624090
           -0.26822567   -0.55078048   -0.89243546
           -0.63065968    0.80708863   -0.35715601

       |   h   k   l |      Real (hkl)       |  Error
-------------------------------------------------------------
  1  H- |   1   0   2 |   1.00   0.01   2.00  |  0.015
  2  H- |   3   2  -1 |   2.98   2.02  -1.00  |  0.026
  3  H- |  -3  -2   0 |  -3.00  -2.00   0.02  |  0.019
  4  H- |   2  -1   4 |   2.00  -1.00   4.00  |  0.000
  5  H- |   1   0   0 |   1.00   0.00   0.00  |  0.000
  6  H- |   1   0  -2 |   0.99   0.00  -2.00  |  0.009
  7  H- |  -3   0  -2 |  -3.01  -0.02  -1.98  |  0.024
  8  H- |   0   1  -1 |   0.00   1.00  -1.00  |  0.000
  9  H- |   1  -1   2 |   1.00  -1.00   2.00  |  0.003
 10  H- |   0   2  -3 |   0.00   2.00  -3.00  |  0.004
 11  H- |   1   2  -2 |   1.00   2.01  -1.99  |  0.015
 12  H- |  -2  -3   3 |  -2.03  -3.02   2.96  |  0.055
 13  H- |  -4  -3  -3 |  -4.02  -3.04  -2.93  |  0.085
 14  H- |   2   1  -4 |   2.02   1.00  -3.99  |  0.026
 15  H- |   3  -1   2 |   3.01  -1.00   1.99  |  0.017
 16  H- |  -5   1  -2 |  -5.00   1.00  -2.01  |  0.006
 17  H- |  -5  -2   1 |  -5.01  -1.99   0.95  |  0.051
 18  H- |  -1   0  -3 |  -1.00   0.00  -3.00  |  0.000
 19  H- |  -3  -2  -1 |  -3.00  -2.02  -0.95  |  0.059
 20  H- |  -3  -1  -2 |  -3.02  -1.00  -1.97  |  0.040
 21  H- |  -4  -1  -2 |  -3.97  -1.01  -2.05  |  0.059
 22  H- |   0   3  -2 |   0.01   3.00  -1.99  |  0.013
 23  H- |  -1  -1  -4 |  -1.00  -1.00  -4.00  |  0.004
 24  H- |   0   0  -1 |  -0.01   0.00  -1.00  |  0.008
 25  H- |   1  -2   2 |   0.98  -2.01   2.00  |  0.026
 26  H- |  -2   3  -3 |  -1.95   3.03  -3.01  |  0.062
-------------------------------------------------------------
Odd [%] |  31  25  19 |
-------------------------------------------------------------
  26h and  26H vectors out of  26.    Quality : 1.000

 Primitive cell :
                          8.916   10.825   10.848
                         87.88    78.25    77.34

 Volume of the cell  :     1000.00

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```

The scaling factor determined using the algorithm described in Appendix A is $S = 5.78807$Å. The corresponding volume of the cell is $V = S^3 = 193.91$Å^3. With the default volume of 1000Å^3 used by *IndX_Laue*, the parameters a, b and c resulting from *IndX_Laue* need to be multiplied by $(193.91/1000)^{1/3} = 0.578807$. Thus, the primitive cell parameters are $a = 5.161$, $b = 6.266$ and $c = 6.279$. The integers m determining the order of reflections are

equal to 1 in all cases except the reflections 5, 8, 9 and 24 for which they are 2, 3, 2 and 4, respectively. The relationship between the resulting reflection indices $\mathtt{h}$ and the indices $\mathtt{h}_{Li}$ is $\pm T\,\mathtt{h} = \mathtt{h}_{Li}$, where

$$T = \begin{bmatrix} -3 & 19 & 17 \\ 2 & -12 & -11 \\ 0 & -1 & -1 \end{bmatrix} .$$

The only exception is the reflection 24 with the indices related via $-T\,\mathtt{h} = 2\,\mathtt{h}_{Li}$.

On recommendation of an anonymous reviewer, below is a derivation of the formula for determination of the scattering vector $\boldsymbol{H}$ from positions of edges of an EBSD band.

