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The Least Set of Conditions to Specify a Bravais Lattice Uniquely in its Parameter Space

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Abstract

A necessary and sufficient region to express a Bravais lattice uniquely in its six-dimensional parameter space is newly obtained. The incorrect method and result of the previous paper [M.Hosoya, *J. Phys. A:Math. Gen.*, 19:1801 (1986)] are revised. The region is specified by only six conditions which cut a convex polytope in the parameter space. It is shown that the region is equivalent to that given from the conditions to specify the reduced bases. Transformation matrices are shown explicitly which convert the parameters of the reduced basis into those within the region in one-to-one correspondence.

Introduction

In order to investigate crystal structures generally in their parameter-space, we must first determine the necessary and sufficient region to represent all the possible structures uniquely¹⁾. In the simplest case which only deals with the structures with an atom per primitive cell, its necessary and sufficient region must be equivalent to that given by the conditions to specify the reduced bases of lattices, for they were also established to represent all the Bravais lattices uniquely (Niggli²⁾, Buerger^{3,4)}, Mighell, et al.⁵⁾, Mighell,⁶⁾). However the region given by the reduced bases has a disadvantage for theoretical treatment of crystal structures. Using the following six scalar products of the edge vectors a , b , c of a primitive cell

$$A = \mathbf{a} \cdot \mathbf{a} \quad B = \mathbf{b} \cdot \mathbf{b} \quad C = \mathbf{c} \cdot \mathbf{c} \quad D = \mathbf{b} \cdot \mathbf{c} \quad E = \mathbf{c} \cdot \mathbf{a} \quad F = \mathbf{a} \cdot \mathbf{b}, \quad (1)$$

the reduced basis must satisfy the following conditions⁵⁾.

A.Type-I cell

Main conditions:

$$A \leq B \leq C; \quad D \leq B/2; \quad E \leq A/2; \quad F \leq A/2 \quad (2a)$$

$$D > 0; \quad E > 0; \quad F > 0. \quad (2b)$$

Special conditions:

$$\text{if } A=B \quad \text{then } D \leq E \quad (3a)$$

$$\text{if } B=C \quad \text{then } E \leq F \quad (3b)$$

$$\text{if } D=B/2 \quad \text{then } F \leq 2E \quad (3c)$$

$$\text{if } E=A/2 \quad \text{then } F \leq 2D \quad (3d)$$

$$\text{if } F=A/2 \quad \text{then } E \leq 2D. \quad (3e)$$

B.Type-II cell

Main conditions:

$$A \leq B \leq C; -D \leq B/2; -E \leq A/2; -F \leq A/2; \quad (4a)$$

$$-D-E-F \leq (A+B)/2 \quad (4b)$$

$$D \leq 0; E \leq 0; F \leq 0. \quad (4c)$$

Special conditions:

$$\text{if } A=B \quad \text{then } -D \leq -E \quad (5a)$$

$$\text{if } B=C \quad \text{then } -E \leq -F \quad (5b)$$

$$\text{if } -D=B/2 \quad \text{then } F=0 \quad (5c)$$

$$\text{if } -E=A/2 \quad \text{then } F=0 \quad (5d)$$

$$\text{if } -F=A/2 \quad \text{then } E=0 \quad (5e)$$

$$\text{if } -D-E-F = (A+B)/2 \quad \text{then } A \leq -2E-F. \quad (5f)$$

Hence the region specified by the above conditions consists of the two distinct parts in the parameter-space which have no connection to each other except at a hyperplane, because the reduced bases are divided into type I and II according to whether all interaxial angles are acute or obtuse (Fig.1). Then any two points which correspond to physically adjacent structures are not necessarily close in the parameter-space but separated far from each other. Thus the necessity of a new region without this disadvantage is obvious. In the previous paper¹⁾, the author obtained a set of conditions which bound a single lump in the parameter-space. Unfortunately it has been found that the method used there contains a wrong procedure, and therefore gives a wrong result. Since the fault is fatal, the present paper is provided to deal with the problem totally again with appropriate abbreviation.

The representation space of Bravais lattices

Any primitive cell is represented as a point in the space of the six variables (A, B, C, D, E, F) defined in (1). In the definition of the previous paper¹⁾ the negative sign must be added in front of each quantity if the system of (a, b, c) is left-handed, but the rule is abandoned here for simplicity. There are infinite number of cells which correspond to the same lattice so that there are also infinite number of equivalent points in the space. The transformations between these equivalent points make the group of primitive transformations^{1), 7)}. The group is most simply represented by the following 3×3 matrices t operating on (a, b, c) :

$$\begin{bmatrix} a' \\ b' \\ c' \end{bmatrix} = \begin{bmatrix} t_{11} & t_{12} & t_{13} \\ t_{21} & t_{22} & t_{23} \\ t_{31} & t_{32} & t_{33} \end{bmatrix} \begin{bmatrix} a \\ b \\ c \end{bmatrix} \quad (6)$$

Here all of the components t_{ij} are indices and the determinants of the matrices are unity. They are translated to 6×6 matrices operating on the above six-dimensional position vectors as follows:

