Niggli cell

Usage of the code

The code is written in C and a python wrapper is prepared in `python` directory. The C code is used to compile with your code. Usual library interface is not prepared. The python code is used as a module. To use this, `numpy` is required.

In both C and python codes, there are two input arguments, `lattice` and `eps`. `lattice` is a `double` array with nine elements,

$$(a_x, b_x, c_x, a_y, b_y, c_y, a_z, b_z, c_z).$$

In python, the input array will be fattened in the module. Therefore, e.g., the following 3×3 shape of a numpy array or a python list is accepted:

$$\begin{pmatrix} a_x & b_x & c_x \\ a_y & b_y & c_y \\ a_z & b_z & c_z \end{pmatrix}.$$

The `double` variable of `eps` is used as the tolerance parameter. The value should be much smaller than lattice parameters, e.g., 1e-8. How it works is shown in the following section.

Test

The test is found in `python` directory as a python code. A set of lattice parameters is found in `lattices.dat` and the references, which are the reduced lattice parameter made in the version 0.1.1, are stored in `reduced_lattices.dat`.

Example

An example is found in `python` directory as a python code.

Algorithm to determine Niggli cell

Reference

1. A Unified Algorithm for Determining the Reduced (Niggli) Cell, I. Krivý and B. Gruber, Acta Cryst., A32, 297-298 (1976)
2. The Relationship between Reduced Cells in a General Bravais lattice, B. Gruber, Acta Cryst., A29, 433-440 (1973)
3. Numerically stable algorithms for the computation of reduced unit cells, R. W. Grosse-Kunstleve,

N. K. Sauter and P. D. Adams, Acta Cryst., A60, 1-6 (2004)

Algorithm

Update variables

The following variables used in this algorithm are initialized at the beginning of the algorithm and updated at the every end of A1-8 steps.

Define following variables as

$$
\begin{aligned}
A &= \mathbf{a} \cdot \mathbf{a} \\
B &= \mathbf{b} \cdot \mathbf{b} \\
C &= \mathbf{c} \cdot \mathbf{c} \\
\xi &= 2\mathbf{b} \cdot \mathbf{c} \\
\eta &= 2\mathbf{c} \cdot \mathbf{a} \\
\zeta &= 2\mathbf{a} \cdot \mathbf{b}.
\end{aligned}
$$

They are elements of metric tensor where the off-diagonal elements are doubled. Therefore the metric tensor $\mathbf{G}$ is represented as

$$
\mathbf{G} = \begin{pmatrix} A & \zeta/2 & \eta/2 \\ \zeta/2 & B & \xi/2 \\ \eta/2 & \xi/2 & C \end{pmatrix}.
$$

ξ, η, ζ are sorted by their ranges of angles as shown below.

Angle	value
Acute	1
Obtuse	-1
Right	0

These values are stored in variables l, m, n as follows.

- Set initially $l = m = n = 0$.
- If $\xi < -\varepsilon, l = -1$.
- If $\xi > \varepsilon, l = 1$.
- If $\eta < -\varepsilon, m = -1$.
- If $\eta > \varepsilon, m = 1$.
- If $\zeta < -\varepsilon, n = -1$.
- If $\zeta > \varepsilon, n = 1$.

$\mathbf{C}$ found in each step is the transformation matrix that is applied to basis vectors:

$$
(\mathbf{a}', \mathbf{b}', \mathbf{c}') = (\mathbf{a}, \mathbf{b}, \mathbf{c})\mathbf{C}.
$$

A1

If $A > B + \varepsilon$ or ($\overline{|A - B| > \varepsilon}$ and $|\xi| > |\eta| + \varepsilon$),

$$\mathbf{C} = \begin{pmatrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$

A2

If $B > C + \varepsilon$ or ($\overline{|B - C| > \varepsilon}$ and $|\eta| > |\zeta| + \varepsilon$),

$$\mathbf{C} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & -1 & 0 \end{pmatrix}.$$

Go to A1.

A3

If $lmn = 1$:

- $i = -1$ if $l = -1$ else $i = 1$
- $j = -1$ if $m = -1$ else $j = 1$
- $k = -1$ if $n = -1$ else $k = 1$

$$\mathbf{C} = \begin{pmatrix} i & 0 & 0 \\ 0 & j & 0 \\ 0 & 0 & k \end{pmatrix}.$$

A4

If $l = -1$, $m = -1$, and $n = -1$, do nothing in A4.

If $lmn = 0$ or $lmn = -1$:

Set $i = j = k = 1$. r is used as a reference to i, j, or k, and is initially undefined.

- $i = -1$ if $l = 1$
- $r \to i$ if $l = 0$
- $j = -1$ if $m = 1$
- $r \to j$ if $j = 0$
- $k = -1$ if $n = 1$
- $r \to k$ if $k = 0$

If $ijk = -1$:

- i, j, or k refered by r is set to -1.

$$\mathbf{C} = \begin{pmatrix} i & 0 & 0 \\ 0 & j & 0 \\ 0 & 0 & k \end{pmatrix}.$$

A5

If $|\xi| > B + \varepsilon$ or $(\overline{|B - \xi| > \varepsilon}$ and $2\eta < \zeta - \varepsilon)$ or $(\overline{|B + \xi| > \varepsilon}$ and $\zeta < -\varepsilon)$:

$$\mathbf{C} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & -\mathrm{sign}(\xi) \\ 0 & 0 & 1 \end{pmatrix}.$$

Go to A1.

A6

If $|\eta| > A + \varepsilon$ or $(\overline{|A - \eta| > \varepsilon}$ and $2\xi < \zeta - \varepsilon)$ or $(\overline{|A + \eta| > \varepsilon}$ and $\zeta < -\varepsilon)$:

$$\mathbf{C} = \begin{pmatrix} 1 & 0 & -\mathrm{sign}(\eta) \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

Go to A1.

A7

If $|\zeta| > A + \varepsilon$ or $(\overline{|A - \zeta| > \varepsilon}, 2\xi < \eta - \varepsilon)$ or $(\overline{|A + \zeta| > \varepsilon}$ and $\eta < -\varepsilon)$:

$$\mathbf{C} = \begin{pmatrix} 1 & -\mathrm{sign}(\zeta) & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

Go to A1.

A8

If $\xi + \eta + \zeta + A + B < -\varepsilon$ or $(\overline{|\xi + \eta + \zeta + A + B| > \varepsilon}$ and $2(A + \eta) + \zeta > \varepsilon)$:

$$\mathbf{C} = \begin{pmatrix} 1 & 0 & 1 \\ 0 & 1 & 1 \\ 0 & 0 & 1 \end{pmatrix}.$$

Go to A1.