

## Regular Paper

Regular and Multi-regular  $t$ -bonded SystemsMIKHAIL BOUNIAEV<sup>1,a)</sup> NIKOLAI DOLBILIN<sup>2,b)</sup>

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**Abstract:** The concept of  $t$ -bonded sets was briefly introduced by the second author in 1976 under the name of  $d$ -connected sets, though it has not received due consideration. This concept is a generalization of the concept of Delone  $(r, R)$ -systems. In light of the developments in the local theory for crystals that occurred since 1976 and demands in chemistry and crystallography, we believe the local theory for  $t$ -bonded sets deserves to be developed to describe materials whose atomic structures is multi-regular “microporous” point set. For a better description of such “microporous” structures it is worthwhile to take into consideration a parameter that represents atomic bonds within the matter. The overarching goal of this paper is to prove that analogous local conditions that guarantee that a Delone set is a regular (or multi-regular) system also guarantee that a  $t$ -bonded set is a regular (or multi-regular)  $t$ -bonded system.

**Keywords:** local theory, Delone sets, regular systems, crystals,  $t$ -bonded sets

## 1. Introduction

In this section we present basic definitions related to the mathematical concept of crystal in the light of the local theory with the overarching goal to extend the theory’s results to the broader class of sets ( $t$ -bonded sets, Definition 2.1).

The above mentioned definitions single the family of crystals out of the family of more general sets, which fulfills the requirements for point sets to be uniformly discrete (see the  $r$ -condition below), and relatively dense (the  $R$ -condition below). Sets with these conditions were introduced and studied by B. Delone who called them  $(r, R)$ -systems (Refs. [2], [3]).

**Definition 1.1** (Delone Set) A subset  $X$  of Euclidean space  $\mathbb{R}^d$  is called a *Delone set* if there are positive numbers  $r$  and  $R$  such that the two conditions hold

$r$ -condition: any open ball  $B(r)$  of radius  $r$  has at most one point from  $X$  (uniform discreteness), and

$R$ -condition: any closed ball  $B(R)$  of radius  $R$  has at least one point from  $X$  (relative density).

**Remark 1.1** A set  $X$  with  $r$ -condition is called *uniformly discrete*. In principle, the parameters  $r$  and  $R$  can be chosen as the supremum of all numbers for which the set  $X$  satisfies  $r$ -condition, and as the infimum of all numbers for which  $X$  satisfies  $R$ -condition, respectively.

**Definition 1.2** (Regular System) A Delone set  $X$  is called a *regular system* if for any two points  $x$  and  $y$  from  $X$  there is a symmetry  $s$  of  $X$  such that  $s(x) = y$ , i.e., if the symmetry group  $\text{Sym}(X)$  acts transitively on  $X$ .

**Remark 1.2** It follows immediately from definition 1.2 that a regular point set  $X$  is an orbit  $G \cdot x$ , where  $x$  is a point from  $X$ , and

$G$  is, generally speaking, a subgroup of  $\text{Sym}(X)$ . We remind that  $G$ -orbit of  $x$  is the set  $G \cdot x = \{g(x) | g \in G\}$ .

Let  $\text{Iso}(d)$  be the complete group of all isometries of  $\mathbb{R}^d$ .

**Definition 1.3** (Discrete Group) A group  $G \subset \text{Iso}(d)$  is called a *discrete subgroup*, if the orbit  $G \cdot x$  of any point  $x \in \mathbb{R}^d$  is a uniformly discrete set.

**Definition 1.4** (Fundamental Domain) Let  $G$  be a discrete subgroup of  $\text{Iso}(d)$ . We call a closed domain  $F(G)$  in  $\mathbb{R}^d$  a *fundamental domain* of group  $G$  if:

(i) for any point  $x$  from  $\mathbb{R}^d$ , the intersection of  $F(G)$  and the orbit  $G \cdot x$  is not empty;

(ii) for any point  $x$  from  $\mathbb{R}^d$ , the interior of  $F(G)$  contains at most one point from  $G \cdot x$ .

**Remark 1.3** For a discrete group  $G$  a fundamental domain does exist. It suffices to take an orbit  $G \cdot x$  of a non-fixed point  $x$  with respect to  $G$  and construct the Voronoi tessellation for the  $G \cdot x$ . The Voronoi domain is a fundamental domain of the group. A fundamental domain can be chosen in a non-unique way, sometimes it can be unbounded.

**Definition 1.5** (Crystallographic Group) A group  $G \subset \text{Iso}(d)$  is called *crystallographic* if any orbit  $G \cdot x$  is a discrete set, and the fundamental domain of  $G$  is compact.

Fundamental results for crystallographic groups were obtained in Refs. [4], [5].