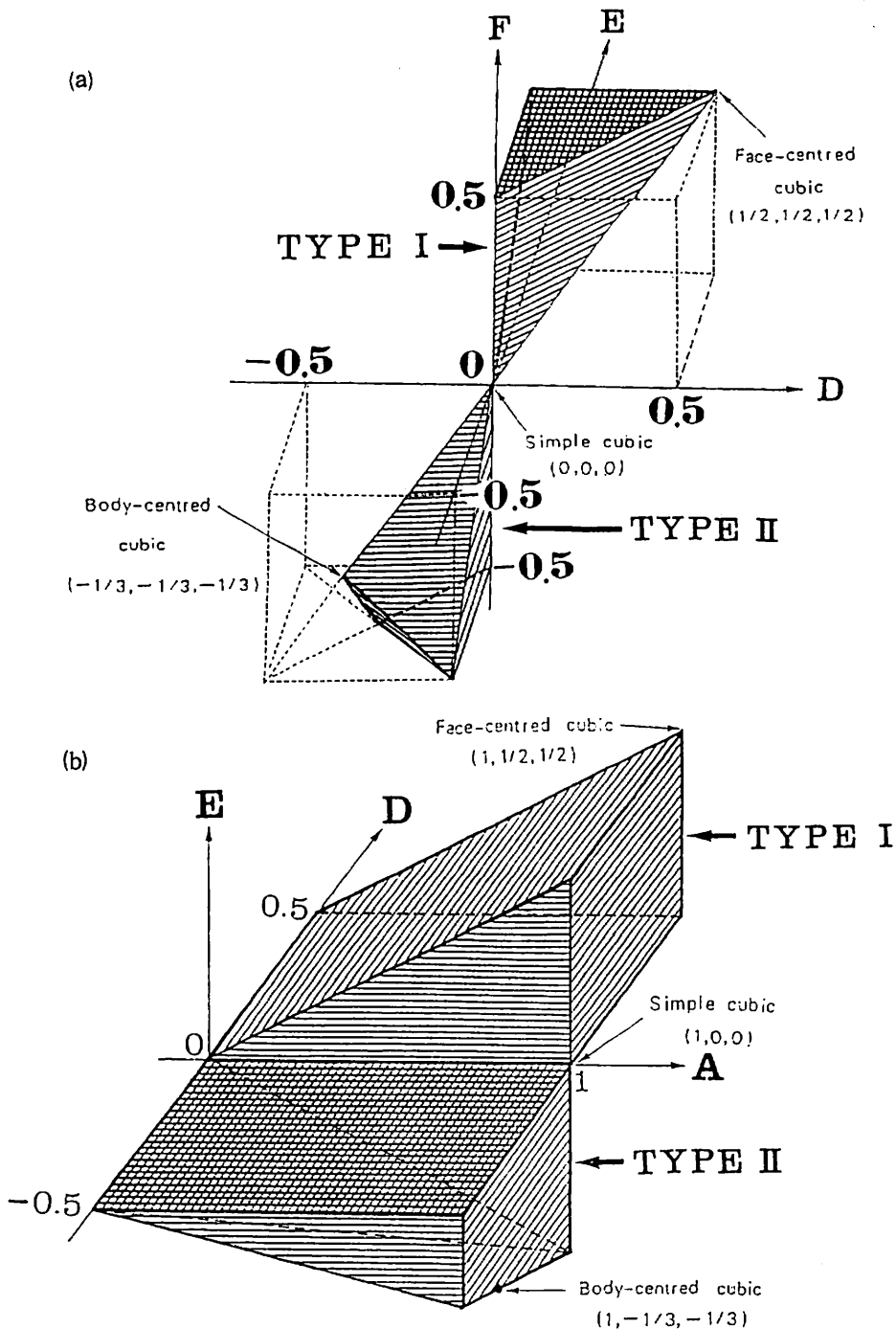


Fig. 1. The three-dimensional cross-sections of the region for the reduced bases. All the hatched lines are parallel to the horizontal plane in each figure. The figures (a) and (b) correspond to the condition $(A=B=C=1)$ and $(B=C=1$ and $E=F)$ respectively. For simplicity, the special conditions are neglected.

