Acta Cryst A FOUNDATIONS ADVANCES

ISSN 2053-2733

Bounding the regularity radius for regular crystals

Dirk Frettloeh*

Technische Fakultät, Universität Bielefeld, Germany. *Correspondence e-mail: frettloe@math.uni-bielefeld.de

Received 8 November 2018
Accepted 9 November 2018

Keywords: Delone sets; regularity radius; crystallinity; Engel sets.

A central question in crystallography is how (or if) a globally crystallographic pattern – a crystal – can be determined by local rules. Therefore it is natural to ask 'how far is local?'. In the previous issue of *Acta Cryst. A*, Baburin *et al.* (2018) give a partial answer for a particular class of (mathematical, idealized) crystals: they consider only 'regular systems'. A regular system is essentially a crystal with only one type of atom, where each atom is surrounded in the same way by its neighbours. They show that in arbitrary dimension d 'local' means at least $2dR$. Here R denotes the radius of the largest empty ball in the crystal (compare the grey ball in Fig. 1). For instance, for the primitive lattice $\mathbb{Z}^2$ in dimension two we obtain $d = 2$ and $R = 2^{1/2}/2$, and hence $2dR = 2(2^{1/2})$. The result says for this example that we need to know at least all neighbourhoods of each atom with radius $2(2^{1/2})$ in order to ensure that it is indeed a crystal.

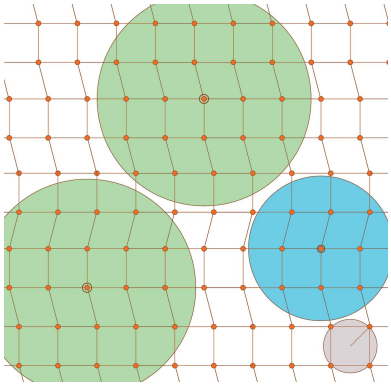
Commonly used mathematical models for crystals (or quasicrystals, or more general structures) are Delone sets. A Delone set is an (infinite, discrete) point set X such that (i) there is $r > 0$ such that each open ball of radius r contains at most one point of X, and (ii) there is $R > r > 0$ such that each closed ball of radius R contains at least one point of X. The points of X represent the (ideal) atomic positions of some structure. One milestone in mathematical crystallography is the Local Theorem (Delone *et al.*, 1976): it provides a necessary and sufficient local condition for a Delone set X being a crystal. In a nutshell this result states that the Delone set X is a crystal if and only if the number of different local patterns of X of radius ρ stays bounded if ρ tends to infinity. For a more precise version of the statement see Delone *et al.* (1976).

In order to count the number of different local patterns properly it is useful to define the cluster-counting function. For $x \in X$ let $C(\rho, x)$ denote the (centred) ρ-cluster $X \cap B(\rho, x)$, where $B(\rho, x)$ denotes the ball of radius ρ centred in x. The cluster-counting function $N(\rho, X)$ is the number of different (centred) ρ-clusters in X. Note that it is important to consider *centred* clusters: for instance, in the integer lattice $\mathbb{Z}^2$ there are several different ρ-clusters of the form $\mathbb{Z}^2 \cap B(\rho, x)$ if x is arbitrary, but there is only one kind of ρ-cluster $C(\rho, x)$ for any particular value ρ if x is required to lie in $\mathbb{Z}^2$.

From now on we consider this particular case where there is only one kind of ρ-cluster. If ρ is very small (*e.g.* $\rho \leq r$) this does not imply anything on X: all ρ-clusters in X consist of only one point. If ρ is large, and there is only one kind of ρ-cluster in X (up to congruence), then by the Local Theorem X is necessarily crystallographic. Hence it is natural to ask for good (upper and lower) bounds on the value $\widehat{\rho}_d$ such that, if there is only one ρ-cluster in some Delone set X in d-dimensional Euclidean space, then X is necessarily crystallographic. Thus $\widehat{\rho}_d$ depends on the dimension d, but is universal for all Delone sets X in d-dimensional Euclidean space.

A commonly used mathematical model of a crystal is the orbit of one point, or of several (inequivalent) points under a crystallographic group in d-dimensional Euclidean space. In the first case the corresponding (infinite) Delone set is called a regular system, in the latter case the Delone set is called a multiregular system. One particular instance of the question of the origin of crystallinity is to find good bounds on the value $\widehat{\rho}_d$ described above for regular systems. Let us call the smallest such $\widehat{\rho}_d$ the regularity radius (of all regular systems X in a given dimension d).

