

Function: KiKoCh2 is a program for crystal orientation determination based on indexing diffraction data given in the form of normalized scattering vectors. The data can be obtained from EBSD patterns, Kikuchi patterns, Laue patterns, Kossel patterns et cetera.

Files:

KiKoCh2.exe – 32-bit executable compiled under MS Windows,
 exmpl_TEM_hex.kk2 – example data file,
 KiKoCh2.pdf – this file.

Distribution: Free for academic use.

Method: To be described in a journal paper.

Execution: Run KiKoCh2 and respond to the question about filename, or run KiKoCh2 filename.kk2. The filename must **not** contain spaces; otherwise, use KiKoCh2 "filename with spaces.kk2". The extension .kk2 is mandatory.

Input file: To learn the structure of the input file examine example.kk2. The input file contains keywords followed by appropriate data. The keywords are listed in Table below. The last of the keywords must be `_PatternData`. It is mandatory, and it is followed by properly formatted data for individual diffraction patterns. For each pattern, there are

- a line with arbitrary content; it must be present but the content is not read,
- a line with the number of scattering vectors, say N ,
- N lines, each with three components of nonzero scattering vectors specified by their Cartesian coordinates in sample reference frame \mathbf{e}_i^s ($i = 1, 2, 3$).

The number of scattering vectors N must be in the range $[2, 32]$. (The upper limit can be changed in the source code. It is specified there by the parameter `max_numOfScattVects`.) The beginning of the data block may look like this

```
_PatternData
  Pattern no 1
    5
      0.5122664   0.5300164  -0.6757705
      0.8116305   0.5572611  -0.1752597
      0.8408079  -0.2067043  -0.5003153
     -0.5705720   0.7394485  -0.3573004
     -0.5049917   0.8383213  -0.2054283
  Pattern no 2
    7
      0.5444633   0.8370910  -0.0532769
      0.2874883  -0.9149224  -0.2833151
      ...         ...         ...
```

The list of optional keywords includes:

	Type	Range	Default
<code>_LatticeBasis</code>	3×3 matrix of F		Identity matrix
<code>_NumberOfFamiliesOfReflectingPlanes</code>	I	[1, 128]	4
<code>_FamiliesOfReflectingPlanes</code>	list of triplets I		(see below)
<code>_NumberOfSymmetryOperations</code>	I	≤ 24	24
<code>_SymmetryOperations</code>	list of quadruplets F		point group O
<code>_IndexingStrategy</code>	I	{1, 2, 3, 4}	3
<code>_ParametersOfStrategy</code>	FF	[0.1°, 10.0°]	{2.0°, 3.5°}
<code>_NumberOfPatterns</code>	I	[1, HUGE(I)]	HUGE(I)

If present, the specification of the parameter `_NumberOfFamiliesOfReflectingPlanes` must precede `_FamiliesOfReflectingPlanes`.

If present, the specification of `_NumberOfSymmetryOperations` must precede the keyword `_SymmetryOperations`.

- The keyword `_LatticeBasis` must be followed by three lines with three basis vectors $\{\mathbf{a}, \mathbf{b}, \mathbf{c}\} = \{\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3\}$ of the (direct) crystal lattice. Each vector is given the form of its three components in the Cartesian system \mathbf{e}_i^c ($i = 1, 2, 3$) attached to the crystal, i.e., the matrix M below `_LatticeBasis` has the entries $M_{ij} = \mathbf{a}_i \cdot \mathbf{e}_j^c$ ($i, j = 1, 2, 3$). For instance, for hexagonal lattice of Zn (with lattice parameters in Å) one may have

```

_LatticeBasis
  2.6649  0.0000  0.0000
 -1.3325  2.3079  0.0000
  0.0000  0.0000  4.9468

```

This means that the basis vectors are

$$\begin{aligned}
 \mathbf{a} &= \mathbf{a}_1 = 2.6649 \mathbf{e}_1^c + 0.0000 \mathbf{e}_2^c + 0.0000 \mathbf{e}_3^c, \\
 \mathbf{b} &= \mathbf{a}_2 = -1.3325 \mathbf{e}_1^c + 2.3079 \mathbf{e}_2^c + 0.0000 \mathbf{e}_3^c, \\
 \mathbf{c} &= \mathbf{a}_3 = 0.0000 \mathbf{e}_1^c + 0.0000 \mathbf{e}_2^c + 4.9468 \mathbf{e}_3^c.
 \end{aligned}$$

The default `_LatticeBasis` is the identity matrix (cubic lattice).

- The keyword `_NumberOfFamiliesOfReflectingPlanes` must be followed by a line with an integer indicating the number of families of reflections expected to be detected in the diffraction pattern. For instance, one may have

```

_NumberOfFamiliesOfReflectingPlanes
  6

```

This number cannot be smaller than 1 and it cannot exceed 128. (The upper limit can be changed in the source code. It is specified there by the parameter `max_n_of_hkl`.)