$$\begin{aligned}
 \begin{pmatrix} A' \\ B' \\ C' \\ D' \\ E' \\ F' \end{pmatrix} &= \begin{pmatrix} T_{11} & T_{12} & T_{13} & T_{14} & T_{15} & T_{16} \\ T_{21} & T_{22} & T_{23} & T_{24} & T_{25} & T_{26} \\ T_{31} & T_{32} & T_{33} & T_{34} & T_{35} & T_{36} \\ T_{41} & T_{42} & T_{43} & T_{44} & T_{45} & T_{46} \\ T_{51} & T_{52} & T_{53} & T_{54} & T_{55} & T_{56} \\ T_{61} & T_{62} & T_{63} & T_{64} & T_{65} & T_{66} \end{pmatrix} \begin{pmatrix} A \\ B \\ C \\ D \\ E \\ F \end{pmatrix} \\
 &= \begin{pmatrix} t_{11}^2 & t_{12}^2 & t_{13}^2 & 2t_{11}t_{13} & 2t_{13}t_{11} & 2t_{11}t_{12} \\ t_{21}^2 & t_{22}^2 & t_{23}^2 & 2t_{21}t_{23} & 2t_{23}t_{21} & 2t_{21}t_{22} \\ t_{31}^2 & t_{32}^2 & t_{33}^2 & 2t_{31}t_{33} & 2t_{33}t_{31} & 2t_{31}t_{32} \\ t_{21}t_{31} & t_{22}t_{32} & t_{23}t_{33} & t_{22}t_{33} + t_{23}t_{32} & t_{23}t_{31} + t_{21}t_{33} & t_{21}t_{32} + t_{22}t_{31} \\ t_{31}t_{11} & t_{32}t_{12} & t_{33}t_{13} & t_{32}t_{13} + t_{33}t_{12} & t_{33}t_{11} + t_{31}t_{13} & t_{31}t_{12} + t_{32}t_{11} \\ t_{11}t_{21} & t_{12}t_{22} & t_{13}t_{23} & t_{12}t_{23} + t_{13}t_{22} & t_{13}t_{21} + t_{11}t_{23} & t_{11}t_{22} + t_{12}t_{21} \end{pmatrix} \begin{pmatrix} A \\ B \\ C \\ D \\ E \\ F \end{pmatrix} \quad (7)
 \end{aligned}$$

Thus the six-dimensional space is a representation space of the group of primitive transformations. Only a small part of the space is necessary and sufficient to represent every possible lattice, because the other part is reducible to this region by the operations T_{ij} . Such a region is called group-theoretically a fundamental region of the group. Then our purpose is to find a fundamental region of the group of primitive transformations.

A point in the representation space is invariant under some operations of the group. Such operations make up a subgroup of the original infinite group. Hence every point is specified by the corresponding subgroup. The most symmetrical points correspond to the maximal subgroups. In the present case the maximal subgroups are given by the following four symmetrical Bravais lattices⁹⁾: simple cubic (SC), face-centred cubic (FCC), body-centred cubic (BCC) and hexagonal (HEX). Among an infinite number of versions their primitive-cell vectors shown in Fig. 2 are best fitted for the present purpose. It should be noted that they are not the same as that in the previous paper¹⁾. Their cartesian coordinates are as follows:

simple cubic	$a = (a_1, 0, 0)$ $b = (0, a_1, 0)$ $c = (0, 0, a_1)$
face-centred cubic	$a = (0, a_2, a_2)$ $b = (a_2, 0, a_2)$ $c = (a_2, a_2, 0)$
body-centred cubic	$a = (2a_3, 0, 0)$ $b = (a_3, a_3, a_3)$ $c = (a_3, -a_3, a_3)$
hexagonal	$a = (2a_4, 0, 0)$ $b = (a_4, \sqrt{3} a_4, 0)$ $c = (0, 0, c)$

Here a_1, a_2, a_3, a_4 and c are arbitrary positive values (Fig.2).

