A Influence of systematic absences on Ito's method

Here, the notation in Section 2 is adopted. We shall determine why the use of Ito's equation is not appropriate for establishing a powder auto-indexing method for all types of systematic absence. Let $P_1(L^*)$ be the set consisting of all the primitive vectors of L^*. In the case of space groups, unlike in the case of wallpaper groups, some types of systematic absence have the latter property:

(i) $\Gamma_{ext} \cap P_1(L^*)$ is contained in a union of finite hyperplanes.

(ii) $\Gamma_{ext} \cap P_1(L^*)$ is not contained in any union set of finite hyperplanes.

Table 1 lists all types of systematic absences corresponding to the latter case.

In the methods by Ito and de Wolff, if the q-values q_1, q_2, q_3, q_4 of observed diffraction peaks satisfy $2(q_1 + q_2) = q_3 + q_4$, they are assumed to have $l_1^*, l_2^* \in L^*$ satisfying the following and used to obtain a zone:

$$q_1 = |l_1^*|^2,\ q_2 = |l_2^*|^2,\ q_3 = |l_1^* + l_2^*|^2,\ q_4 = |l_1^* - l_2^*|^2. \tag{A.1}$$

Candidates for the 3×3 metric tensor of L^* are made from combinations of zones. To simplify the procedure, it is very desirable that $\{l_1^*, l_2^*\}$ in (A.1) be a primitive set of L^*. Otherwise, metric tensors of 3D sublattices $L_2^* \subsetneq L^*$ might have been obtained, which complicates and slows the powder auto-indexing method.

In fact, according to the following fact, $\{l_1^*, l_2^*\}$ is never a primitive set of L^* for some types of systematic absence, as long as l_1^*, l_2^* satisfies (A.1).

Fact A.1. *If the type of systematic absence belongs to the category B or N, there exists no primitive set $\{l_1^*, l_2^*\}$ of L^* such that none of l_1^*, l_2^*, $l_1^* \pm l_2^*$ belong to Γ_{ext}.*

In order to eliminate the adverse effects of systematic absences, equations other than Ito's equation have been proposed (de Wolff, 1957). However, it has not been ascertained whether the equations work appropriately for all types of systematic absence. The following was also proposed to obtain 3×3 metric tensors directly:

$$|l_1^*|^2 + |l_2^*|^2 + |l_3^*|^2 + |l_1^* + l_2^* + l_3^*|^2 = |l_1^* + l_2^*|^2 + |l_1^* + l_3^*|^2 + |l_2^* + l_3^*|^2. \tag{A.2}$$

The above formula has a similar property to Ito's equation:

Fact A.2. *If the type of systematic absence belongs to the category B, C, F, G, or N, there exists no basis $\langle l_1^*, l_2^*, l_3^* \rangle$ of L^* such that none of l_1^*, l_2^*, l_3^*, $l_1^* + l_2^*$, $l_1^* + l_3^*$, $l_2^* + l_3^*$, $l_1^* + l_2^* + l_3^*$ belong to Γ_{ext}.*

B A proof of Lemma 1

In this section, a self-contained proof of Lemma 1 is provided. In the following, L is a 3D lattice in the Euclidean space $\mathbb{R}^3$. $\mathcal{S}^3$ is the 6-dimensional linear space consisting of all 3-by-3 metric tensors. $\mathcal{S}^3_{\succ 0} \subset \mathcal{S}^3$ is its subset consisting of all positive definite metric tensors.

For any $\Phi \in V_3$ (see Section 3.2 for definition), $D(\Phi) \subset \mathcal{S}^3_{\succ 0}$ is defined as follows:

$$D(\Phi) := \{S \in \mathcal{S}^3_{\succ 0} : {}^t u S u = \min\{{}^t(u + 2l) S (u + 2l) : l \in L\} \text{ for any } u \in \Phi\}. \tag{A.3}$$

From the definition, $D(\Phi)$ is the convex cone defined by the inequalities:

$${}^t u S u \le {}^t(u + 2l) S (u + 2l)\ (u \in \Phi, l \in L). \tag{A.4}$$

Note that when $L = \mathbb{Z}^3$ and $\Phi_0 = \{\pm {}^t(c_1, c_2, c_3) : c_j = 0, 1\}$, any $S \in \mathcal{S}^3_{\succ 0}$ is Selling (Delaunay) reduced if and only if $S \in D(\Phi_0)$.

The following lemma is used in the proof of Lemma 1:

Lemma B.1. *For any fixed basis $\langle l_1, l_2, l_3 \rangle$ of L, we define $l_4 := -l_1 - l_2 - l_3$ and $\Phi := \{\pm \sum_{i=1}^3 c_i l_i : c_i = 0, 1\} \in V_3$. In this case, $D(\Phi)$ is the convex cone in $\mathcal{S}^3_{\succ 0}$ defined by the following inequalities:*

$${}^t(l_i + l_j) S (l_i + l_j) \le {}^t(l_i - l_j) S (l_i - l_j)\ (1 \le i < j \le 4). \tag{A.5}$$

Table 1: Types of systematic absence having Γ_{ext} that is not contained in a union of finite hyperplanes[a].