**Statement 1.1** A Delone set  $X$  is a regular system if and only if there is a crystallographic group  $G$  such that  $X$  is a  $G$ -orbit of some point  $x$ .

E.S. Fedorov defined crystal as a finite union of regular systems [6].

**Definition 1.6** (Crystal) We say that a subset  $X$  of  $\mathbb{R}^d$  is a *crystal* if  $X$  is the  $G$ -orbit of a finite set  $X_0 = \{x_1, \dots, x_k\}$ , i.e.,  $X = \bigcup_{i=1}^k G \cdot x_i$ .

The main goal of the local theory for crystals is to develop a sound mathematical theory that would explain how symmetry of

<sup>1</sup> University of Texas Rio Grande Valley, Brownsville-Edinburg-Harlingen, USA

<sup>2</sup> Steklov Mathematical Institute of Russian Academy of Science, Moscow, Russian Federation

<sup>a)</sup> mikhail.bouniaev@utrgv.edu

<sup>b)</sup> dolbilin@mi.ras.ru

crystalline structure can be derived from the pairwise identity of fragments (clusters, see below) around each atom. However, before 1970s, there were no rigorously proven mathematical statements in this regard until B. Delone and R. Galiulin put the problem, and Delone's students N. Dolbilin, M. Stogrin, and others (see for instance, Refs. [7], [8], [9], [11], [14], [15]) developed a mathematically sound local theory of crystals.

**Statement 1.2** For a Delone set  $X$  and for any two points  $x$  and  $x' \in X$  there is a finite sequence  $x = x_0, x_1, \dots, x_m = x'$  of points from  $X$  such that  $|x_{i-1}x_i| \leq 2R$ ,  $i \in [1, m]$ .

We call such sequence a  $2R$ -chain and denote it as  $[x, \dots, x']$ . Each pair  $(x_{i-1}, x_i)$  is called a *bond* of the  $2R$ -chain.

One should note that in proofs of theorems in the local theory we use Statement 1.2, i.e., the fact that any two points of a Delone set can be linked by a chain with the length of bonds not greater than some number  $t$ . We note that by Statement 1.2 for a Delone set  $t$  does not exceed  $2R$ . Moreover, the upper bounds for the size of a cluster of  $X$ , which determines a global symmetry of the structure, depends on the value of  $t$ . It follows that the lesser the value of  $t$  the smaller cluster. On the other hand, there are Delone sets for which the 'bond length' parameter  $t$  is significantly lesser than  $2R$  as well as there are uniformly discrete sets whose any two points can be also connected by a  $t$ -chain.

These observations inspired us to develop the local theory for the  $t$ -bonded sets. In fact, this concept was introduced in Ref. [1] under the name of  $d$ -connected sets. In the theory of  $t$ -bonded sets we do not require (unless it is stated as a premise) that a set  $X$  under consideration is a Delone set, and therefore these sets do not possess some properties that were used in developing the local theory for Delone sets.

## 2. Definition of $t$ -bonded Sets and Related Concepts

As we have already mentioned, in this paper we consider sub-sets (that we denote  $X, Y, Z, \dots$  etc.) of  $d$ -space  $\mathbb{R}^d$  that are uniformly discrete point sets, i.e. sets which fulfil  $r$ -condition in Definition 1.1. Thus  $X$  is, generally speaking, not a Delone set. Like for a Delone set we will choose  $r$  as the supremum of all numbers such that the set  $X$  satisfies  $r$ -condition.

**Definition 2.1** ( $t$ -bonded Set) A set  $X \subset \mathbb{R}^d$  is said to be a  $t$ -bonded set in  $\mathbb{R}^d$ , where  $t$  is some positive number if:

- (1) any open ball  $B(r)$  of radius  $r$  has at most one point from  $X$  ( $r$ -condition);
- (2)  $\text{aff}X = \mathbb{R}^d$ , where  $\text{aff}X$  stands for the affine hull of  $X$ ;
- (3) for any two points  $x$  and  $x' \in X$  there is a  $t$ -chain, finite sequence  $x_0 = x, x_1, \dots, x_m = x'$  of points from  $X$  such that  $|x_{i-1}x_i| \leq t$ ,  $i \in [1, m]$ .

We say that a pair  $(x_{i-1}, x_i)$  of points with  $|x_{i-1}x_i| \leq t$  is a  $t$ -bond.

It is clear that for a  $t$ -bonded set  $X$  we have  $t \geq 2r$ . By Statement 1.2 for a Delone set we  $t \leq R$ . However, for some Delone sets the value of  $t$  can be less than  $2R$ . For instance, if  $X = \mathbb{Z}^d$  is the cubic lattice, then  $t$  can be chosen as the edge length of the cube. Since the largest ball empty from points of  $X$  is the circum ball around a cube with the edge length  $t$ . Therefore for  $\mathbb{Z}^d$  we have  $2R = t\sqrt{d}$ .

