Supporting information

Appendix

Calculations of the lower bounds on the mixed volumes for system (1) from the main text for 3- and 2-dimensional crystals

An individual polynomial equation of system (1) is:

$$\left(1+\sum_{j=1}^{N-1}\xi_j^h\eta_j^k\zeta_j^l\right)\left(1+\sum_{j=1}^{N-1}\frac{1}{\xi_j^h\eta_j^k\zeta_j^l}\right)-I_{hkl}=0 \qquad \text{(A1)}$$

For a given j, the projection of the 3(N-1)-dimensional Newton polytope given by the left-hand side polynomial onto the 3-dimensional space of powers of ξ_j, η_j and ζ_j is a centrosymmetric line segment with the ends at (-h, -k, -l) and (h, k, l). Because this projection is two-dimensional, i.e. its dimensionality is less than 3, the 3(N-1)-dimensional volume of this Newton polytope ($V_{3D,1}$) is zero. By the same argument, the volume of the Newton polytope for the analogous polytope defined for a two-dimensional crystal ($V_{2D,1}$) is zero.

We will consider the Minkowski sum of two analogous Newton polytopes, one defined for (h_1, k_1, l_1) and the other for (h_2, k_2, l_2). Here, the projection of this sum onto the 3-dimensional space of powers of ξ_j, η_j and ζ_j (for any given j) is a parallelogram and; therefore, the volume of the Minkowski sum polytope ($V_{3D,2}$) is zero. A different scenario arises for the analogous Minkowski sum for a 2-dimensional crystal, where one polytope is defined for (h_1, k_1) and the other for (h_2, k_2). The corresponding equations can be written as:

$$\left(1+\sum_{j=1}^{N-1}X_{1,j}\right)\left(1+\sum_{j=1}^{N-1}\frac{1}{X_{1,j}}\right)-I_{h_1k_1}=0 \tag{A2}$$

$$\left(1+\sum_{j=1}^{N-1}X_{2,j}\right)\left(1+\sum_{j=1}^{N-1}\frac{1}{X_{2,j}}\right)-I_{h_2k_2}=0 \tag{A3}$$

where

$$X_{1,j}=\xi_j^{h_1}\eta_j^{k_1}\text{ , } j = 1, 2, \ldots, N\text{-}1 \tag{A4}$$

$$X_{2,j}=\xi_j^{h_2}\eta_j^{k_2}\text{ , } j = 1, 2, \ldots, N\text{-}1 \tag{A5}$$

The new system A2-A5 is a system of polynomial equations that is equivalent to the original one. As a result of this substitution, the Newton polytopes for eqs. A2 and A3 are so-called *h*-polytopes defined and analyzed by our group for the case of a one-dimensional crystal (Al-Asadi *et al.*, 2012), where h = 1. Because $X_{1,j}$ and $X_{2,j}$ can be viewed as new independent variables, the volume of the convex hull of the Minkowski sum of the Newton polytopes defined by eqs. A3 and A4 is equal to the product of the volumes of two *h*-polytopes with h = 1, derived previously by our group (Al-Asadi *et al.*, 2012). In order to calculate the volume in the original coordinates, one can treat eqs. A4 and A5 as N-1 pairwise shrinking coordinate transformations, with each pair being independent with respect to index j. Therefore, the final volume is:

$$V_{2D,2}=\left(\frac{\left(2\left(N-1\right)\right)!}{\left(\left(N-1\right)!\right)^3}\right)^2\left|h_1k_2-h_2k_1\right|^{N-1} \tag{A6}$$

The term $|h_1k_2\text{-}h_2k_1|$ is equal to the area of a parallelogram with vertices at (0, 0), (h_1, k_1), (h_2, k_2) and (h_1+h_2, k_1+k_2). A generalization of this formula to the Minkowski sum of m Newton polytopes corresponding to m equations for I_{hk} for m different pairs (h_p, k_p), p = 1, 2, …, m yields a lower bound on the respective volume of the sum:

$$V_{2\mathrm{D},m} \geq \left(\frac{\left(2(N-1)\right)!}{\left((N-1)!\right)^3} \right)^2 \left(\sum_{\substack{p_1=1 \\ p_1<p_2}}^{m} \left| h_{p_1} k_{p_2} - h_{p_2} k_{p_1} \right| \right)^{N-1} \quad \text{(A7)}$$

The summation term is equal to the total area of parallelograms formed as described above by all possible combinations of two distinct pairs (h_p, k_p), or the convex hull of the Minkowski sum of the m sets {(0,0), (h_p, k_p)}. The right hand side in inequality A7 is a lower bound and not an exact volume due to additional elements present in the sum polytope for $m > 2$ that cannot be readily accounted for in an expression general for all m. The Minkowski sum polytope coincides with the lower bound when the reflections are located on the axes of the reciprocal lattice. Owing to the monotonicity property of the mixed volume (with respect to polytope containment), one obtains a lower bound on the mixed volume of Newton polytopes by using the lower bound of the Minkowski sums defined by inequality (A7).