Space group G (No.[b])	R_H^c	Coordinates
A (Face-centered lattice)		
$F\ d\ d\ 2$ (43)	C_2	$(0,0,z)$
$F\ d\ d\ d$ (70)	C_2	$(x,0,0)$
$F\ d\ d\ d$ (70)	D_2	$(0,0,0)$
$F\ d\ d\ d$ (70)	D_2	$(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
$F\ d\ \bar{3}$ (203)	C_2	$(x,0,0)$
$F\ d\ \bar{3}$ (203)	T	$(0,0,0)$
$F\ d\ \bar{3}$ (203)	T	$(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
$F\ 4_1\ 3\ 2$ (210)	C_2	$(x,0,0)$
$F\ 4_1\ 3\ 2$ (210)	T	$(0,0,0)$
$F\ 4_1\ 3\ 2$ (210)	T	$(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
$F\ d\ \bar{3}\ m$ (227)	C_{2v}	$(x,0,0)$
$F\ d\ \bar{3}\ m$ (227)	T_d	$(0,0,0)$
$F\ d\ \bar{3}\ m$ (227)	T_d	$(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
A (Body-centered lattice)		
$I\ 4_1$ (80)	C_2	$(0,0,z)$
$I\ 4_1/a$ (88)	C_2	$(0,0,z)$
$I\ 4_1/a$ (88)	S_4	$(0,0,0)$
$I\ 4_1/a$ (88)	S_4	$(0,0,\frac{1}{2})$
$I\ 4_1\ 2\ 2$ (98)	C_2	$(0,0,z)$
$I\ 4_1\ 2\ 2$ (98)	D_2	$(0,0,0)$
$I\ 4_1\ 2\ 2$ (98)	D_2	$(0,0,\frac{1}{2})$
$I\ 4_1\ m\ d$ (109)	C_{2v}	$(0,0,z)$
$I\ \bar{4}\ 2\ d$ (122)	C_2	$(0,0,z)$
$I\ \bar{4}\ 2\ d$ (122)	S_4	$(0,0,0)$
$I\ \bar{4}\ 2\ d$ (122)	S_4	$(0,0,\frac{1}{2})$
$I\ 4_1/a\ m\ d$ (141)	C_2	$(x,x,0)$
$I\ 4_1/a\ m\ d$ (141)	C_{2v}	$(0,0,z)$
$I\ 4_1/a\ m\ d$ (141)	D_{2d}	$(0,0,0)$
$I\ 4_1/a\ m\ d$ (141)	D_{2d}	$(0,0,\frac{1}{2})$
$I\ 4_1/a\ c\ d$ (142)	C_2	$(x,x,\frac{1}{4})$
B (Face-centered lattice)		
$F\ d\ d\ d$ (70)	C_i	$(\frac{1}{8},\frac{1}{8},\frac{1}{8})$
$F\ d\ d\ d$ (70)	C_i	$(\frac{5}{8},\frac{5}{8},\frac{5}{8})$
$F\ d\ \bar{3}$ (203)	C_{3i}	$(\frac{1}{8},\frac{1}{8},\frac{1}{8})$
$F\ d\ \bar{3}$ (203)	C_{3i}	$(\frac{5}{8},\frac{5}{8},\frac{5}{8})$
$F\ 4_1\ 3\ 2$ (210)	D_3	$(\frac{1}{8},\frac{1}{8},\frac{1}{8})$
$F\ 4_1\ 3\ 2$ (210)	D_3	$(\frac{5}{8},\frac{5}{8},\frac{5}{8})$
$F\ d\ \bar{3}\ m$ (227)	D_{3d}	$(\frac{1}{8},\frac{1}{8},\frac{1}{8})$
$F\ d\ \bar{3}\ m$ (227)	D_{3d}	$(\frac{5}{8},\frac{5}{8},\frac{5}{8})$
B (Body-centered lattice)		
$I\ 4_1/a$ (88)	C_i	$(0,\frac{1}{4},\frac{1}{8})$
$I\ 4_1/a$ (88)	C_i	$(\frac{1}{4},0,\frac{3}{8})$
$I\ 4_1/a\ m\ d$ (141)	C_{2h}	$(0,\frac{1}{4},\frac{1}{8})$
$I\ 4_1/a\ m\ d$ (141)	C_{2h}	$(0,\frac{1}{4},\frac{5}{8})$
C		
$I\ 4_1/a\ m\ d$ (141)	C_2	$(x,\frac{1}{4},\frac{1}{8})$
$I\ 4_1/a\ c\ d$ (142)	C_2	$(\frac{1}{4},y,\frac{1}{8})$
D		
$P\ 3\ 1\ c$ (159)	C_3	$(\frac{1}{3},\frac{2}{3},z)$
$P\ \bar{3}\ 1\ c$ (163)	C_3	$(\frac{1}{3},\frac{2}{3},z)$
$P\ \bar{3}\ 1\ c$ (163)	D_3	$(\frac{2}{3},\frac{1}{3},\frac{1}{4})$
$P\ \bar{3}\ 1\ c$ (163)	D_3	$(\frac{1}{3},\frac{2}{3},\frac{1}{4})$
$P\ 6_3$ (173)	C_3	$(\frac{1}{3},\frac{2}{3},z)$
$P\ 6_3/m$ (176)	C_3	$(\frac{1}{3},\frac{2}{3},z)$
$P\ 6_3/m$ (176)	C_{3h}	$(\frac{2}{3},\frac{1}{3},\frac{1}{4})$
$P\ 6_3/m$ (176)	C_{3h}	$(\frac{1}{3},\frac{2}{3},\frac{1}{4})$
$P\ 6_3\ 2\ 2$ (182)	C_3	$(\frac{1}{3},\frac{2}{3},z)$
$P\ 6_3\ 2\ 2$ (182)	D_3	$(\frac{2}{3},\frac{1}{3},\frac{1}{4})$
$P\ 6_3\ 2\ 2$ (182)	D_3	$(\frac{1}{3},\frac{2}{3},\frac{1}{4})$
$P\ 6_3\ m\ c$ (186)	C_{3v}	$(\frac{1}{3},\frac{2}{3},z)$
$P\ \bar{6}\ 2\ c$ (190)	C_3	$(\frac{1}{3},\frac{2}{3},z)$
$P\ \bar{6}\ 2\ c$ (190)	C_{3h}	$(\frac{2}{3},\frac{1}{3},\frac{1}{4})$
$P\ \bar{6}\ 2\ c$ (190)	C_{3h}	$(\frac{1}{3},\frac{2}{3},\frac{1}{4})$
$P\ 6_3/m\ m\ c$ (194)	C_{3v}	$(\frac{1}{3},\frac{2}{3},z)$
$P\ 6_3/m\ m\ c$ (194)	D_{3h}	$(\frac{2}{3},\frac{1}{3},\frac{1}{4})$
$P\ 6_3/m\ m\ c$ (194)	D_{3h}	$(\frac{1}{3},\frac{2}{3},\frac{1}{4})$
E		
$P\ 6_2$ (171)	C_2	$(\frac{1}{2},\frac{1}{2},z)$
$P\ 6_4$ (172)	C_2	$(\frac{1}{2},\frac{1}{2},z)$
$P\ 6_2\ 2\ 2$ (180)	C_2	$(\frac{1}{2},0,z)$
$P\ 6_2\ 2\ 2$ (180)	D_2	$(\frac{1}{2},0,0)$
$P\ 6_2\ 2\ 2$ (180)	D_2	$(\frac{1}{2},0,\frac{1}{2})$
$P\ 6_4\ 2\ 2$ (181)	C_2	$(\frac{1}{2},0,z)$
$P\ 6_4\ 2\ 2$ (181)	D_2	$(\frac{1}{2},0,0)$
$P\ 6_4\ 2\ 2$ (181)	D_2	$(\frac{1}{2},0,\frac{1}{2})$
F (Primitive lattice)		
$P\ 4_2\ 3\ 2$ (208)	C_2	$(x,\frac{1}{2},0)$
$P\ 4_2\ 3\ 2$ (208)	C_2	$(x,0,\frac{1}{2})$
$P\ \bar{4}\ 3\ n$ (218)	C_2	$(x,\frac{1}{2},0)$
$P\ \bar{4}\ 3\ n$ (218)	C_2	$(x,0,\frac{1}{2})$
$P\ m\ \bar{3}\ n$ (223)	C_2	$(\frac{1}{4},y,y+\frac{1}{2})$
$P\ m\ \bar{3}\ n$ (223)	C_{2v}	$(x,\frac{1}{2},0)$
$P\ m\ \bar{3}\ n$ (223)	C_{2v}	$(x,0,\frac{1}{2})$
F (Body-centered lattice)		
$I\ \bar{4}\ 3\ d$ (220)	C_3	(x,x,x)
$I\ a\ \bar{3}\ d$ (230)	C_3	(x,x,x)
G		
$P\ 4_2\ 3\ 2$ (208)	D_2	$(\frac{1}{4},0,\frac{1}{2})$
$P\ 4_2\ 3\ 2$ (208)	D_2	$(\frac{1}{4},\frac{1}{2},0)$
$P\ \bar{4}\ 3\ n$ (218)	S_4	$(\frac{1}{4},0,\frac{1}{2})$
$P\ \bar{4}\ 3\ n$ (218)	S_4	$(\frac{1}{4},\frac{1}{2},0)$
$P\ m\ \bar{3}\ n$ (223)	D_{2d}	$(\frac{1}{4},0,\frac{1}{2})$
$P\ m\ \bar{3}\ n$ (223)	D_{2d}	$(\frac{1}{4},\frac{1}{2},0)$
H		
$P\ 4_3\ 3\ 2$ (212)	D_3	$(\frac{1}{8},\frac{1}{8},\frac{1}{8})$
$P\ 4_3\ 3\ 2$ (212)	D_3	$(\frac{5}{8},\frac{5}{8},\frac{5}{8})$
$P\ 4_1\ 3\ 2$ (213)	D_3	$(\frac{3}{8},\frac{3}{8},\frac{3}{8})$
$P\ 4_1\ 3\ 2$ (213)	D_3	$(\frac{7}{8},\frac{7}{8},\frac{7}{8})$
I		
$I\ 4_1\ 3\ 2$ (214)	D_3	$(\frac{1}{8},\frac{1}{8},\frac{1}{8})$
$I\ 4_1\ 3\ 2$ (214)	D_3	$(\frac{7}{8},\frac{7}{8},\frac{7}{8})$
J		
$I\ 4_1\ 3\ 2$ (214)	D_2	$(\frac{1}{8},0,\frac{1}{4})$
$I\ 4_1\ 3\ 2$ (214)	D_2	$(\frac{5}{8},0,\frac{1}{4})$
$I\ \bar{4}\ 3\ d$ (220)	S_4	$(\frac{7}{8},0,\frac{1}{4})$
$I\ \bar{4}\ 3\ d$ (220)	S_4	$(\frac{3}{8},0,\frac{1}{4})$
K		
$I\ 4_1\ 3\ 2$ (214)	C_2	$(x,0,\frac{1}{4})$
$I\ \bar{4}\ 3\ d$ (220)	C_2	$(x,0,\frac{1}{4})$
$I\ a\ \bar{3}\ d$ (230)	C_2	$(\frac{1}{8},y,-y+\frac{1}{4})$
L		
$I\ a\ \bar{3}\ d$ (230)	C_2	$(x,0,\frac{1}{4})$
M		
$I\ a\ \bar{3}\ d$ (230)	D_2	$(\frac{1}{8},0,\frac{1}{4})$
$I\ a\ \bar{3}\ d$ (230)	S_4	$(\frac{3}{8},0,\frac{1}{4})$
N		
$I\ a\ \bar{3}\ d$ (230)	D_3	$(\frac{1}{8},\frac{1}{8},\frac{1}{8})$