In the local theory the concept of cluster plays a significant role. In principle, this concept can be introduced by different ways. In this paper we will consider a version of the cluster which was used in the local set for Delone sets.

**Definition 2.2** (Cluster) For  $\rho > 0$ , a  $\rho$ -cluster  $C_x(\rho)$  centered at point  $x \in X$  is defined as a set of all points  $x' \in X$  such that  $|xx'| \leq \rho$ , i.e.,

$$C_x(\rho) = X \cap B_x(\rho).$$

The parameter  $t$  in a  $t$ -bonded set plays a role similar to that of the parameter  $2R$  in a Delone set. However, as we will see that there are essential differences between properties of  $2R$ -clusters and of  $t$ -clusters.

In particular, in a Delone set a  $2R$ -cluster always has the rank, i.e., dimension of the affine hull of the cluster, equal to  $d$ . At the same time in a  $t$ -bonded set the rank of a  $t$ -cluster can be arbitrary between 2 and  $d$ .

Later we will introduce some conditions that guarantee that given cluster has rank  $d$  (Theorem 3.1).

**Statement 2.2** Given a  $t$ -bonded set  $X$ ,  $\rho > 0$ , let  $X \setminus C_x(\rho) \neq \emptyset$ . Then there is a point  $x' \in X$  such that  $x' \in C_x(\rho + t) \setminus C_x(\rho)$ , and it is connected to the center  $x$  by a  $t$ -chain contained in  $C_x(\rho + t)$ .

Indeed, if we assume the contrary, i.e., we assume that the spherical layer  $B_x(\rho + t) \setminus B_x(\rho)$  contains no points of  $X$ . Since  $X$  is a  $t$ -bonded set we get  $X \setminus C_x(\rho) = \emptyset$ .

Here it should be noted that both  $C_x(\rho)$  and  $C_x(\rho + t)$  are not necessarily  $t$ -bonded set itself. In the spherical layer  $B_x(\rho + t) \setminus B_x(\rho)$ , besides  $x'$ , generally speaking, there can also be points  $x'' \in X$  that are connected to  $x$  just by a 'long'  $t$ -chain starting at the center  $x$  of the cluster  $C_x(\rho + t)$ , leaving it, and then coming back to the cluster  $C_x(\rho + t)$  to get eventually connected to  $x''$ .

**Definition 2.4** (Cluster Equivalence) Given a  $t$ -bonded set  $X$  in  $\mathbb{R}^d$ ,  $\rho > 0$  and two points  $x$  and  $x' \in X$ , we say that the  $\rho$ -clusters  $C_x(\rho)$  and  $C_{x'}(\rho)$  are equivalent, if there is an isometry  $g$  of  $\mathbb{R}^d$ , such that  $g(x) = x'$  and  $g(C_x(\rho)) = C_{x'}(\rho)$ .

In Section 4 we prove two theorems (Theorem 4.1 and Theorem 4.2) for  $t$ -bonded sets that are similar to the Criterion for Regular (Delone) Systems and Criterion for Crystals (see, e.g., Refs. [7], [8], [10], [12], [13], [16]). Though the statements of the theorems are almost identical for both Delone sets and  $t$ -bonded sets the main challenge of the proofs is related to the rank of the clusters, which as we have already mentioned is  $d$  for  $2R$ -clusters in Delone sets, however, in case of  $t$ -bonded sets it may not be equal to  $d$  for  $\rho$ -clusters when  $\rho$  is equal to  $t$ . The cluster's rank naturally affects the structure of the group  $S_x(\rho)$  of the cluster's symmetries. The statements of both theorems, as well as their proofs, depend on the concept of cluster counting function that we define below.

For a given  $\rho > 0$ , the set of all  $\rho$ -clusters  $C_x(\rho)$ ,  $x \in X$ , is divided into equivalence classes. If a  $t$ -bonded set  $X$  is finite the cardinality of the set of equivalence classes is an integer positive number. If  $X$  is an infinite set then the cardinality of the set of equivalence  $\rho$ -classes, generically saying, can be infinite.

**Definition 2.5** (Set of Finite Type) A set  $X$  is said to be of *finite type* if for any positive number  $\rho$  the cardinality of the set of all classes of  $\rho$ -clusters  $C_x(\rho)$  is finite. The cardinality in this case

defined for all  $\rho \geq 0$  function which is called the *cluster counting function*. denoted by  $N(\rho)$ .