Analogously, for a three-dimensional crystal we obtain a lower bound on the volume of the convex hull of the Minkowski sum of $m > 2$ polytopes corresponding to eq. A1 for m triplets (h, k, l):

$$V_{3\mathrm{D},m} \geq \left(\frac{\left(2\left(N-1\right)\right)!}{\left(\left(N-1\right)!\right)^3} \right)^3 \left(\sum_{\substack{p_1=1 \\ p_1<p_2<p_3}}^{m} \left| h_{p_1}\left(k_{p_2} l_{p_3} - k_{p_3} l_{p_2}\right) - k_{p_1}\left(h_{p_2} l_{p_3} - h_{p_3} l_{p_2}\right) + l_{p_1}\left(h_{p_2} k_{p_3} - h_{p_3} k_{p_2}\right) \right| \right)^{N-1}$$

(A8)

The summation term in the parentheses of the right-hand side of inequality A9 is equal to the total volume of parallelepipeds ($V_{p_1 p_2 p_3}$) constructed by Minkowski addition operations on the origin (0, 0, 0) and all possible combinations of three distinct triplets (h_p, k_p, l_p), analogously to the parallelogram construction in the two-dimensional case.

The lower bounds on the volumes of the Minkowski sum polytopes are used to calculate the respective bounds on the mixed volume, owing to the monotonicity property of mixed volume. By analogy with our previous report (Al-Asadi *et al.*, 2012), a direct substitution of the right-hand side eq. (A8) into the definition of a mixed volume (given in Supplemental Information to the above ref.) yields:

$$V_{\mathrm{mix,3D}} \geq \left(\frac{[2(N-1)]!}{\left((N-1)!\right)^3} \right)^3 (N-1)! \sum_{q=1}^{[3(N-1)]!/[(N-1)!(3!)^{N-1}]} \left(\prod_{(p1,p2,p3)}^{N-1} V_{p_1 p_2 p_3} \right) \qquad \text{(A9)}$$

Here, the product is calculated over all different N-1 triplets (p_1, p_2, p_3), in which each index is used only once in each product. The outside summation is performed over all of such triplet combinations. The multiplier (N-1)! is a coefficient in front of every term, equal to the number of permutations that yields each product, as it originates from raising the sum of the individual volumes to the power of N-1 in eq. (A8). Analogously, for a two dimensional crystal:

$$V_{\mathrm{mix,2D}} \geq \left(\frac{[2(N-1)]!}{\left((N-1)!\right)^3} \right)^2 (N-1)! \sum_{q=1}^{[2(N-1)]!/[(N-1)!(2!)^{N-1}]} \left(\prod_{(p1,p2)}^{N-1} A_{p_1 p_2} \right) \tag{A10}$$

where areas of the parallelepipeds defined above are used instead of the volumes and the combinatorics are changed accordingly. For example, for N = 3 in the two-dimensional case, the summation terms raised to the power of N-1 in eq. (A7) in the mixed volume calculation simplify to the term:

$2A_{12}A_{34}+2A_{14}A_{23}+2A_{13}A_{24}$, where

$A_{pq} = |h_p k_q - h_q k_p|$

Here, $(N - 1)!=2!$, which is the factor of 2 in this equation.

The sum of the products of the parallelepiped volumes on the right-hand side of (A9) generally cannot be calculated in the close form. We estimate it based on a scaling argument, as follows. For a one-dimensional crystal the analogous term is exactly equal to (N-1)! (Al-Asadi *et al.*, 2012). For a three-dimensional crystal, the half-ball in the reciprocal space (h ≥ 0) enclosing 3(N-1) of reflections has the radius R determined by the relationship: $(2\pi/3)R^3 \approx 3(N\text{-}1)$, i.e.