[a] Every type of systematic absence is removed from the list if $L^* \setminus \Gamma_{ext}$ is contained in the reciprocal lattice L_2^* of some $L_2 \supsetneq L$.

[b] Number assigned to every space group in the International Tables

[c] The point group corresponding to the site symmetry group H

Proof. Any $S \in D(\Phi)$ clearly satisfy the inequalities in (A.5). Conversely, assume that $S \in \mathcal{S}^3_{\succ 0}$ satisfies the inequalities in (A.5). From the assumption, we have ${}^t l_i S l_j \le 0$ for any $1 \le i < j \le 4$. For any $u := \sum_{i=1}^3 \alpha_i l_i$, the following holds if we put $\alpha_4 := 0$:

$$ {}^t u S u = - \sum_{1 \le i < j \le 4} (\alpha_i - \alpha_j)^2 \, {}^t l_i S l_j. \tag{A.6} $$

It follows from this that S satisfies all the inequalities in (A.4). □

As seen from Lemma B.1, $D(\Phi)$ includes interior points. If $\Phi_1, \Phi_2 \in V_3$ are distinct, $D(\Phi_1)$ and $D(\Phi_2)$ cannot have common interior points, because they are separated by the hyperplane defined by ${}^t k_1 S k_1 = {}^t k_2 S k_2$, where k_i $(1 \le i \le 2)$ are chosen from $\Phi_i \setminus (\Phi_1 \cap \Phi_2)$ so that they satisfy $k_1 - k_2 \in 2L$. (Such k_1, k_2 always exist because the map $\Phi_i \to L/2L$ given by $l \mapsto l + 2L$ is onto, and $u_1, u_2 \in \Phi_i$ are mapped to the same class of $L/2L$ if and only if $u_1 = \pm u_2$.)

Proof of Lemma 1. From the assumption, there exist k_1, k_2 such that $\Phi_1 = (\Phi_1 \cap \Phi_2) \cup \{\pm k_1\}$ and $\Phi_2 = (\Phi_1 \cap \Phi_2) \cup \{\pm k_2\}$. In this case, either of the following holds:

(a) $k_1 = \pm l_i$ for some $1 \le i \le 4$,

(b) $k_1 = \pm(l_i + l_j)$ for some $1 \le i < j \le 3$.

In the former case, $D(\Phi_2) \subset D(\Phi_1)$ follows from $l_i + l_j \in \Phi_2$ $(1 \le i < j \le 3)$ and Lemma B.1. This is impossible because of $\Phi_1 \ne \Phi_2$.