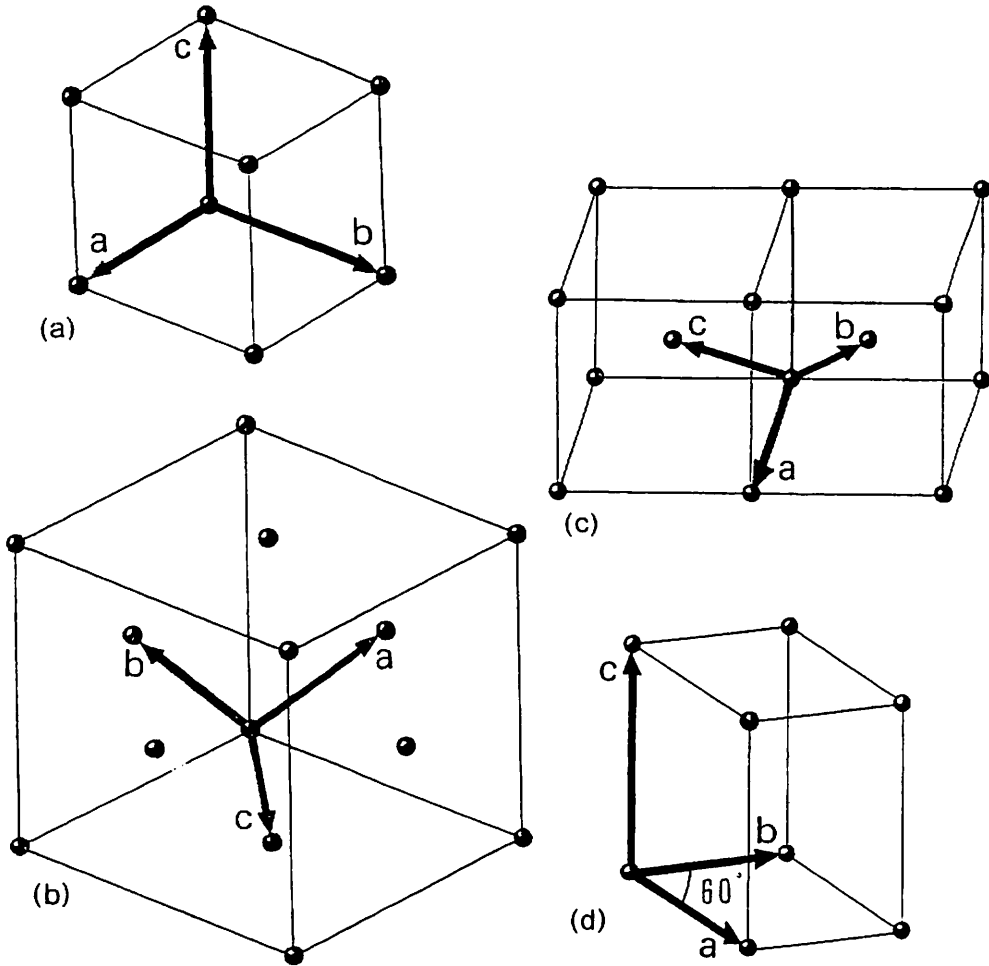


Fig. 2. The edge vectors of the primitive cells for the most symmetrical Bravais lattices, (a) simple cubic, (b) face-centred cubic, (c) body-centred cubic and (d) hexagonal.

They correspond to the following points:

simple cubic

$$(x_1, x_1, x_1, 0, 0, 0)$$

face-centred cubic

$$(2x_2, 2x_2, 2x_2, x_2, x_2, x_2)$$

body-centred cubic

$$(4x_3, 3x_3, 3x_3, x_3, 2x_3, 2x_3)$$

hexagonal

$$(2x_4, 2x_4, z, 0, 0, x_4)$$

Here x_1, x_2, x_3, x_4 and z are arbitrary positive values. These points are called the highest symmetrical positions (HSP) below.

The corresponding subgroups are generated by the following operators which are given below in detail:

simple cubic	(24)	C_3, C_4
face-centred cubic	(24)	C_3, C_4'
body-centred cubic	(24)	C_3', C_4
hexagonal	(12)	$C_6, C_4 \cdot C_3$

where the order of each group is shown in each parenthesis.

$$C_3 = (001000/100000/010000/000001/000100/000010) \quad (8)$$

$$C_4 = (100000/001000/010000/000100/00000\bar{1}/000010) \quad (9)$$

$$C_4' = (011\bar{2}00/11000\bar{2}/010000/01000\bar{1}/010\bar{1}00/010\bar{1}\bar{1}\bar{1}) \quad (10)$$

$$C_3' = (011\bar{2}00/11000\bar{2}/001000/000\bar{1}10/00\bar{1}\bar{1}00/010\bar{1}\bar{1}\bar{1}) \quad (11)$$

$$C_6 = (11000\bar{2}/100000/001000/000010/000\bar{1}10/10000\bar{1}) \quad (12)$$

Here the contracted description of a matrix is introduced as follows with the conventional indication of a negative quantity by placing a minus sign above it:

$$\begin{aligned}
 & (T_{11}T_{12}T_{13}T_{14}T_{15}T_{16}/\dots/T_{61}T_{62}T_{63}T_{64}T_{65}T_{66}) \\
 = & \begin{bmatrix} T_{11} & T_{12} & T_{13} & T_{14} & T_{15} & T_{16} \\ T_{21} & T_{22} & T_{23} & T_{24} & T_{25} & T_{26} \\ T_{31} & T_{32} & T_{33} & T_{34} & T_{35} & T_{36} \\ T_{41} & T_{42} & T_{43} & T_{44} & T_{45} & T_{46} \\ T_{51} & T_{52} & T_{53} & T_{54} & T_{55} & T_{56} \\ T_{61} & T_{62} & T_{63} & T_{64} & T_{65} & T_{66} \end{bmatrix} \quad (13)
 \end{aligned}$$

The order of each group is half of that of the corresponding point group, because the translation from matrices (t_{ij}) to (T_{ij}) is two-to-one as is seen in (7).

Since we have to distinguish only a fundamental region from its neighbour regions, only the elements which transform a point in it into the adjacent regions must be checked. The elements of the above four HSP are sufficient for this object, for the HSP are found to be located on a certain region. The total number of the elements is 84, but some elements are common in different groups, so that the net number is 65⁷⁾.

Construction of a fundamental region

The method used in the previous paper is almost the same as that of determining the Wigner-Seitz cell in the reciprocal space¹⁾. The boundary of a region is constructed by the set of planes which bisect perpendicularly the lines connecting the equivalent points. If all the operations were simultaneously orthogonal in some space, this procedure would have no problems. As it is, only the elements of SC are orthogonal in the original space. If we adopt a space in which all the elements of another maximal subgroup, for instance FCC, are orthogonal, then the elements in the other

three maximal subgroups can not be orthogonal. In the previous paper the perpendicular bisecting planes were obtained separately in the transformed spaces in which all the operations of the corresponding subgroup are orthogonal and transferred back into the original space. However this does not give a correct answer as follows. Since several elements are shared among the maximal subgroups, several perpendicular bisecting planes are obtained differently in more than one space. Each of such planes should coincide with the corresponding one in the original space but does not in general. Thus the Wigner-Seitz cell method is not applicable to the present problem even in its modified way.