It is easy to see that for a  $t$ -bonded set  $X$  of finite type the cluster counting function  $N(\rho)$  is a positive, piecewise constant, integer valued, monotonically non-decreasing, and continuous from the left function.

### 3. The Rank and the Symmetry Group of a Cluster

In this section we discuss the *rank* of a cluster, i.e. the dimension of the affine hull of a cluster. Emphasize again, that there is an essential difference between  $2R$ -clusters in Delone sets and  $t$ -clusters in  $t$ -bonded sets: in a Delone set a  $2R$ -cluster always has the rank equal to  $d$  while in a  $t$ -bonded set the rank of a  $t$ -cluster can be arbitrary between 2 and  $d$ .

To shorten the notation, we will use  $d_x(\rho) := \dim(\text{aff}C_x(\rho))$  for the rank of the cluster  $C_x(\rho)$ . In all discussions below  $\Pi^n$  stands for the affine hull of a  $t$ -bonded set  $X$ ,  $n \leq d$ .

**Lemma 3.1** Let  $X \subset \mathbb{R}^d$  be a  $t$ -bonded set,  $\rho$  a positive real number, and  $x, x'$  two points from  $X$  such that  $|xx'| \leq t$ , and the following conditions hold true,

$$d_x(\rho) = d_{x'}(\rho + t) \text{ and } d_{x'}(\rho) = d_x(\rho + t) \quad (1)$$

Then  $\text{aff}C_{x'}(\rho) = \text{aff}C_{x'}(\rho + t) = \text{aff}C_x(\rho + t) = \text{aff}C_x(\rho)$ .

**Proof.** Since  $|xx'| \leq t$ , it follows that  $C_x(\rho) \subset C_{x'}(\rho + t)$  and  $C_{x'}(\rho) \subset C_x(\rho + t)$ . Hence,  $\text{aff}C_x(\rho) \subset \text{aff}C_{x'}(\rho + t)$  and  $\text{aff}C_{x'}(\rho) \subset \text{aff}C_x(\rho + t)$ . From the premises of the lemma  $d_x(\rho) = d_{x'}(\rho + t)$  and  $d_{x'}(\rho) = d_x(\rho + t)$ , it follows that  $\text{aff}C_x(\rho + t) = \text{aff}C_x(\rho) \subset \text{aff}C_{x'}(\rho + t)$ , and  $\text{aff}C_{x'}(\rho + t) = \text{aff}C_{x'}(\rho) \subset \text{aff}C_x(\rho + t)$ . Therefore,  $\text{aff}C_{x'}(\rho) = \text{aff}C_{x'}(\rho + t) = \text{aff}C_x(\rho + t) = \text{aff}C_x(\rho)$ .  $\square$

Using Lemma 3.1 it is not hard to prove the following two theorems.

**Theorem 3.1** Let  $X \subset \mathbb{R}^d$  be a  $t$ -bonded set, assume that there is some  $\rho > 0$  such that for any point  $x$  from  $X$  the following condition holds

$$d_x(\rho) = d_x(\rho + t). \quad (2)$$

Then  $\forall x \in X$   $d_x(\rho) = d_x(\rho + t) \equiv d$  and  $\text{aff}C_x(\rho) = \text{aff}X = \mathbb{R}^d$ .

**Theorem 3.2** Let  $X \subset \mathbb{R}^d$  be a  $t$ -bonded set, such that for every given  $\rho \leq t \cdot (d - 1)$  the rank of a  $\rho$ -cluster at each point of  $X$  is the same ( $d_x(\rho) = d(\rho)$ ,  $\forall x \in X$ ). Then, for any  $\rho' \geq d \cdot t$  and any  $x \in X$ , the rank  $d_x(\rho') \equiv d$ .

**Remark 3.1** Under the conditions of Theorem 3.2 stabilization of the rank of any cluster definitely occurs when  $\rho \geq d \cdot t$ . However, for some sets it might occur even if  $\rho \leq d \cdot t$ .

Now we are going to discuss symmetries of clusters. We keep assuming that  $X$  is a  $t$ -bonded set in  $\mathbb{R}^d$  which by definition implies  $\text{aff}X = \mathbb{R}^d$ . Let us denote by  $O(x, d)$  a group of all isometries of space  $\mathbb{R}^d$  which leave  $x \in \mathbb{R}^d$  fixed.

**Definition 3.1** (The Symmetry of a Cluster) Assume  $x \in X$ , then an isometry  $\tau \in O(x, d)$  is called a *symmetry* of the cluster  $C_x(\rho)$  if  $\tau(C_x(\rho)) = C_x(\rho)$ .

We want to emphasize that since  $\tau \in O(x, d)$ , any symmetry  $\tau$  of a cluster leaves its center  $x$  fixed. We denote by  $S_x(\rho)$  a group of all symmetries  $\tau$  of the cluster  $C_x(\rho)$ .