In the latter case, $k_1 = \pm(l_i + l_j) = \pm(l_m + l_n)$ when $1 \le m, n \le 4$ are chosen so that i, j, m, n are distinct. We shall prove $k_2 = l_i - l_j$ or $l_m - l_n$ holds in this case; we define $\Phi_{i,j} := (\Phi_1 \setminus \{\pm(l_i + l_j)\}) \cup \{\pm(l_i - l_j)\}$ and $\Phi_{m,n} := (\Phi_1 \setminus \{\pm(l_m + l_n)\}) \cup \{\pm(l_m - l_n)\}$. $\Phi_{i,j}$ then equals $\{\pm \sum_{i=1}^3 c_i \tilde{l}_i : c_i = 0, 1\}$ with the following $\tilde{l}_i$:

$$ \tilde{l}_1 := l_i, \ \tilde{l}_2 := -l_j, \ \tilde{l}_3 := l_j + l_m, \ \tilde{l}_4 := -\tilde{l}_1 - \tilde{l}_2 - \tilde{l}_3 = l_j + l_n. \tag{A.7} $$

Hence $\Phi_{i,j}$ belongs to V_3. $\Phi_{m,n} \in V_3$ is also obtained by permuting l_1, l_2, l_3, l_4. In order to prove $k_2 = l_i - l_j$ or $l_m - l_n$, it is sufficient if $D(\Phi_2) \subset D(\Phi_1) \cup D(\Phi_{i,j}) \cup D(\Phi_{m,n})$ is shown. If $S \in D(\Phi_2)$ does not belong to $D(\Phi_1)$, ${}^t l_i S l_j > 0$ or ${}^t l_m S l_n > 0$ holds. We assume ${}^t l_i S l_j \ge {}^t l_m S l_n$ and ${}^t l_i S l_j > 0$ by permuting l_1, l_2, l_3, l_4. From Lemma B.1, such S belongs to $D(\Phi_{i,j})$ if and only if

$$ \begin{aligned} {}^t\tilde{l}_1 S \tilde{l}_2 &= -{}^t l_i S l_j \le 0, && \text{(A.8)} \\ {}^t\tilde{l}_1 S \tilde{l}_3 &= {}^t l_i S (l_j + l_m) = \frac{{}^t l_n S l_n - {}^t(l_n - 2l_i) S (l_n - 2l_i)}{4} \le 0, && \text{(A.9)} \\ {}^t\tilde{l}_1 S \tilde{l}_4 &= {}^t l_i S (l_j + l_n) = \frac{{}^t l_m S l_m - {}^t(l_m - 2l_i) S (l_m - 2l_i)}{4} \le 0, && \text{(A.10)} \\ {}^t\tilde{l}_2 S \tilde{l}_3 &= -{}^t l_j S (l_j + l_m) = \frac{{}^t l_m S l_m - {}^t(l_m + 2l_j) S (l_m + 2l_j)}{4} \le 0, && \text{(A.11)} \\ {}^t\tilde{l}_2 S \tilde{l}_4 &= -{}^t l_j S (l_j + l_n) = \frac{{}^t l_n S l_n - {}^t(l_n + 2l_j) S (l_n + 2l_j)}{4} \le 0, && \text{(A.12)} \\ {}^t\tilde{l}_3 S \tilde{l}_4 &= (l_j + l_m) S (l_j + l_n) = -{}^t l_i S l_j + {}^t l_m S l_n \le 0. && \text{(A.13)} \end{aligned} $$

$S \in D(\Phi_{i,j})$ is obtained from the assumptions ${}^t l_i S l_j \ge {}^t l_m S l_n$, ${}^t l_i S l_j > 0$, $S \in D(\Phi_2)$ and $l_1, l_2, l_3, l_4 \in \Phi_2$. Therefore, $D(\Phi_2) \subset D(\Phi_1) \cup D(\Phi_{i,j}) \cup D(\Phi_{m,n})$. □

C Fundamental group of topographs for 3D lattices

Using a group presentation of $GL(3,\mathbb{Z})$, it is proved that topographs for 3D lattices are connected and their fundamental group is generated by the two circuits presented in Figure 6 of Section 3.2.

For any two bases $\langle l_1, l_2, l_3\rangle$, $\langle k_1, k_2, k_3\rangle$ of a 3D lattice L, $g \in GL(3,\mathbb{Z})$ satisfying the following equation is uniquely determined:

$$\begin{pmatrix} l_1 & l_2 & l_3 \end{pmatrix} g = \begin{pmatrix} k_1 & k_2 & k_3 \end{pmatrix} \tag{A.14}$$

It is easily checked that their corresponding nodes $\Phi_1 := \{\pm \sum_{i=1}^3 c_i l_i : c_i = 0,1\}$ and $\Phi_2 := \{\pm \sum_{i=1}^3 c_i k_i : c_i = 0,1\}$ are same if and only if g or $-g$ gives a permutation of the following vectors:

$$\mathbf{e}_1 := \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \ \mathbf{e}_2 := \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \ \mathbf{e}_3 := \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}, \ \mathbf{e}_4 := \begin{pmatrix} -1 \\ -1 \\ -1 \end{pmatrix}. \tag{A.15}$$

This is equivalent to the condition that g belongs to the subgroup $\tilde{S}_4 \subset GL(3,\mathbb{Z})$ generated by the following matrices:

$$(1\ 2) := \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \ (2\ 3) := \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \ (3\ 4) := \begin{pmatrix} 1 & 0 & -1 \\ 0 & 1 & -1 \\ 0 & 0 & -1 \end{pmatrix}, \ h := \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}. \tag{A.16}$$

The subgroup of $\tilde{S}_4$ generated by the first three matrices can be identified with the permutation group S_4 of degree 4. $\tilde{S}_4$ is the direct product of S_4 and $\langle h\rangle$ generated by h of order 2.

When a basis $\langle l_1, l_2, l_3\rangle$ of L is fixed, a bijection between the set of left cosets $GL(3,\mathbb{Z})/\tilde{S}_4$ and V_3 (the set of all the nodes) is provided by the following map:

$$g\tilde{S}_4 \mapsto \left\{ \pm \begin{pmatrix} l_1 & l_2 & l_3 \end{pmatrix} g \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix} : c_i = 0,1 \right\}. \tag{A.17}$$

Furthermore, $\Phi_1 := \{\pm \sum_{i=1}^3 c_i l_i : c_i = 0,1\}$ and $\Phi_2 := \{\pm \sum_{i=1}^3 c_i k_i : c_i = 0,1\}$ are connected by an edge if and only if $\{k_1, k_2, k_3, -k_1-k_2-k_3\} = \pm\{l_i, -l_j, l_j+l_m, l_j+l_n\}$ for some distinct $1 \le i,j,m,n \le 4$ (*cf.* the proof of Lemma 1 in Appendix B). This is equivalent to the condition that g determined by the equation (A.14) belongs to $\tilde{S}_4\tau\tilde{S}_4$, where τ is the following matrix:

$$\tau := \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 1 \\ 0 & 0 & 1 \end{pmatrix} \tag{A.18}$$

Namely, two nodes corresponding to $g_1\tilde{S}_4$, $g_2\tilde{S}_4$ by the map (A.17) are connected by an edge if and only if $g_1^{-1}g_2$ is contained in $\tilde{S}_4\tau\tilde{S}_4$.