There is no other way than to find the region by trial and error. The obtained region is examined by the following consideration. Since each equivalent point corresponding to a certain Bravais lattice appears once and only once in each fundamental region, if a point in a fundamental region goes out across a boundary, then another equivalent point must enter the region. Hence any point (at a general position) on a boundary plane has its equivalent point at another position on some boundary plane. This imposes that any boundary plane or its partial piece of the obtained region must have its equivalent one among the boundary planes. (Strictly speaking, only one of such paired planes belongs to the region concerned, but for the convenience here we simply consider that all the boundary planes are contained in the region.)

The most helpful clue to find the candidate of a fundamental region is the symmetrical positions which are invariant under some operations other than the identical one. These positions are analogous to a rotation axis in three dimensions, because their dimensions are two or more lower than that of the space itself, so they will be called simply axes hereafter. Any axis must exist on the boundary of a region, because any point on it is the converging limit of two or more equivalent points.

Then we can choose a plane which includes some axis as a temporary boundary. Since several axes intersect each other on the HSP, it may be wise to take a plane which passes as many HSP as possible. Then its equivalent planes obtained by applying the 65 operations may be the other probable boundaries, for one of them may be the pair to the original plane and the others may be the extensions of the boundaries of the other regions. (Both situations are not inevitable, but probable by analogy of the case of usual three-dimensional point groups.)

The closest region surrounded by such planes usually includes a fundamental region entirely, but exceeds it (Fig. 3). The region is divided into the definite and the indefinite parts. The former contains only the points which have no equivalent one within the region, so that it must not be excluded from the aimed region. The latter part constitutes of the regions which are equivalent to each other, and therefore it must be reduced. However since any part may survive among the two or more equivalent ones, it is indefinite where to reduce. To eliminate the excess an arbitrary chosen point on each plane is transformed by the 65 operators and examined by the criterion stated below.

If the transferred points enter the interior (not the boundary) of the region, it means that the original point is on the indefinite boundary, and the transferred point is in the indefinite region. Then it may seem that the new plane transferred by the

corresponding operation should be chosen as a new boundary which partially cuts off the redundant part. However there can be two cases as in Fig. 3: (a) The whole transferred plane is on the outside of the definite part. (b) The transferred plane passes within the definite part. In the case of (a), the transferred plane can be adopted readily as a new boundary. If the case (b) occurs, the transferred plane must be abandoned and another appropriate plane should be discovered. There are no immediate indications to tell which of the case (a) or (b) has occurred. Thus we add the transferred plane to the boundaries, no matter whether the case (a) or (b) occurs,

