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A Unified Algorithm for Determining the Reduced (Niggli) Cell

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An algorithm is proposed which enables one, starting from an arbitrary primitive cell of a three-dimensional Bravais lattice, to reach the Niggli form requisite for the lattice type determination.

Introduction

By a Niggli cell we understand (Santoro & Mighell, 1970; Gruber, 1973) that cell of a three-dimensional Bravais lattice which is based on the reduction theory of the positive definite quadratic forms (Eisenstein, 1851). Its significance is in its uniqueness and in the possibility that it can be used for determining the Bravais type of the lattice (Niggli, 1928; Azároff & Buerger, 1958). However, how to obtain it is not straightforward.

By means of an algorithm which was proposed by Buerger (1957, 1960) and made more economical by Gruber (1973) we can reach fairly simply the Buerger cell, *i.e.* the cell characterized by the shortest three non-coplanar translations. If this Buerger cell in the given lattice is unique, it is simultaneously the Niggli cell and the problem is solved. But this need not be always the case. As Gruber (1973) has shown, there exist Bravais lattices with two, three, four or even five different Buerger cells. Then we have to apply the table given in Santoro & Mighell (1970) which contains transformation matrices by means of which any Buerger cell may be converted into the Niggli cell. It is clear that the application of a table is not welcome if a computer is employed.

However, this two-part procedure may be reduced to one which makes use solely of an algorithm. Moreover, the new algorithm is almost as simple as the original. This is due to the fact that Santoro & Mighell's transformations (which are, by the way, not unique) are very similar to though not identical with those which occur in the Buerger algorithm. Thus they can be, when slightly modified, directly incorporated into it (Křivý, 1973).

The question arises whether it is impossible for the new algorithm to get into an infinite cycle. This danger does not exist in the original algorithm since at every step (save the normalization) the sum $a+b+c$ diminishes. With the present algorithm, however, the sum may remain unchanged. We have not found any better way to overcome this difficulty than to analyse all possible cases which satisfy the new additional conditions. This is a tedious approach but guarantees that the algorithm will end after a finite number of steps. That the resulting values describe a Niggli cell is apparent.

The basis of the algorithm is Gruber's (1973) formulation. Here, however, the function *entier* is avoided since it could, under the new conditions, be equal to zero and the algorithm would fail. It is replaced by the function *sign* (meaning sign $x=1$ for $x>0$ and sign $x=-1$ for $x<0$) which avoids this disadvantage. The points 1,2,3,4 provide the normalization. We can start from any primitive cell

$$a,\ b,\ c,\ \cos\alpha,\ \cos\beta,\ \cos\gamma$$

of the Bravais lattice in question. If

$$A,\ B,\ C,\ \xi,\ \eta,\ \zeta \qquad (1)$$

are the resulting values obtained by performing the algorithm then the matrix

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

stands for the well-known Niggli form and can be immediately used for the lattice type determination (Niggli, 1928; Azároff & Buerger, 1958). The values

$$a'=\sqrt{A}, \qquad b'=\sqrt{B}, \qquad c'=\sqrt{C}$$
$$\cos\alpha'=\xi/2b'c', \quad \cos\beta'=\eta/2a'c', \quad \cos\gamma'=\zeta/2a'b'$$

describe the Niggli cell in the usual way.

Algorithm

0. Put $(a^2,b^2,c^2)\rightarrow(A,B,C)$,
   $(2bc\cos\alpha,\ 2ac\cos\beta,\ 2ab\cos\gamma)\rightarrow(\xi,\eta,\zeta)$.
1. If $A>B$ or $(A=B,\ |\xi|>|\eta|)$, change $(A,\xi)\leftrightarrow(B,\eta)$.
2. If $B>C$ or $(B=C,\ |\eta|>|\zeta|)$, change $(B,\eta)\leftrightarrow(C,\zeta)$ and go to 1.
3. If $\xi\eta\xi>0$, put $(|\xi|,|\eta|,|\zeta|)\rightarrow(\xi,\eta,\zeta)$.
4. If $\xi\eta\zeta\leq 0$, put $(-|\xi|,-|\eta|,-|\zeta|)\rightarrow(\xi,\eta,\zeta)$.
5. If $|\xi|>B$ or $(\xi=B,\ 2\eta<\zeta)$ or $(\xi=-B,\ \zeta<0)$, put
   $B+C-\xi \quad \text{sign}\ \xi\rightarrow C$,
   $\eta-\zeta \quad \text{sign}\ \xi\rightarrow\eta$,
   $\xi-2B \quad \text{sign}\ \xi\rightarrow\xi$
   and go to 1.