The fundamental group of the topograph can be computed from a group presentation of $GL(3,\mathbb{Z})$ by using the above identifications. Recall that for any $N > 0$, $SL(N,\mathbb{Z})$ is generated by the matrices T_{ij} ($1 \le i,j \le N$, $i \ne j$) with 1's on the diagonal or in the (i,j)-entry and 0's elsewhere. When $[x,y]$ represents the commutator $x^{-1}y^{-1}xy$, the following are the fundamental relations among T_{ij} (*cf.* Corollary 10.3, Milnor(1971)).

(a) $[T_{ij}, T_{mn}] = 1$ for $i \ne n$ and $j \ne m$,

(b) $[T_{ij}, T_{jm}] = T_{im}$ for i, j, m distinct,

(c) $(T_{12}T_{21}^{-1}T_{12})^4 = 1$.

The presentation of $GL(3,\mathbb{Z})$ with generators τ and $s \in \tilde{S}_4$ is obtained from these relations. In the following, the element of S_4 which exchanges $\mathbf{e}_i$, $\mathbf{e}_j$ $(1 \le i < j \le 4)$ and fixes the other two vectors is represented as $(i\ j)$. The free product of the groups G_1 and G_2 is denoted by $G_1 * G_2$.

Proposition C.1. *Let φ be the natural map $G := \tilde{S}_4 * \langle\tau\rangle \to GL(3,\mathbb{Z})$ induced by the inclusion $\tilde{S}_4$, $\langle\tau\rangle \subset GL(3,\mathbb{Z})$. Then φ is onto, and the kernel of φ is the normal closure $K \subset G$ of the subgroup generated by*

$$(h\tau)^2, \tag{A.19}$$

$$((3\ 4)\tau)^2, \tag{A.20}$$

$$((1\ 2)\tau)^2(3\ 4)h, \tag{A.21}$$

$$(\tau(1\ 3)(2\ 4))^3 h, \tag{A.22}$$

$$((1\ 3)\tau(1\ 3)\tau(1\ 4)\tau(1\ 4))^2. \tag{A.23}$$

(Hence the map $G/K \to GL(3,\mathbb{Z})$ induced by φ is an isomorphism.)

Proof. It is straightforward to check that K is contained in the kernel. In the following, the map $G/K \to GL(3,\mathbb{Z})$ induced by φ is denoted by φ_2. $s \in S_4$ maps 1, 2, 4 to j, i, 4 respectively, $s(1\ 4)\tau(1\ 4)\tau s^{-1}$ is mapped to T_{ij} by φ. Hence φ_2 is onto. We define another map $\psi : GL(3,\mathbb{Z}) \to G/K$ by $h \mapsto h$ and $T_{ij} \mapsto s(1\ 4)\tau(1\ 4)\tau s^{-1}$ with the above s. In order to verify ψ is well-defined, we shall check that $\psi([T_{ij}, T_{mn}]) = \psi((T_{12}T_{21}^{-1}T_{12})^4) = K$ and $\psi([T_{ij}, T_{jm}]) = \psi(T_{im})$. For the proof, the following obtained from (A.20) and (A.22) is used:

$$(\tau(1\ 4)(2\ 3))^3 hK = (3\ 4)(\tau(1\ 3)(2\ 4))^3(3\ 4)hK = K. \tag{A.24}$$

We shall also utilize $(\tau(2\ 3))^6 = 1$ obtained as follows:

$$\begin{aligned} \tau(2\ 3)\tau(2\ 3)K &= (3\ 4)(1\ 2)\tau(1\ 2)(2\ 3)(3\ 4)(1\ 2)\tau(1\ 2)(2\ 3)K\ (\because (A.21)) \\ &= (3\ 4)(1\ 2)\tau(1\ 4)(1\ 3)\tau(1\ 3)(1\ 2)K. \end{aligned} \tag{A.25}$$

Hence,

$$\begin{aligned} (\tau(2\ 3))^6 K &= (\tau(2\ 3)\tau(2\ 3))^3 K \\ &= (3\ 4)(1\ 2)\tau(1\ 4)(1\ 3)\tau(1\ 3)(3\ 4)\tau(1\ 4)(1\ 3)\tau(1\ 3)(3\ 4)\tau(1\ 4)(1\ 3)\tau(1\ 3)(1\ 2)K \\ &= (3\ 4)(1\ 2)\tau(1\ 4)(1\ 3)\tau(1\ 3)\tau(1\ 3)(1\ 4)\tau(1\ 4)\tau(1\ 4)(1\ 3)\tau(1\ 3)(1\ 2)K\ (\because (A.20)) \\ &= (3\ 4)(1\ 2)\tau(1\ 4)(1\ 3)(1\ 4)\tau(1\ 4)(1\ 3)\tau(1\ 3)(1\ 4)(1\ 3)\tau(1\ 3)(1\ 2)K\ (\because (A.23)) \\ &= (3\ 4)(1\ 2)\tau(3\ 4)\tau(1\ 4)(1\ 3)\tau(3\ 4)\tau(1\ 3)(1\ 2)K \\ &= (3\ 4)(1\ 2)(3\ 4)(1\ 4)(1\ 3)(3\ 4)(1\ 3)(1\ 2)K\ (\because (A.20)) \\ &= K. \end{aligned} \tag{A.26}$$

(a) $\psi([T_{ij}, T_{mn}]) = K$ $(i \ne n, j \ne m)$; by replacing T_{ij}, T_{mn} with $sT_{ij}s^{-1}$, $sT_{mn}s^{-1}$ $(s \in S_4)$ if necessary, it is sufficient for the proof if the relation is obtained in the case of $i = 2$ and $j = 1$. In this case, $m = 2$ or $n = 1$ must hold. If $m = 2$ and $n = 1$, $\psi([T_{21}, T_{21}]) = K$ holds clearly. If $m = 2$ and $n \ne 1$ (hence $n = 3$),

$$\begin{aligned} \psi(T_{23}^{-1}T_{21}) &= (1\ 3)\tau(1\ 4)\tau(1\ 4)(1\ 3)(1\ 4)\tau(1\ 4)\tau K \\ &= (1\ 3)\tau(1\ 4)\tau(3\ 4)\tau(1\ 4)\tau K \\ &= (1\ 3)\tau(1\ 4)(3\ 4)(1\ 4)\tau K\ (\because (A.20)) \\ &= (1\ 3)\tau(1\ 3)\tau K. \end{aligned} \tag{A.27}$$