Let $\boldsymbol{k}_0$ and $\boldsymbol{k}$ denote the wave vectors of the incident and the diffracted beams, respectively. The derivation is based on the Laue equation $\boldsymbol{H} = \boldsymbol{k} - \boldsymbol{k}_0$ and the condition $\boldsymbol{k}^2 = \boldsymbol{k}_0^2$ $(= 1/\lambda^2)$ arising from energy conservation[1]. Edges of EBSD bands are generated by divergent beams, i.e., directions of the vectors $\boldsymbol{k}_0$ are arbitrary. The formula governing the wave vectors of diffracted beams is obtained by eliminating $\boldsymbol{k}_0$; one has

$$\boldsymbol{H} \cdot (\boldsymbol{H} - 2\boldsymbol{k}) = (\boldsymbol{k} - \boldsymbol{k}_0) \cdot ((\boldsymbol{k} - \boldsymbol{k}_0) - 2\boldsymbol{k}) = \boldsymbol{k}_0^2 - \boldsymbol{k}^2 = 0 \ .$$

Thus, the wave vectors $\boldsymbol{k}$ corresponding to the scattering vector $\boldsymbol{H}$ are on the cone described by $\boldsymbol{H} \cdot (\boldsymbol{H} - 2\boldsymbol{k}) = 0$. Similarly, the wave vectors corresponding to $-\boldsymbol{H}$ are on the cone $(-\boldsymbol{H}) \cdot ((-\boldsymbol{H}) - 2\boldsymbol{k}) = \boldsymbol{H} \cdot (\boldsymbol{H} + 2\boldsymbol{k}) = 0$. Let the wave vector $\boldsymbol{k}_1$ be on the first cone and and $\boldsymbol{k}_2$ on the second cone, i.e.,

$$\boldsymbol{H} \cdot (\boldsymbol{H} - 2\boldsymbol{k}_1) = 0 \ , \quad \boldsymbol{H} \cdot (\boldsymbol{H} + 2\boldsymbol{k}_2) = 0 \ .$$

By adding and subtracting the sides of these equations, one gets

$$\boldsymbol{H} \cdot (\boldsymbol{H} - (\boldsymbol{k}_1 - \boldsymbol{k}_2)) = 0 \ , \quad \boldsymbol{H} \cdot (\boldsymbol{k}_1 + \boldsymbol{k}_2) = 0 \ . \tag{1}$$

If $\boldsymbol{H}$, $\boldsymbol{k}_1$ and $\boldsymbol{k}_2$ are coplanar, one can express the scattering vector as a linear combination of $\boldsymbol{k}_1$ and $\boldsymbol{k}_2$. With $\boldsymbol{H} = \alpha_1 \boldsymbol{k}_1 + \alpha_2 \boldsymbol{k}_2$, eqs.(1) can be written in the form

$$\boldsymbol{H} \cdot ((\alpha_1 \boldsymbol{k}_1 + \alpha_2 \boldsymbol{k}_2) - (\boldsymbol{k}_1 - \boldsymbol{k}_2)) = 0 \ , \quad (\alpha_1 \boldsymbol{k}_1 + \alpha_2 \boldsymbol{k}_2) \cdot (\boldsymbol{k}_1 + \boldsymbol{k}_2) = 0 \ .$$

Using $\boldsymbol{H} \cdot \boldsymbol{k}_1 = \boldsymbol{H}^2/2$ and $\boldsymbol{H} \cdot \boldsymbol{k}_2 = -\boldsymbol{H}^2/2$, one obtains

$$(\alpha_1 - \alpha_2 - 2)\boldsymbol{H}^2 = 0 \ , \quad (\alpha_1 + \alpha_2)(1/\lambda^2 + \boldsymbol{k}_1 \cdot \boldsymbol{k}_2) = 0 \ . \tag{2}$$

Both $\boldsymbol{H}^2$ and $1/\lambda^2 + \boldsymbol{k}_1 \cdot \boldsymbol{k}_2$ are positive for physical reasons, and this means that eqs.(2) are solved by $\alpha_1 = 1$ and $\alpha_2 = -1$. Thus, the scattering vector can be expressed as

$$\boldsymbol{H} = \boldsymbol{k}_1 - \boldsymbol{k}_2 = (\widehat{\boldsymbol{k}}_1 - \widehat{\boldsymbol{k}}_2)/\lambda \ , \tag{3}$$

where $\widehat{\boldsymbol{k}}_j = \boldsymbol{k}_j/|\boldsymbol{k}_j| = \lambda \boldsymbol{k}_j$ $(j = 1, 2)$, and the vectors $\widehat{\boldsymbol{k}}_1$ and $\widehat{\boldsymbol{k}}_2$ are coplanar with $\boldsymbol{H}$. When $\widehat{\boldsymbol{k}}_j$ is directed toward the foot of the perpendicular from the pattern center of the j-th edge, the condition of coplanarity is satisfied. Thus, knowing the vectors $\widehat{\boldsymbol{k}}_j$ for the band edges and the wavelength λ, one can determine the scattering vector corresponding to the band by using eq.(3).

References

[1] Lili Li and Ming Han. Determining the Bravais lattice using a single electron backscatter diffraction pattern. *J. Appl. Cryst.*, 48:107–115, 2015.

[1] Formation of EBSD patterns involves inelastic scattering but the energy loss is negligible.