6. If $|\eta| > A$ or $(\eta = A, 2\xi < \zeta)$ or $(\eta = -A, \zeta < 0)$,
   put $A + C - \eta$ sign $\eta \rightarrow C$,
   $\xi - \zeta$ sign $\eta \rightarrow \xi$,
   $\eta - 2A$ sign $\eta \rightarrow \eta$
   and go to 1.
7. If $|\zeta| > A$ or $(\zeta = A, 2\xi < \eta)$ or $(\zeta = -A, \eta < 0)$,
   put $A + B - \zeta$ sign $\zeta \rightarrow B$,
   $\xi - \eta$ sign $\zeta \rightarrow \xi$,
   $\zeta - 2A$ sign $\zeta \rightarrow \zeta$
   and go to 1.
8. If $\xi + \eta + \zeta + A + B < 0$ or
   $[\xi + \eta + \zeta + A + B = 0, 2(A + \eta) + \zeta > 0]$,
   put $A + B + C + \xi + \eta + \zeta \rightarrow C$,
   $2B + \xi + \zeta \rightarrow \xi$,
   $2A + \eta + \zeta \rightarrow \eta$
   and go to 1.

Example

Suppose the values

$$a = 3{\cdot}000 \quad b = 5{\cdot}196 \quad c = 2{\cdot}000$$
$$\alpha = 103°55' \quad \beta = 109°28' \quad \gamma = 134°53'$$

characterize a primitive cell of the lattice L. According to point 0 of the algorithm we put

$$A = 9, \quad B = 27, \quad C = 4, \quad \xi = \bar{5}, \quad \eta = \bar{4}, \quad \zeta = \overline{22}.$$

Table 1. *The progress of the algorithm*

	A	B	C	ξ	η	ζ		
2.	9	27	4	$\bar{5}$	$\bar{4}$	$\overline{22}$		
1.	9	4	27	$\bar{5}$	$\overline{22}$	$\bar{4}$		
5.	4	9	27	$\overline{22}$	$\bar{5}$	$\bar{4}$		
6.	4	9	14	$\bar{4}$	$\bar{9}$	$\bar{4}$		
7.	4	9	9	$\bar{8}$	$\bar{1}$	$\bar{4}$	B	
3.	4	9	9	$\bar{9}$	$\bar{1}$	4		
5.	4	9	9	9	1	4	B	
3.	4	9	9	$\bar{9}$	$\bar{3}$	4		
	4	9	9	9	3	4	B	N

The error is nowhere greater than 0·025%. The algorithm then runs as in Table 1. The first column of Table 1 indicates the points of the algorithm which are applied to the values in the same row. The letters B, N denote [after normalizing the values (1)] the Buerger* and Niggli cells, respectively. The Niggli matrix form reads

$$\begin{pmatrix} 4 & 9 & 9 \\ \frac{9}{2} & \frac{3}{2} & 2 \end{pmatrix}$$

and shows that L is triclinic. The parameters of the Niggli cell are

$$a' = 2{\cdot}000 \quad b' = 3{\cdot}000 \quad c' = 3{\cdot}000$$
$$\alpha' = 60°00' \quad \beta' = 75°31' \quad \gamma' = 70°32'.$$

This example is, deliberately, rather an exceptional case. As a rule, when reaching a Buerger cell which is not a Niggli cell, we get the Niggli cell in the next step. Only when

$$A < B, \quad \xi + \eta = -B, \quad -A/2 < \eta < 0, \quad \zeta = -A$$

[the values (1) being normalized] do we need two steps. This can be ascertained from the Table compiled by Gruber (1973) which lists all ambiguities between Buerger cells.

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* A Buerger cell can be recognized by fulfilling the inequalities $|\xi| \leq B$, $|\eta| \leq A$, $|\zeta| \leq A$, $\xi + \eta + \zeta + A + B \geq 0$ [supposing the values (1) are normalized] or by minimizing the sum $A + B + C$.

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