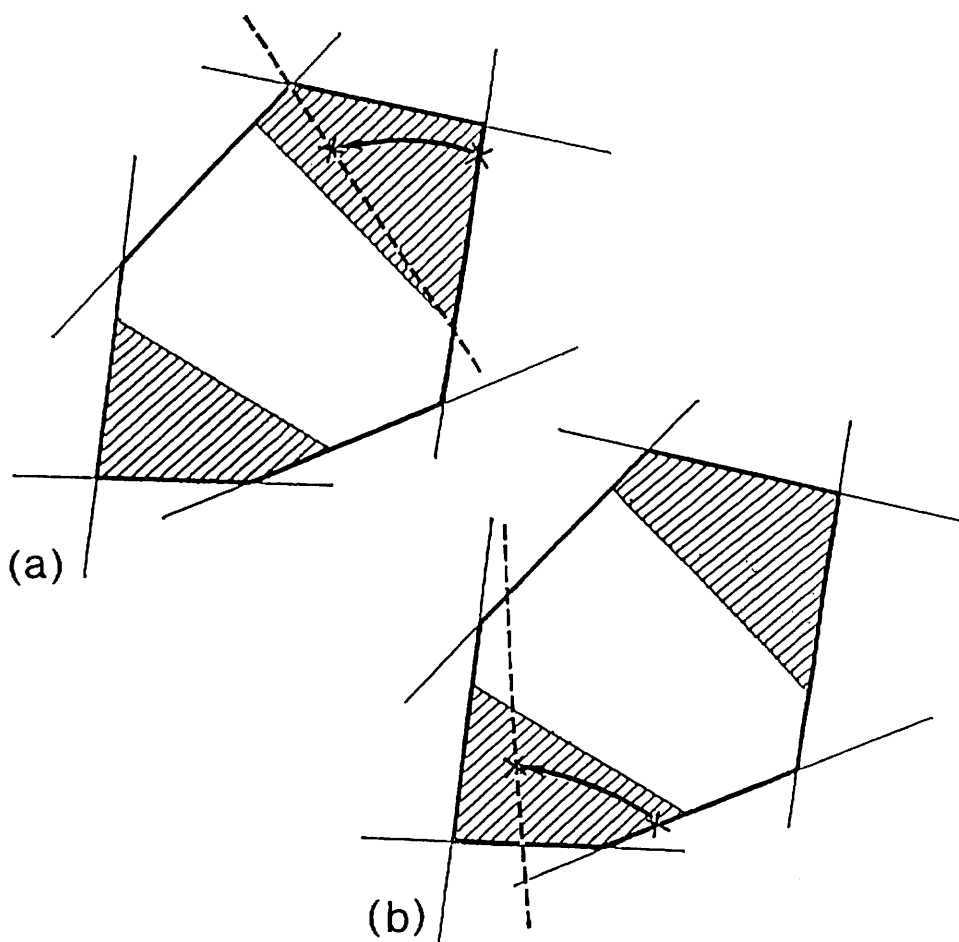


Fig. 3. A schematic view of eliminating the excessive parts of the candidate of a fundamental region. The tentative region (surrounded by the solid lines) can be divided into the definite (blank) part and the indefinite (shaded) one. If a point on the boundaries enter the region under some symmetry operation, it means that either case of the (a) or (b) has occurred; (a) the transferred plane is entirely outside of the definite part, (b) the transferred plane passes within the definite part. In case (a), the transferred plane can be adopted as a new boundary, while in case (b) another appropriate plane must be discovered.

and continue to examine if any point on the boundaries have its pair on somewhere on the boundaries. If the test is passed by for a sufficiently many times, the case is recognized as (a) and transferred plane is adopted as a new boundary. Once there is a point which has no pair, we know that the definite part has been cut off and the case (b) has occurred. Then the transferred plane must be replaced by another one. This needs another heuristic procedure. A new plane is often successfully chosen in order that the axis of the corresponding transfer should be contained in it. Sometimes symmetric considerations with respect to the permutations of the variables may be helpful. Anyway there is no infallible way to find it. Its appropriateness is proved only by the criterion that every point on the boundaries should have its pair at another position on the boundaries.

The successful course in the above way is as follows. We start from the plane $E-F=0$ on which the three HSP: SC, FCC and BCC are situated. Applying the 65 operations, we get 15 equivalent planes. The closest region around the four HSP is found to be surrounded by the following 7 inequalities:

$$\begin{aligned} -E+F \geq 0, \quad -D+E \geq 0, \quad D+E \geq 0, \quad A-E-F \geq 0, \\ A+D-E-F \geq 0, \quad B-D-F \geq 0, \quad B+D-E-F \geq 0. \end{aligned} \quad (10)$$

(In order to find the most inner planes a Monte Carlo method by computer is used as in the previous paper¹⁾.)

A test is made to see where arbitrary chosen points on the 7 planes are transformed by the 65 operations. (This is carried out by computer using also a Monte Carlo method.) Then it turns out that the operator $(11000\bar{2}/010000/001000/000\bar{1}00/000\bar{1}10/01000\bar{1})$ transforms a point on the plane $D+E=0$ into one on $2D-E=0$ which is within the region. Hence the transferred plane $2D-E=0$ is added. Now the closest region is bounded as follows:

$$-E+F \geq 0, \quad -D+E \geq 0, \quad A-E-F \geq 0, \quad B-D-F \geq 0, \quad 2D-E \geq 0. \quad (11)$$

A further test shows that a point on the plane $B-D-F=0$ enters the interior under the operation $(011\bar{2}00/1010\bar{2}0/001000/0010\bar{1}0/001\bar{1}00/001\bar{1}\bar{1}1)$. However the transferred plane $A-C+D-F=0$ is inadequate as a boundary, for it cuts the region so narrow that some points on the boundaries have no equivalent one on them. Then planes passing the axis should be examined. The axis that is invariant under the above operation is given by $(a, a+d-e, d+e, d, e, f)$ where a, d, e and f are arbitrary. A plane $C-D-E=0$ is found to be convenient. Fortunately this completes the process and we get the final result as follows:

$$A \quad -E-F \quad \geq 0, \quad (16)$$

$$B \quad -D \quad -F \quad \geq 0, \quad (17)$$

$$C-D-E \quad \geq 0, \quad (18)$$

$$-D+E \quad \geq 0, \quad (19)$$

$$-E+F \quad \geq 0, \quad (20)$$

$$2D-E \quad \geq 0. \quad (21)$$

When a sign of equality holds in either of expressions (16)–(21), its equation represents a boundary plane. A point on each plane has its equivalent one on the same plane. Operations transversing the equivalent points on each plane to one another are as follows in the corresponding order of expressions (16)–(21):

The three-dimensional cross sections of this region are shown in Fig. 4.

