

# 1 Making a new lattice

Given a set of cartesian basis vectors  $\mathbf{L}$  and a matrix  $\mathbf{M}$  in Hermite normal form, construct a new lattice

$$\mathbf{L}' = \mathbf{L}\mathbf{M} \quad (1)$$

The integer matrix  $\mathbf{M}$  has the following form:

$$\mathbf{M} = \begin{pmatrix} a & d & e \\ 0 & b & f \\ 0 & 0 & c \end{pmatrix} \quad (2)$$

with

$$d, e \in [-(a-1)/2, -(a-1)/2 + 1, \dots, (a-1)/2] ; a \text{ odd} \quad (3)$$

$$d, e \in [-a/2 + 1, -a/2 + 2, \dots, a/2], a \text{ even} \quad (4)$$

$$f \in [-(b-1)/2, -(b-1)/2 + 1, \dots, (b-1)/2] ; b \text{ odd} \quad (5)$$

$$f \in [-a/2 + 1, -a/2 + 2, \dots, a/2] ; b \text{ even} \quad (6)$$

$$a > 0 \quad (7)$$

$$b > 0 \quad (8)$$

$$c > 0 \quad (9)$$

$$(10)$$

The determinant of  $\mathbf{M}$  describes the volume ratio of the newly chosen cell to the original cell. As the determinant of  $\mathbf{M}$  is equal to  $abc$ , all matrices with a certain determinant  $\Delta$  can be easily constructed by finding all triples  $(a, b, c)$  for which  $\Delta = abc$ . A simple use of a brute force integer factorisation (known as trial factorisation) algorithm, can return these triples fast.

The construction of a new lattice is thus relatively straightforward.

# 2 Unit cell comparison

Say we have a basis  $\mathbf{L}_r$  in the reference setting. Transform it to the Niggli setting:

$$\mathbf{L}_n = \mathbf{R}_n \mathbf{L}_r \mathbf{R}_n^{-1} \quad (11)$$

Do the same for a *target* lattice:

$$\mathcal{L}_n = \mathcal{R}_n \mathcal{L}_r \mathcal{R}_n^{-1} \quad (12)$$

We are looking for a matrix  $\mathbf{M}$  and affine (*similarity*) transform of the lattice  $\mathbf{S}$  for which

$$\mathcal{L}_n \approx \mathbf{S}\mathbf{L}_n\mathbf{M}\mathbf{S}^{-1} \quad (13)$$

If one desires to explore all matrices  $\mathbf{M}$  with determinant equal to 10, only 217 matrices need to be checked. The big computational cost are the number of affine transformations to check. One hopes all unimodular matrices are sufficient.

### 3 What happens to the coordinates?

Say a match between two lattices is found (i.e.  $\mathbf{M}$  and  $\mathbf{S}$  are known), how to compare coordinates? It would be instructive to figure out how a set of coordinates transform. As the only thing that is done in this analyses, is change coordinates systems, it is usefull to stress that the cartesian coordinates of the molecules in the lattice under question remain the same upon the action of  $\mathbf{M}$ :

$$\mathbf{x}_c = \mathbf{L}_n\mathbf{x}_{f,n} \quad (14)$$

$$\mathbf{x}_c = \mathbf{L}'\mathbf{x}'_f \quad (15)$$

$$(16)$$

and thus

$$\mathbf{L}_n\mathbf{x}_{f,n} = \mathbf{L}_n\mathbf{M}\mathbf{x}'_f \quad (17)$$

$$\mathbf{x}_{f,n} = \mathbf{M}\mathbf{x}'_f \quad (18)$$

and here it stops because 1) I am not sure where to go from this 2) I am not sure which question to ask I would like to get a full set of transformation laws of course that allow me generate new miller indices from old ones, and be able to tell something about which rotation needs to be carried out to bring coordinates from  $\mathcal{L}'$  to  $\mathbf{L}$ . One thing that worries me are origin shifts and how to take them into account.