$R^{3D} \approx [9/(2\pi)(N\text{-}1)]^{1/3}$

Analogously, for a two-dimensional crystal, the radius of the corresponding half-disk is

$R^{2D} \approx [4/\pi(N\text{-}1)]^{1/2}$

Therefore, to a good approximation, the volume and area products on the right-hand side of eqs. (A9) and (A10) are equal to $[9/(2\pi)]^{N-1}(N\text{-}1)!$ and $[4/\pi]^{N-1}(N\text{-}1)!$ for a three- and a two-dimensional crystal, respectively. Multiplying by the number of such terms in the summation yields for a three-dimensional crystal

$$V_{\text{mix,3D}} \geq \left(\frac{[2(N-1)]!}{\left((N-1)!\right)^3} \right)^3 (N-1)! \frac{[3(N-1)]! \left(\frac{9}{2\pi} \right)^{N-1} (N-1)!}{6^{N-1}(N-1)!} \tag{A11}$$

Similarly, for a two-dimensional crystal

$$V_{\text{mix,2D}} \geq \left(\frac{[2(N-1)]!}{\left((N-1)!\right)^3} \right)^2 (N-1)! \frac{[2(N-1)]! \left(\frac{4}{\pi} \right)^{N-1} (N-1)!}{4^{N-1}(N-1)!} \tag{A12}$$

Note that these expressions become increasingly accurate with increasing *N*, except for very small *N*, since the ball and the circle are poor approximations of the distributions of reflections for small numbers of reflections. For small *N*, accurate calculations can be performed by exact computation of the mixed volumes by using existing software, as described in the text.

Newton polytopes and the Bernstein's theorem on the number of roots of polynomial systems

Here, we give the algebraic terminology and the Bernstein's theorem formulation used in the main text.

A Laurent polynomial is a function of *N* independent complex variables $\eta_1,\ldots,$ η_N defined as a sum of monomial terms $a_k \eta_1^{\beta,k} \ldots \eta_N^{\beta_{N,k}}$, where a_k are complex coefficients and $\beta_{1,k},\ldots, \beta_{N,k}$ are integer powers, which can be positive, zero or negative. This means that for each monomial there is one point in Euclidian space $\boldsymbol{R}^N$ whose coordinates are $(\beta_{1,k}, \ldots, \beta_{N,k})$. For a given Laurent polynomial, these points define vertices of a polytope in $\boldsymbol{R}^N$. The convex hull of this polytope is called the Newton polytope of this polynomial. (A geometrical object is convex when a line segment between any two points that belong to this object lies entirely in that object. A convex hull of a polytope is a minimal convex polytope that contains the given polytope.) The Minkowski sum of two polytopes A and B is a polytope, whose vertices are defined by vector sums of each vertex of polytope A and each vertex of polytope B.

The Bernstein's theorem states that a system of *d* Laurent polynomial equations with *d* unknowns has at most the number of roots equal to the so-called mixed volume of this system, V_{mix}, defined by the following linear combination of *d*-dimensional volumes $V_{M,p}$:

$$V_{mix} = \sum_{p=1}^{d} (-1)^{d-p} V_{M,p} \tag{B1}$$

where for a given *p*, $V_{M,p}$ are volumes of convex hulls of the Minkowski sums of all combinations of *p* different Newton polytopes of this system. For example, for a system of 3 polynomial equations with 3 unknowns:

$$\begin{aligned} V_{mix} = {} & V(\mathbf{conv}(A_1 + A_2 + A_3)) - V(\mathbf{conv}(A_1 + A_2)) - V(\mathbf{conv}(A_1 + A_3)) - V(\mathbf{conv}(A_2 + A_3)) \\ & + V(A_1) + V(A_2) + V(A_3), \end{aligned} \tag{B2}$$

where A_k is the Newton polytope of the *k*-th polynomial in the system, the "+" symbol applied to the polytopes denotes their Minkowski addition, "conv" is the convex hull operator.

In practical cases where monomial coefficients are sufficiently generic (*e.g.* the monomial terms do not cancel out and the polynomials are not linearly dependent), the above mixed volume is known to be equal to the number of roots of the polynomial system. Therefore, the Bernstein's theorem provides a general approach to analyzing the number of roots of a multivariate polynomial system of d equations with d unknowns when variable elimination is not possible.

References

1. Al-Asadi, A., Chudin, E. & Tsodikov, O. V. (2012). *Acta crystallographica. Section A, Foundations of crystallography* **68**, 313-318.