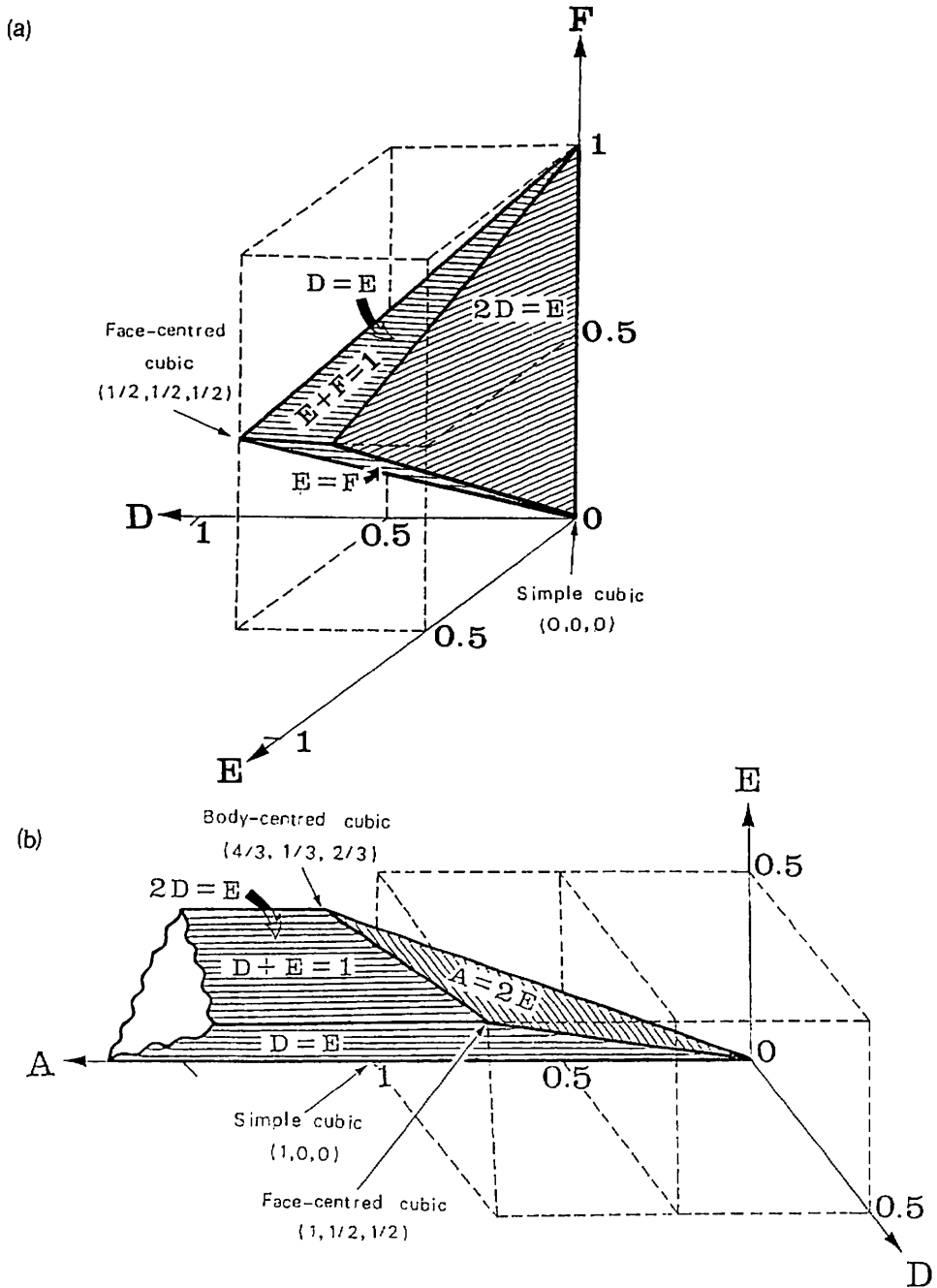


Fig. 4. The three-dimensional cross-sections of the region obtained here. All the hatched lines are parallel to the horizontal plane in each figure. The figures (a) and (b) correspond to the condition $(A=B=C=1)$ and $(B=C=1 \text{ and } E=F)$, respectively.

$$T_1 = (100000/1010\bar{2}0/11000\bar{2}/1001\bar{1}\bar{1}/10000\bar{1}/1000\bar{1}0) \quad (22)$$

$$T_2 = (011\bar{2}00/010000/11000\bar{2}/01000\bar{1}/010\bar{1}\bar{1}\bar{1}/010\bar{1}00) \quad (23)$$

$$T_3 = (011\bar{2}00/1010\bar{2}0/001000/0010\bar{1}0/001\bar{1}00/001\bar{1}\bar{1}\bar{1}) \quad (24)$$

$$T_4 = (010000/100000/001000/000010/000100/000001) \quad (25)$$

$$T_5 = (100000/001000/010000/000100/000001/000010) \quad (26)$$

$$T_6 = (100000/11000\bar{2}/001000/000\bar{1}10/000010/10000\bar{1}) \quad (27)$$

Strictly speaking, only a half of each boundary plane must belong to the fundamental region. The conditions for this limitation are easily obtained. For example, if $-D+E=0$ holds, there are two equivalent points on this plane; (A,B,C,D,E,F) and (B,A,C,E,D,F) according to (25). The two points should coincide with each other if $A=B$, for $D=E$ holds already by the assumption itself. This means that the hyperplane $A=B$ is the limit to which the paired points converge. Hence either $A \geq B$ or $B \geq A$ must be adopted. Such consideration gives the following conditions:

$$\text{if } A-E-F=0 \text{ then } C+F \geq B+E, \quad (28)$$

$$\text{if } B-D-F=0 \text{ then } C+F \geq A+D, \quad (29)$$

$$\text{if } C-D-E=0 \text{ then } B+E \geq A+D, \quad (30)$$

$$\text{if } -D+E=0 \text{ then } B \geq A, \quad (31)$$

$$\text{if } -E+F=0 \text{ then } C \geq B, \quad (32)$$

$$\text{if } 2D-E=0 \text{ then } A \geq 2F. \quad (33)$$

They correspond to the special conditions in the case of reduced bases.