Hence,

$$\begin{aligned}
\psi(T_{21}^{-1}T_{23}^{-1}T_{21}T_{23}) &= \tau(1\ 4)\tau(1\ 4)(1\ 3)\tau(1\ 3)\tau(1\ 3)(1\ 4)\tau(1\ 4)\tau(1\ 3)K \\
&= (1\ 3)\tau(1\ 3)(1\ 4)\tau(1\ 4)(1\ 3)(1\ 4)\tau(1\ 4)\tau(1\ 3)K\ (\because (A.23)) \\
&= (1\ 3)\tau(1\ 3)(1\ 4)\tau(3\ 4)\tau(1\ 4)\tau(1\ 3)K \\
&= (1\ 3)\tau(1\ 3)(1\ 4)(3\ 4)(1\ 4)\tau(1\ 3)K\ (\because (A.20)) \\
&= K. \qquad\qquad (A.28)
\end{aligned}$$

If $m \neq 2$ and $n = 1$ (hence $m = 3$), we have

$$\begin{aligned}
\psi(T_{21}T_{31}) &= (1\ 4)\tau(1\ 4)\tau(2\ 3)(1\ 4)\tau(1\ 4)\tau(2\ 3)K \\
&= (1\ 4)\tau(1\ 4)(2\ 3)(1\ 4)\tau(2\ 3)(1\ 4)(1\ 4)\tau(2\ 3)hK\ (\because (A.24)) \\
&= (1\ 4)\tau(2\ 3)\tau(2\ 3)\tau(2\ 3)hK. \qquad\qquad (A.29)
\end{aligned}$$

Hence

$$\psi(T_{21}^{-1}T_{31}^{-1}) = (2\ 3)\psi((T_{21}T_{31})^{-1})(2\ 3) = \tau(2\ 3)\tau(2\ 3)\tau(1\ 4)(2\ 3)hK. \qquad (A.30)$$

Therefore,

$$\psi(T_{21}^{-1}T_{31}^{-1}T_{21}T_{31}) = (\tau(2\ 3))^6K = K. \qquad (A.31)$$

(b) $\psi([T_{ij}, T_{jm}]) = \psi(T_{im})$; it may be assumed $i = 2$, $j = 1$ and $m = 3$.

$$\begin{aligned}
\psi(T_{13}) &= (1\ 3)(2\ 3)(1\ 4)\tau(1\ 4)\tau(2\ 3)(1\ 3)K \\
&= (2\ 3)(2\ 4)(1\ 2)\tau(1\ 2)(2\ 4)(1\ 2)\tau(1\ 2)(2\ 3)K \\
&= (2\ 3)(2\ 4)\tau(3\ 4)(2\ 4)(3\ 4)\tau(2\ 3)K\ (\because (A.21)) \\
&= (2\ 3)(2\ 4)\tau(2\ 3)\tau(2\ 3)K \\
&= (3\ 4)(2\ 3)\tau(2\ 3)\tau(2\ 3)K. \qquad\qquad (A.32)
\end{aligned}$$

Therefore,

$$\begin{aligned}
\psi(T_{13}T_{21}^{-1}T_{13}^{-1}) &= (3\ 4)(2\ 3)\tau(2\ 3)\tau(2\ 3)\tau(1\ 4)\tau(1\ 4)(2\ 3)\tau(2\ 3)\tau(2\ 3)(3\ 4)K \\
&= (3\ 4)(2\ 3)\tau(2\ 3)\tau(2\ 3)\tau(1\ 4)(1\ 4)(2\ 3)\tau(1\ 4)(2\ 3)(2\ 3)\tau(2\ 3)(3\ 4)hK\ (\because (A.24)) \\
&= (3\ 4)(2\ 3)\tau(2\ 3)\tau(2\ 3)\tau(2\ 3)\tau(1\ 4)\tau(2\ 3)(3\ 4)hK \\
&= (3\ 4)\tau(2\ 3)\tau(2\ 3)(1\ 4)\tau(2\ 3)(3\ 4)hK\ (\because (A.26)) \\
&= (3\ 4)\tau(2\ 3)(2\ 3)(1\ 4)\tau(2\ 3)(1\ 4)(2\ 3)(3\ 4)K\ (\because (A.24)) \\
&= (3\ 4)\tau(1\ 4)\tau(1\ 4)(3\ 4)K \\
&= \tau(1\ 3)\tau(1\ 3)K\ (\because (A.20)) \qquad\qquad (A.33) \\
&= \psi(T_{21}^{-1}T_{23}).\ (\because (A.27)) \qquad\qquad (A.34)
\end{aligned}$$

Hence $\psi([T_{21}, T_{13}]) = \psi(T_{23})$ follows from $\psi([T_{21}, T_{23}]) = \psi([T_{13}, T_{23}]) = K$.

(c) $(T_{12}T_{21}^{-1}T_{12})^4 = 1$;

$$\begin{aligned}
\psi(T_{12}T_{21}^{-1}) &= (1\ 2)(1\ 4)\tau(1\ 4)\tau(1\ 2)\tau(1\ 4)\tau(1\ 4)K \\
&= (1\ 2)(1\ 4)\tau(1\ 4)(1\ 2)(3\ 4)h(1\ 4)\tau(1\ 4)K\ (\because (A.21)) \\
&= (1\ 2)(1\ 4)\tau(1\ 3)(2\ 4)\tau(1\ 4)hK \\
&= (1\ 2)(1\ 4)(1\ 3)(2\ 4)\tau(1\ 3)(2\ 4)(1\ 4)K\ (\because (A.22)) \\
&= (1\ 3)(3\ 4)\tau(3\ 4)(1\ 3)(1\ 2)K \\
&= (1\ 3)\tau(1\ 3)(1\ 2)K.\ (\because (A.20)) \qquad\qquad (A.35)
\end{aligned}$$

Hence,

$$\begin{aligned}
\psi(T_{12}T_{21}^{-1}T_{12}) &= (1\ 3)\tau(1\ 3)(1\ 4)\tau(1\ 4)\tau(1\ 2)K && \text{(A.36)}\\
&= \tau(1\ 4)\tau(1\ 4)(1\ 3)\tau(1\ 3)(1\ 2)K.\ (\because (A.23)) && \text{(A.37)}
\end{aligned}$$

By the equalities (A.36) and (A.37),

$$\begin{aligned}
\psi((T_{12}T_{21}^{-1}T_{12})^2) &= (1\ 3)\tau(1\ 3)(1\ 4)\tau(1\ 4)\tau(1\ 2)\tau(1\ 4)\tau(1\ 4)(1\ 3)\tau(1\ 3)(1\ 2)K\\
&= (1\ 3)\tau(1\ 3)(1\ 4)\tau(1\ 4)(1\ 2)(3\ 4)h(1\ 4)\tau(1\ 4)(1\ 3)\tau(1\ 3)(1\ 2)K\ (\because (A.21))\\
&= (1\ 3)\tau(1\ 3)(1\ 4)\tau(1\ 3)(2\ 4)\tau(1\ 4)(1\ 3)\tau(1\ 3)(1\ 2)hK\\
&= (1\ 3)\tau(1\ 3)(1\ 4)(1\ 3)(2\ 4)\tau(1\ 3)(2\ 4)(1\ 4)(1\ 3)\tau(1\ 3)(1\ 2)K\ (\because (A.22))\\
&= (1\ 3)\tau(2\ 3)(3\ 4)\tau(3\ 4)(2\ 3)\tau(1\ 3)(1\ 2)K\\
&= (1\ 3)\tau(2\ 3)\tau(2\ 3)\tau(1\ 3)(1\ 2)K.\ (\because (A.20)) && \text{(A.38)}
\end{aligned}$$