Since we may scale any crystallographic Delone set X arbitrarily, the bounds on $\widehat{\rho}_d$ ought to be expressed in terms of R (the radius of the largest empty ball in X). In dimensions $d = 1$ and $d = 2$ the exact values of the corresponding $\widehat{\rho}_d$ are known: $\widehat{\rho}_1 = 2R$ and $\widehat{\rho}_2 = 4R$ (see *e.g.* Barburin *et al.*, 2018; Dolbilin, 2018). Similar arguments as in



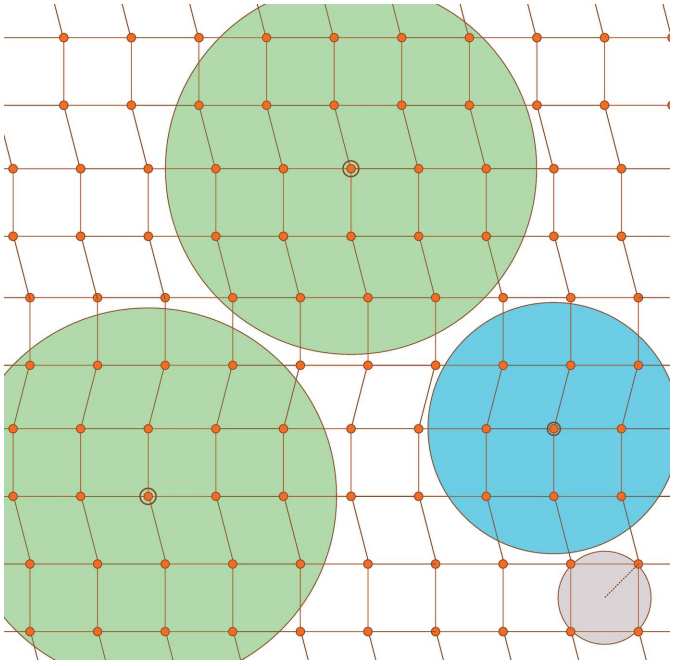


Figure 1
The orange points form a non-crystalline point set. The green balls of radius $2(2^{1/2})$ can detect the non-crystallinity of the point set. Smaller balls like the blue one cannot: they all look alike.

Dolbilin (2018) yield that $\widehat{\rho}_d$ is at least $4R$ for any $d \geq 2$. Engel conjectured that in dimension three we have $4R \leq \widehat{\rho}_3 \leq 6R$ (Engel, 1986).

A good lower bound on $\widehat{\rho}_d$ for Delone sets in arbitrary dimension is obtained in Barburin *et al.* (2018): it is shown that $\widehat{\rho}_d$ is at least $2dR$ (Theorem 5.8). In particular, $\widehat{\rho}_d$ grows at least linearly in the dimension d. Hence there is no general bound on $\widehat{\rho}_d$ independent of d. The result is obtained by a sophisticated construction of Delone sets X ('Engel sets') with only one kind of centred ρ-cluster of radius $\rho < 2dR$ such that X still is not a regular system. The construction works in any dimension $d \geq 3$.

This recent result shows that there are still profound questions and answers found in mathematical crystallography today. A next step might be to treat the corresponding question for multiregular systems. Here one cannot expect a regularity radius $\widehat{\rho}_d$ such that beyond that radius there exists only one congruence class of ρ-clusters. Rather one would require that beyond $\widehat{\rho}_d$ there are at most m types of ρ-clusters, where m is the number of different orbits with respect to the underlying crystallographic group.

References

Baburin, I. A., Bouniaev, M., Dolbilin, N., Erokhovets, N. Y., Garber, A., Krivovichev, S. V. & Schulte, E. (2018). *Acta Cryst.* A**74**, 616–629.

Delone, B. N., Dolbilin, N. P., Stogrin, M. I. & Galiulin, R. V. (1976). *Sov. Math. Dokl.* **17**, 319–322.

Dolbilin, N. P. (2018). *Discrete Geometry and Symmetry*, edited by M. D. E. Conder, A. Deza & A. Ivic Weiss, *Springer Proceedings in Mathematics and Statistics*, Vol. 234, pp. 109–125. Springer International Publishing.

Engel, P. (1986). *Geometric Crystallography, an Axiomatic Introduction to Crystallography*. Dordrecht: Kluwer.