Comparison with the reduced bases

Our region specified by the six inequalities in (16)–(21) should be equivalent to that restricted by the reduced bases. Fortunately this is confirmed by the one-to-one correspondence between them as below. If a reduced basis is given in either range of the following list, its parameters can be transformed into the new region by the matrix on its right side. The coincidence of the two regions which were obtained independently and quite differently^{3,4)} proves the correctness of the both.

Type I. ($A \leq B \leq C$; $D \leq B/2$; $E \leq A/2$; $F \leq A/2$; $D > 0$; $E > 0$; $F > 0$.)

Range	Transformation matrix
$-E+F \geq 0, 2D-F \geq 0, -D+E \geq 0$	$(100000/010000/001000/000100/000010/000001)$
$-2D+E \geq 0, -E+F \geq 0$	$(100000/11000\bar{2}/001000/000\bar{1}10/000010/10000\bar{1})$
$-2D+F \geq 0, E-F \geq 0$	$(100000/1010\bar{2}0/010000/000\bar{1}01/000001/1000\bar{1}0)$
$E-F \geq 0, 2D-F \geq 0, -D+F \geq 0$	$(100000/001000/010000/000100/000001/000010)$
$-D+E \geq 0, -D+2F \geq 0, D-F \geq 0$	$(001000/100000/010000/000001/000100/000010)$
$D-2F \geq 0, -D+E \geq 0$	$(001000/1010\bar{2}0/010000/00010\bar{1}/000100/0010\bar{1}0)$
$E-2F \geq 0, D-E \geq 0$	$(001000/011\bar{2}00/100000/0000\bar{1}\bar{1}/000010/001\bar{1}00)$
$D-E \geq 0, -E+2F \geq 0, E-F \geq 0$	$(001000/010000/100000/000001/000010/000100)$
$D-F \geq 0, 2E-F \geq 0, -E+F \geq 0$	$(010000/001000/100000/000010/000001/000100)$
$-2E+F \geq 0, D-F \geq 0$	$(010000/011\bar{2}00/100000/0000\bar{1}\bar{1}/000001/010\bar{1}00)$

$$\begin{array}{ll}
D-2E \geq 0, -D+F \geq 0 & (010000/11000\bar{2}/001000/0001\bar{1}0/000100/01000\bar{1}) \\
-D+F \geq 0, -D+2E \geq 0, D-E \geq 0 & (010000/100000/001000/000010/000100/000001)
\end{array}$$

Type II. ($A \leq B \leq C$; $-D \leq B/2$; $-E \leq A/2$; $-F \leq A/2$; $-D-E-F \leq (A+B)/2$; $D \leq 0$;
 $E \leq 0$; $F \leq 0$.)

Range	Transformation matrix
$-C-D-E-F \geq 0, -C-2D-E \geq 0, D-E \geq 0$	(101020/010000/001000/000100/001010/000101)
$C+D+E+F \geq 0, -D+F \geq 0, D-F \geq 0$	(101020/001000/010000/000100/000101/001010)
$D-F \geq 0, -E+F \geq 0, C+D+E+F \geq 0$	(101020/100000/010000/000001/000101/100010)
$D-E \geq 0, E-F \geq 0, C+D+2E \geq 0$	(110002/100000/001000/000010/000110/100001)
$-D+E \geq 0, D-F \geq 0, C+2D+E \geq 0$	(110002/010000/001000/000100/000110/010001)
$E-F \geq 0, -D+F \geq 0, C+D+E+F \geq 0$	(011200/010000/100000/000001/000011/010100)
$C+D+E+F \geq 0, -E+F \geq 0, -D+E \geq 0$	(011200/001000/100000/000010/000011/001100)
$C+D+2E \geq 0, -C-2D-E \geq 0, -C-D-E-F \geq 0$	(011200/111222/001000/001110/001100/011211)
$-C-D-E-F \geq 0, -C-D-2E \geq 0, -D+E \geq 0$	(011200/100000/001000/000010/001100/000011)
$C+2D+E \geq 0, -C-D-2E \geq 0, -C-D-E-F \geq 0$	(101020/111222/001000/001110/001010/101121)

Discussion

As was stated in the previous paper¹⁾, the region obtained here will play an analogous important role as the first Brillouin zone does. Its future applications can not be predicted thoroughly, but, for example, the phenomenological theory of the phase transitions between different crystal structures will be developed using this region. If we can assign a function as the thermodynamic potential of a crystal in the region, we will find the most stable structure at the minimum position in it. The minimum point moves in accordance with the change of the temperature and pressure. Then the shape of the region should be as simple as possible, in order that we may track the minimum point without a discontinuous jump on a boundary plane. Since at least six planes are necessary to cut out a solid angle in the six-dimensional space (for example, Sommerville,⁹⁾), our six inequalities in (16)-(21) are the simplest set of conditions. The coefficients of the boundary equations are also simple enough. Thus we may have obtained one of the best regions.

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