If the keyword `_NumberOfFamiliesOfReflectingPlanes` is used, the next keyword must be `_FamiliesOfReflectingPlanes`.

- The keyword `_FamiliesOfReflectingPlanes` must be followed by lines with triplets of Miller indices of families of reflecting planes (i.e., indices of high intensity reflections expected to be detected in the diffraction pattern). For instance,

```

_FamiliesOfReflectingPlanes
  0   1   0
  0   0   2
  0   1   1
  0   1   2
  1   1   0
  0   1   3

```

means that these families are $\{010\}$, $\{002\}$, $\{011\}$, $\{012\}$, $\{110\}$ and $\{013\}$.

If the keyword `_FamiliesOfReflectingPlanes` is used in a given data file, it must be preceded by the keyword `_NumberOfFamiliesOfReflectingPlanes`.

The default value of `_NumberOfFamiliesOfReflectingPlanes` is 4, and the default families of reflecting planes are $\{111\}$, $\{002\}$, $\{022\}$ and $\{113\}$ (fcc lattice).

- The keyword `_NumberOfSymmetryOperations` must be followed by a line with an integer in with the number of proper rotations in the Laue (point) group of the crystal. For instance,

```

_NumberOfSymmetryOperations
  12

```

means that the number of proper rotations in the Laue group is 12.

If the keyword `_NumberOfSymmetryOperations` is used in a give file, the next keyword must be `_SymmetryOperations`.

- The keyword `_SymmetryOperations` must be followed by lines with symmetry operations of the Laue group. The operations are specified by the coordinates of the rotation axis in the Cartesian system \mathbf{e}_i^c ($i = 1, 2, 3$) attached to the crystal and the rotation angle in degrees. For instance, one may have

```

_SymmetryOperations
  0.0000  0.0000  1.0000  0.000
  0.0000  0.0000  1.0000  60.000
  0.0000  0.0000  1.0000  120.000
  ...    ...    ...    ...

```

i.e., the first symmetry is the identity operation, the second and third are rotations about \mathbf{e}_3^c by the angles of 60° and 120° , respectively. If the keyword `_SymmetryOperations` is used, it must be preceded by the keyword `_NumberOfSymmetryOperations`.

The default value of `_NumberOfSymmetryOperations` is 24, and the default symmetry operations are those from the chiral octahedral point group O (432).

- The keyword `_IndexingStrategy` must be followed by one of the integers 1, 2, 3 or 4. The integer indicates the strategy to be used in computation. The numbers 1, 2, 3 and 4 correspond to the strategies A, B, C and D, respectively. For instance,

```
_IndexingStrategy
      2
```

means that the strategy B will be used. The default value of `_IndexingStrategy` is 3.

- The keyword `_ParametersOfStrategy` must be followed by a line with two positive real numbers specifying parameters p_1 and p_2 . For instance, if the data are

```
_ParametersOfStrategy
      2.0   1.1
```

the program will run with $p_1 = 2.0^\circ$ and $p_2 = 1.1^\circ$. The range of each of these parameters is $[0.1^\circ, 10.0^\circ]$. The default values are $p_1 = 2.0^\circ$ and $p_2 = 3.5^\circ$.

- The keyword `_NumberOfPatterns` must be followed by a line with an integer specifying the number of patterns to be processed. For instance, with

```
_NumberOfPatterns
      100000
```

that there should be at least 100.000 data sets (patterns) in the section `_PatternData`; if there are more sets, only the first 100.000 will be processed. The minimal value of `_NumberOfPatterns` is 1. The largest allowed (and default) value of `_NumberOfPatterns` is HUGE(I) (= 2147483647).

Output file: A run of KiKoCh2 on `filename.kk2` will produce a file `filename_kk2.res`. E.g., KiKoCh2 `example.kk2` gives `example_kk2.res`. The file contains `_NumberOfPatterns` rows and seven columns. Each row corresponds to one data set (pattern).

The data in the columns are:

column 1 (**no**) – pattern number,

columns 2–4 (**ph1_1 Phi phi_2**) – Euler angles $\varphi_1, \phi, \varphi_2$ (in degrees) in Bunge’s convention,

column 5 (**used**) – number of scattering vectors (reflections) used in indexing,

column 6 (**all**) – number of scattering vectors provided in data file,

column 7 (**fit**) – the average angular deviation (in degrees) between used scattering vectors and the directions of corresponding reciprocal lattice vectors.

The special orthogonal matrix $O = O(\varphi_1, \phi, \varphi_2)$ determined by the resulting Euler angles φ_1, ϕ and φ_2 relates the Cartesian reference frames \mathbf{e}_i^s and \mathbf{e}_i^c via $\mathbf{e}_i^c \approx \sum_j O_{ij} \mathbf{e}_j^s$. The Miller indices $(hkl) = (h_1 h_2 h_3)$ of the reflection $\mathbf{s} = \sum_i s_i \mathbf{e}_i^s$ are $h_i \tilde{\propto} \sum_{j,k} M_{ij} O_{jk} s_k$.