Now let  $\text{aff}C_x(\rho) = \Pi_x^n$  where  $\Pi_x^n$  is an  $n$ -dimensional affine subspace,  $x \in \Pi_x^n$ , and  $n \leq d$ . We denote by  $\bar{S}_x(\rho)$  a group of all isometries from  $O(x, n)$  that leave invariant the affine subspace  $\Pi_x^n$  and the cluster  $C_x(\rho)$ .

If  $n = d$ , then  $\bar{S}_x(\rho) = S_x(\rho)$ . Let  $n < d$ , then we denote the affine hull of  $C_x(\rho)$  by  $\Pi_x^n$ , and the complementary orthogonal  $(d - n)$ -affine subspace passing through  $x$  by  $Q_x^{d-n}$ . Let  $s \in S_x(\rho)$  be a symmetry of the  $\rho$ -cluster  $C_x(\rho)$ . It is clear that any such symmetry is an orthogonal transformation of the  $d$ -space which is a product of the transformation  $\bar{s}$  of  $\Pi_x^n$  and of an arbitrary transformation  $g \in O(x, d - n)$  of the complementary affine subspace.

Two lemmas below summarize some facts on the cluster symmetry group.

**Lemma 3.2** The following statements hold true.

- (1) If  $\text{aff}C_x(\rho) = \Pi_x^n$  and  $n < d$ , then  $S_x(\rho) = \bar{S}_x(\rho) \oplus O(x, d - n)$ , where  $\bar{S}_x(\rho) \subset O(x, n)$ , and  $O(x, d - n)$  is the full group of isometries of the affine subspace  $Q_x^{d-n}$  complementary to  $\Pi_x^n$  and passing through the point  $x$ .
- (2) The group  $\bar{S}_x(\rho)$  is a finite subgroup of  $O(x, n)$ . Particularly, if  $\text{aff}C_x(\rho) = \mathbb{R}^d$ , then group  $S_x(\rho) = \bar{S}_x(\rho)$  is a finite subgroup of  $O(x, d)$ .
- (3) The group  $S_x(\rho)$  is finite if and only if  $\text{aff}C_x(\rho) = \mathbb{R}^d$  or  $\text{aff}C_x(\rho) = \mathbb{R}^{d-1}$ .

**Lemma 3.3** Assume  $\bar{S}_x(\rho_0)$  and  $\bar{S}_x(\rho_0 + t)$  are finite groups as defined at the beginning of the paragraph for clusters  $C_x(\rho_0)$  and  $C_x(\rho_0 + t)$  respectively. The following statements hold true.

- (1) If  $S_x(\rho_0 + t) = S_x(\rho_0)$ , then  $\text{aff}C_x(\rho_0) = \text{aff}C_x(\rho_0 + t) = \Pi_x^n$ ,  $n \leq d$ .
- (2) The equality  $S_x(\rho_0) = S_x(\rho_0 + t)$  is equivalent to  $\bar{S}_x(\rho_0) = \bar{S}_x(\rho_0 + t)$ .

Let us remind that according to Definition 2.4 given a  $t$ -bonded set  $X$  in  $\mathbb{R}^d$  and  $\rho > 0$ , the  $\rho$ -cluster  $C_x(\rho)$  is equivalent to the  $\rho$ -cluster  $C_{x'}(\rho)$ , if there is a space isometry  $g$  of  $\mathbb{R}^d$ , such that  $g(x) = x'$  and  $g(C_x(\rho)) = C_{x'}(\rho)$ .

The following two statements are easy to prove.

**Statement 3.1** Given  $t$ -bonded set  $X \subset \mathbb{R}^d$  and  $\rho_0 > 0$ , if clusters  $C_x(\rho_0)$  and  $C_{x'}(\rho_0)$  are equivalent, then groups  $S_x(\rho_0)$  and  $S_{x'}(\rho_0)$  are conjugate.

**Statement 3.2** Let  $X$  be a  $t$ -bonded set in  $\mathbb{R}^d$ , and there is a point  $x \in X$  and  $\rho_0 > 0$  such that  $S_x(\rho_0) = S_x(\rho_0 + t)$ . If the cluster  $C_x(\rho_0 + t)$  is equivalent to a centered at some point  $x'$  cluster  $C_{x'}(\rho_0 + t)$ , then  $S_{x'}(\rho_0) = S_{x'}(\rho_0 + t)$ .

Now we will prove a theorem which plays an important role in proving theorems of the local theory.