Therefore,

$$\psi((T_{12}T_{21}^{-1}T_{12})^4) = (1\ 3)(\tau(2\ 3))^6(2\ 3)(1\ 3)(1\ 2)K = K. \qquad \text{(A.39)}$$

In order to prove φ_2 is an isomorphism, it is only necessary to show that ψ is an onto map because $\varphi_2 \circ \psi$ is the identity map on $GL(3,\mathbb{Z})$. If $s \in G$ belongs to the image of ψ, $(i\ j)s(i\ j)$ also does for any $1 \le i < j \le 3$. Hence, ψ is onto if τK, $(1\ 2)K$ and $(3\ 4)K$ belong to the image. From (A.38), we have

$$\begin{aligned}
\psi((T_{13}T_{31}^{-1}T_{13})^2) &= (2\ 3)(1\ 3)\tau(2\ 3)\tau(2\ 3)\tau(1\ 3)(1\ 2)(2\ 3)K\\
&= (1\ 2)(2\ 3)\tau(2\ 3)\tau(2\ 3)\tau(2\ 3)(1\ 2)(1\ 3)K\\
&= (1\ 2)\tau(2\ 3)\tau(2\ 3)\tau(1\ 2)(1\ 3)K\ (\because (A.26))\\
&= \tau(3\ 4)h(1\ 3)\tau(3\ 4)h(1\ 3)\tau(3\ 4)h(1\ 3)K\ (\because (A.21))\\
&= \tau(3\ 4)(1\ 3)\tau(1\ 4)\tau(1\ 3)hK. && \text{(A.40)}
\end{aligned}$$

Therefore,

$$\begin{aligned}
\psi((T_{13}T_{31}^{-1}T_{13})^2T_{23}^{-1}h) &= \tau(3\ 4)(1\ 3)(1\ 4)(1\ 3)K\\
&= \tau K. && \text{(A.41)}\\
\psi((T_{13}T_{31}^{-1}T_{13})^2T_{12}T_{21}^{-1}T_{12}h) &= \tau(3\ 4)(1\ 3)\tau(1\ 4)(1\ 3)(1\ 4)\tau(1\ 4)\tau(1\ 2)K\ (\because (A.36))\\
&= \tau(3\ 4)(1\ 3)(3\ 4)(1\ 4)\tau(1\ 2)K\ (\because (A.20))\\
&= (1\ 2)K. && \text{(A.42)}
\end{aligned}$$

Because $(3\ 4) = ((1\ 2)\tau)^2$ holds, $(3\ 4)K$ is also in the image of ψ. Hence ψ is onto. □

Corollary C.1. *The fundamental group of topographs for 3D lattices is generated by the two circuits of lengths 3 and 6 presented in Figure 6 of Section 3.2.*

Proof. By the identification between V_3 and $GL(3,\mathbb{Z})/\tilde{S}_4$, topographs for 3D lattices are connected because $\tilde{S}_4$ and τ generate $GL(3,\mathbb{Z})$. The relations (A.22) and (A.23) correspond to the circuits of lengths 3 and 6 respectively. The other relations correspond to contractible circuits because they have a length less than 3. □

D Proofs of theorems (Case of 3D lattices)

In the following, we fix a type of systematic absence corresponding to a space group G and a site symmetry group $H \subset G$. Let M be the order of the point group R_G of G,

Γ_{ext}, $\mathcal{H}$ and $\Omega \subset L^*/ML^*$ be as described in Fact 1 of Section 2. From the definition, we have

$$\Omega = \{l^* + ML^* : l^* \in \Gamma_{ext} \setminus \mathcal{H}\}. \tag{A.43}$$

In powder auto-indexing, it may be assumed that L^* is generated by elements of $L^* \setminus \Gamma_{ext}$. It is not difficult to prove our theorems if $\Gamma_{ext} \subset \mathcal{H}$ holds. (This is always true for 2D lattices.) As a result, it is sufficient if all the types in Table 1 are considered as special cases. Because too many case-by-case considerations are required for the cases, the most difficult part of the theorems was confirmed by direct computation by executing a program using the space group library of Z-Rietveld code (Oishi-Tomiyasu et. al., 2012). We verified that the program outputs exactly the same list as the International Tables.

In the following, for a lattice L of dimension N and an integer $1 \le m \le N$, the set of all the primitive set $\{l_1, \ldots, l_m\}$ of L is denoted by $P_m(L)$. The following lemma is proved for the proofs of the theorems:

Lemma D.1. *Let $L \subset \mathbb{R}^N$ be a lattice of dimension N, and $1 \le m \le N$ be an integer. Then, any open cone $C \subset \mathbb{R}^N$ contains a primitive set $\{l_1, \ldots, l_m\} \in P_m(L)$. Furthermore, if $M > 0$ is a positive integer and $\{k_1, \ldots, k_m\} \in P_m(L)$, C contains infinitely many $\{l_1, \ldots, l_m\} \in P_m(L)$ satisfying $l_i - k_i \in ML$ for any $1 \le i \le m$.*

Proof. We prove the first statement by induction. Since $\{al : a \in \mathbb{Q}, l \in L\} = \{al : 0 \ne a \in \mathbb{Q}, l \in P_1(L)\}$ is dense in $\mathbb{R}^N$, there exist $0 \ne a \in \mathbb{Q}$ and $l \in P_1(L)$ such that $al \in C$. Hence, $l \in C$ is obtained. Next suppose that $m < N$ and there is $T \in P_m$ contained in C. Then there exists $l \in L$ such that $T \cup \{l\} \in P_{m+1}$. For any arbitrarily fixed $l_2 \in T$, there is $\epsilon > 0$ such that $C_2 := \{x \in \mathbb{R}^N : (1-\epsilon)|x|^2|l_2|^2 \le (x \cdot l_2)^2\}$ is contained in C. In this case, $l + sl_2 \in C_2$ holds for sufficiently large integer $s > 0$. As a result, $T \cup \{l + sl_2\}$ is a subset of C and primitive. In order to prove the second statement, it is sufficient if some $\{l_1, \ldots, l_m\} \in P_m(L)$ satisfies the desired property. We fix a basis $l_1, \ldots, l_N \in C$ of L and $g \in GL(N, \mathbb{Z})$ satisfying $k_i = gl_i$ for any $1 \le i \le m$. When the subgroup of $GL(N, \mathbb{Z})$ with positive entries is denoted by $GL_+(N, \mathbb{Z})$, the natural map $GL_+(N, \mathbb{Z}) \longrightarrow G := \{g \in GL(N, \mathbb{Z}/M\mathbb{Z}) : \det g = \pm 1 \bmod M\}$ is an epimorphism. Let $g_0 \in GL_+(N, \mathbb{Z})$ be an element belonging to the inverse image of $g \bmod M$. Then $g_0 l_1, \ldots, g_0 l_N$ are all contained in C and satisfy $g_0 l_i - k_i \in ML$ $(1 \le i \le m)$. □

Because Theorem 2 is obtained from Theorem 3, it is sufficient if Theorems 3 and 4 are proved.