**Theorem 3.3** ( $t$ -extension) Assume in the  $t$ -bonded set  $X$  for two points  $x$  and  $x' \in X$  and some  $\rho_0 > 0$ , clusters  $C_x(\rho_0 + t)$  and  $C_{x'}(\rho_0 + t)$  are equivalent, and the groups  $S_x(\rho_0)$  and  $S_{x'}(\rho_0 + t)$  coincide:

$$S_x(\rho_0) = S_{x'}(\rho_0 + t). \quad (3)$$

Then any isometry  $g \in \text{Iso}(\mathbb{R}^d)$  such that  $g(x) = x'$  and that maps  $C_x(\rho_0)$  onto  $C_{x'}(\rho_0)$  (i.e.,  $g(C_x(\rho_0)) = C_{x'}(\rho_0)$ ) also maps  $(\rho_0 + t)$ -cluster  $C_x(\rho_0 + t)$  onto  $C_{x'}(\rho_0 + t)$  (i.e.,  $g(C_x(\rho_0 + t)) = C_{x'}(\rho_0 + t)$ ).

**Proof.** By the assumption of the theorem, clusters  $C_x(\rho_0 + t)$  and  $C_{x'}(\rho_0 + t)$  are equivalent. Therefore there is an isometry  $g \in \text{Iso}(d)$  such that  $g(x) = x'$  and  $g(C_x(\rho_0 + t)) = C_{x'}(\rho_0 + t)$ .

Let  $f$  be an arbitrary isometry that maps  $\rho_0$ -cluster  $C_x(\rho_0)$  onto  $\rho_0$ -cluster  $C_{x'}(\rho_0)$ . Let us take the composition  $f^{-1} \circ g$ . Then we have

$$(f^{-1} \circ g)(C_x(\rho_0)) = f^{-1}(g(C_x(\rho_0))) = f^{-1}(C_{x'}(\rho_0)) = C_x(\rho_0). \quad (4)$$

From Eq. (4) it follows that  $f^{-1} \circ g \in S_x(\rho_0)$ . Hence, by condition (3.3) of Theorem 3.3  $f^{-1} \circ g \in S_x(\rho_0) = S_{x'}(\rho_0 + t)$ . Let us put  $f^{-1} \circ g := s$ ,  $s \in S_x(\rho_0 + t)$ . Thus,  $f = g \circ s^{-1}$ . Since  $g$  maps  $C_x(\rho_0 + t)$  onto  $C_{x'}(\rho_0 + t)$  and  $s^{-1}$  maps  $C_x(\rho_0 + t)$  onto  $C_x(\rho_0 + t)$ , we conclude that  $f$  maps  $C_x(\rho_0 + t)$  onto  $C_{x'}(\rho_0 + t)$ .  $\square$

#### 4. Criteria for Regular and Multi-regular $t$ -bonded Systems

Let us remind that by Definition 2.5 a cluster counting function  $N(\rho)$  is equal to the cardinal number of equivalence classes of clusters with radius  $\rho$  provided the cardinal number is finite.

**Definition 4.1** (Regular  $t$ -bonded System) A  $t$ -bonded set  $X$  is called a *regular  $t$ -system* if for any two points  $x$  and  $y$  from  $X$  there is a symmetry  $g$  of  $X$  such that  $g(x) = y$ , i.e., if the symmetry group  $\text{Sym}(X)$  acts transitively on  $X$ .

**Theorem 4.1** Given  $t$ -set  $X$  in  $\mathbb{R}^d$ , assume that there is  $\rho_0$  such that the following two conditions hold:

- (1)  $N(\rho_0 + t) = 1$ ;
- (2) for some point  $x_0 \in X$ ,  $S_{x_0}(\rho_0) = S_{x_0}(\rho_0 + t)$ .

Then:

- (1) Group  $G \subset \text{Iso}(\mathbb{R}^d)$  of all symmetries of  $X$  acts on  $X$  transitively.
- (2) For any point  $x \in X$   $\text{aff}(C_x(\rho_0)) = \text{aff}C_x(\rho_0 + t) = \text{aff}X = \mathbb{R}^d$ .

**Proof.** First of all, note that because of Statement 3.2 and Condition (1) of Theorem 4.1 (any two  $(\rho_0 + t)$ -clusters are equivalent), Condition (2) holds true not only for the point  $x_0$ , but for any point  $x \in X$  ( $S_x(\rho_0) = S_x(\rho_0 + t)$ ).

Let us prove that the subgroup  $G \subset \text{Iso}(\mathbb{R}^d)$  of all symmetries of  $X$  acts on  $X$  transitively.

By condition (1) of the theorem for any two points  $x$  and  $x'$  from  $X$ , there exists  $g \in \text{Iso}(\mathbb{R}^d)$  such that  $g$  maps  $C_x(\rho_0 + t)$  onto  $C_{x'}(\rho_0 + t)$  and  $g(x) = g(x')$ . We will prove that  $g$  maps  $X$  onto  $X$ .

Let us take an arbitrary point  $z \in X$  and connect  $x$  to  $z$  by a  $t$ -chain  $x = x_0, x_1, \dots, x_n = z$ . We will show that  $g$ -images of all points of the chain starting with  $x_1$  and ending with  $x_n = z$  belong to  $X$ .

Since  $|xx_1| \leq t$ , it follows that  $C_{x_1}(\rho_0) \subset C_x(\rho_0 + t)$  and  $g(C_{x_1}(\rho_0)) = C_{y_1}(\rho_0)$  where  $y_1 = g(x_1) \in C_{y_1}(\rho_0 + t) \subset X$ . By Theorem 3.3  $g(C_{x_1}(\rho_0 + t)) = C_{y_1}(\rho_0 + t)$ .

Hence we proved that  $g(C_{x_1}(\rho_0 + t)) = C_{y_1}(\rho_0 + t)$  and  $g(x_1) = y_1 \in X$ . Since the distance  $|x_i x_{i-1}| \leq t$  for all  $i$  such that  $1 \leq i \leq n-1$ , applying the same argument to points  $x_i$  and  $x_{i+1}$  as we applied to  $x_0$  and  $x_1$ , we prove that for all non-negative integers  $i \leq n-1$ ,  $g(x_{i+1}) = y_{i+1} \in X$  and  $g(C_{x_{i+1}}(\rho_0 + t)) = C_{y_{i+1}}(\rho_0 + t)$ .

Hence,  $g(z) = g(x_n) = y_n \in X$ , and  $g(X) \subseteq X$ .

To show that  $g$  is a surjection we note that the inverse isometry  $g^{-1}$  maps  $x'$  onto  $x$  and  $C_{x'}(\rho_0)$  onto  $C_x(\rho_0)$ . Applying the same argument to  $g^{-1}$  as we applied to  $g$  we show that  $g^{-1}$  maps  $X$  into  $X$ . Therefore, for any  $y \in X$ ,  $g^{-1}y \in X$ . Hence,  $g$  is a surjection.

As we already mentioned,  $S_x(\rho_0) = S_x(\rho_0 + t)$  for any point

$x \in X$ . Therefore, by Lemma 3.3 (part 1)  $\text{aff}C_x(\rho) = \Pi_x^n = \text{aff}C_x(\rho_0 + t) = \Pi_x^n$ , i.e. for every  $x \in X$  the following condition holds

$$d_x(\rho) = d_x(\rho + t). \quad (5)$$

Then, by Theorem 3.1  $\forall x \in X$   $d_x(\rho) = d_x(\rho + t) \equiv d$ , and  $\text{aff}C_x(\rho_0) = \text{aff}C_x(\rho_0 + t) = \text{aff}X \subseteq \mathbb{R}^d$ .  $\square$

**Definition 4.2** A  $t$ -bonded set  $X \subset \mathbb{R}^d$  is a *multi-regular  $t$ -bonded system* if there is a finite set  $X_0 = \{x_1, \dots, x_m\}$  such that

$$X = \bigcup_{i=1}^m \text{Sym}(X) \cdot x_i.$$

Definition 4.2 is analogous to Definition 1.6 of a crystal. However, the situation is quite different in some respects. For instance, in case of crystal we deal with Delone sets which are always infinite sets. Therefore the requirement to represent a Delone set as a disjoint union of a finite number of regular systems selects a proper subfamily from the full family of all Delone sets.

However, if  $X$  is a finite set then  $X$  can be obviously thought as a  $t$ -bonded set for some suitable value of  $t$  and, moreover,  $X$  can be thought as a multi-regular system. In fact the finite set  $X$  can be presented as a finite collection of orbits with respect to the trivial group. Nevertheless, the following refined version of the question makes sense for finite sets as well as for infinite  $t$ -bonded sets.

Let us call a  $t$ -bonded set an  *$m$ -regular  $t$ -bonded system* if the number of classes in  $X/\text{Sym}(X) = m$ . Are there conditions which guarantee that a  $t$ -bonded set  $X$  is an  $m$ -regular system? The following criterion answers the question.

**Theorem 4.2** (Local Criterion for  $m$ -regular  $t$ -systems) A  $t$ -bonded set  $X \subset \mathbb{R}^d$  is an  $m$ -regular  $t$ -system if and only if there is some  $\rho_0 > 0$  such that two conditions hold:

- 1)  $N(\rho_0) = N(\rho_0 + t) = m$ ;
- 2)  $S_x(\rho_0) = S_x(\rho_0 + t)$ ,  $\forall x \in X$ .