Proof of Theorem 3. By Lemma D.1, for any open convex cone $C \subset \mathbb{R}^N$ satisfying $C \cap \mathcal{H} = \emptyset$, there exists $\{l_1^*, l_2^*, l_3^*\} \in P_3(L^*)$ such that $\{\sum_{i=1}^3 m_i l_i^* : m_i \in \mathbb{Z}_{\ge 0}\} \subset C$ holds. In this case, $\{l_1^*, l_2^* + kl_3^*\} \in P_2(L^*)$ is included in C for any integer $k \ge 0$, and their expanding 2D lattices are different from each other. If $\Gamma_{ext} \subset \mathcal{H}$ holds, every such $\{l_1^*, l_2^* + kl_3^*\}$ satisfies the property stated in the theorem. (Here, $l^* \in \Gamma_{ext} \Leftrightarrow -l^* \in \Gamma_{ext}$ was used.)

Hence, it may be assumed that systematic absence is one of the types in Table 1. We define

$$P_{2,M}(L^*) \;:=\; \{\{l_1^* + ML^*, l_2^* + ML^*\} : \{l_1^*, l_2^*\} \in P_2(L^*)\}, \tag{A.44}$$

$$\tilde{P}_{2,M}(L^*) \;:=\; \{\{l_1^* + ML^*, l_2^* + ML^*\} \in P_{2,M}(L^*) : ml_1^* + (m-1)l_2^* + ML^* \notin \Omega \text{ for any } m \in \mathbb{Z}\}. \tag{A.45}$$

By direct calculation, it is verified that $\tilde{P}_{2,M}(L^*) \ne \emptyset$ holds for any type of systematic absence in Table 1 (see Table 2). Therefore, from Lemma D.1, there exists $\{l_1^*, l_2^*, l_3^*\} \in P_3(L^*)$ contained in Csuch that $\{l_1^* + ML^*, l_2^* + ML^*\} \in \tilde{P}_{2,M}(L^*)$ holds. In this case, $\{l_1^*, l_2^* + kMl_3^*\} \in P_2(L^*)$ is included in C for any integer $k \ge 0$, and their expanding 2D latices satisfy the required property. □

Table 2: Density of $L^* \setminus \Gamma_{ext}$ in L^*.

Type	$\tilde{P}_{2,M}(L^*)$ in $P_{2,M}(L^*)$	$\tilde{P}_{3,M}(L^*)$ in $P_{3,M}(L^*)$
A	0.321	0.286
B	0.286	0.143
C	0.476	0.190
D	0.341	0.209
E	0.736	0.604
F	0.714	0.571
G	0.214	0.027
H	0.429	0.058
I	0.714	0.571
J	0.071	0.022
K	0.857	0.786
L	0.107	0.004
M	0.036	0.004
N	0.036	0.004

[a] Here, the densities are computed by dividing the number of elements of $\tilde{P}_{i,M}(L^*)$ by that of $P_{i,M}(L^*)$ $(i = 2, 3)$.

[b] The densities of G, H, J, L, M, N, which consist of only primitive and body-centered cubic lattices, are rather small. As a practical measure against small densities, Conograph also uses Ito's equation to enumerate powder auto-indexing solutions, in addition to $3|l_1^*|^2 + |l_1^* + 2l_2^*|^2 = |2l_1^* + l_2^*|^2 + 3|l_2^*|^2$. (This is effective except for the category N, owing to Fact A.1.) Furthermore, the condition (b) of Theorem 4 is not required to hold for infinitely many m in the actual algorithm. Subgraphs with relatively many edges are given priority.

Proof of Theorem 4. By Lemma D.1, any open convex cone $C \subset \mathbb{R}^N \setminus \mathcal{H}$ contains some $\{l_1^*, -l_1^* + l_2^*, -l_1^* + l_3^*\} \in P_3(L^*)$. In this case, C also includes $\pm l_1^* + l_2^* + l_3^*$, $(m+1)l_1^* + m(-l_1 + l_i^*)$, $ml_1^* + (m+1)(-l_1^* + l_i^*)$ and $ml_1^* + (-l_1^* + l_i^*)$ for any $m \in \mathbb{Z}_{\geq 0}$. Consequently, if Γ_{ext} is contained in $\mathcal{H}$, the statement is obtained immediately.

When systematic absence is one of the types in Table 1, we define

$$P_{3,M}(L^*) := \{(l_1^* + ML^*, l_2^* + ML^*, l_3^* + ML^*) : \{l_1^*, l_2^*, l_3^*\} \in P_3(L^*)\}, \tag{A.46}$$

$$\tilde{P}_{3,M}(L^*) := \left\{ (l_1^* + ML^*, l_2^* + ML^*, l_3^* + ML^*) \in P_{3,M}(L^*) : \begin{array}{c} \pm l_1^* + l_2^* + l_3^* + ML^* \in \Omega, \\ \{l_1^* + ML^*, -l_1^* - l_i^* + ML^*\} \\ \text{or } \{l_i^* + ML^*, -l_1^* - l_i^* + ML^*\} \\ \text{belongs to } \tilde{P}_{2,M}(L^*) \text{ for both } i = 2, 3 \end{array} \right\}. \tag{A.47}$$

By direct calculation, it is verified that $\tilde{P}_{3,M}(L^*) \neq \emptyset$, regardless of the type of systematic absence (see Table 2). From Lemma D.1, there exist infinitely many $\{l_1^*, -l_1^* + l_2^*, -l_1^* + l_3^*\} \in P_3(L^*)$ contained in C such that $\{l_1^* + ML^*, l_2^* + ML^*, l_3^* + ML^*\} \in \tilde{P}_{3,M}(L^*)$ holds. In this case, l_1^*, l_2^*, l_3^* satisfy the property stated in the theorem. □