**Proof.** We precede a proof of Theorem 4.2 with Lemma 4.1, which from our point of view also has its own value. The idea of the proof is similar to that of an analogous criterion for a crystal (see, e.g., Refs. [8], [10], [16]). On the other hand, in order to prove this criterion for  $t$ -bonded sets we do not need to prove that the group  $\text{Sym}(X)$  is crystallographic. The local criterion for regular systems (Theorem 4.1) is a particular case of Theorem 4.2. Indeed, the condition  $N(\rho_0 + t) = 1$  implies  $N(\rho_0) = N(\rho_0 + t) = 1$ .

**Lemma 4.1** Let a  $t$ -bonded set  $X$  fulfill conditions 1) and 2) of Theorem 4.2 and  $X_i$  a subset of  $X$  of all points from  $X$ , whose  $\rho_0$ -clusters are equivalent and belong to the  $i$ -th class,  $i \in [1, m]$ . If  $G_i$  is a group generated by all isometries  $f$  such that  $f(x) = x'$  and  $f(C_x(\rho_0)) = C_{x'}(\rho_0)$ ,  $\forall x, x' \in X_i$ , then:

- 1)  $G_i$  acts transitively on a set  $X_i$ ,  $\forall i \in [1, m]$ ;
- 2) Group  $G_i$  does not depend on  $i$  and for any  $i \in [1, m]$ ,  $G_i = \text{Sym}(X)$ .

**Proof.** Since for any  $i$ ,  $X_i$  is not empty, for any two points  $x, x' \in X_i$  there is an isometry  $g$  that maps  $C_x(\rho_0)$  onto  $C_{x'}(\rho_0)$  and  $x$  onto  $x'$ . Therefore for any  $i$ ,  $G_i$  is not empty. Because of the way we defined  $X_i$ , at least one isometry exists in  $G_i$  though it could be more than one.

To prove that for any point  $z \in X$ ,  $g(z) \in X$  we can apply the



same method that was used to prove Theorem 4.1, though due to the fact that unlike the conditions of Theorem 4.1, not all points in the set  $X$  are  $(\rho_0 + t)$ -equivalent, and therefore we must be sure that the  $t$ -extension theorem (Theorem 3.3) is applicable to the situation under consideration.

Let us take an arbitrary point  $z \in X$  and connect  $x$  to  $z$  by a  $t$ -chain  $x = x_0, x_1, \dots, x_n = z$ . We will show that  $g$ -images of all points in the chain starting with  $x_0$  and ending with  $x_n = z$  belong to  $X$ .

Since  $|xx_1| \leq t$ , it follows that  $C_{x_1}(\rho_0) \subset C_x(\rho_0 + t)$  and  $g(C_{x_1}(\rho_0)) = C_{y_1}(\rho_0)$  where  $y_1 = g(x_1) \in C_{y_1}(\rho_0) \subset X$ . Since  $g(C_{x_1}(\rho_0)) = C_{y_1}(\rho_0)$  and  $y_1 = g(x_1)$ , it follows that  $x_1$  and  $y_1$  belong to the same set  $X_j$ . Therefore it follows from Theorem 3.3 that  $g(C_{x_1}(\rho_0 + t)) = C_{y_1}(\rho_0 + t)$ .

Hence, we proved that  $g(C_{x_1}(\rho_0 + t)) = C_{y_1}(\rho_0 + t)$  and  $g(x_1) = y_1 \in X_j \subseteq X$ .

Since for any positive integer  $i \leq m$  the distance  $|x_i x_{i+1}| \leq t$ , applying the same argument to the points  $x_i$  and  $x_{i+1}$  as we applied to  $x_0$  and  $x_1$ , we prove that for any positive integer  $i \leq m$ ,  $g(C_{x_{i+1}}(\rho_0 + t)) = C_{y_{i+1}}(\rho_0 + t)$  and  $g(x_{i+1}) = y_{i+1} \in X_j \subseteq X$  for some  $j \leq m$ .

Hence,  $g(z) = g(x_n) = y_n \in X$ , and  $g(X) \subseteq X$ .

To show that  $g$  restricted to  $X$  is a surjective mapping of  $X$  onto itself, we notice that the inverse isometry  $g^{-1}$  maps  $x'$  onto  $x$  and  $C_{x'}(\rho)$  onto  $C_x(\rho_0)$ . Applying the same argument to  $g^{-1}$  as we applied to  $g$  we show that  $g^{-1}$  maps  $X$  into  $X$ . Therefore, for any  $y \in X$   $g^{-1}y \in X$ . Hence,  $g$  is a surjection on  $X$ . Therefore  $G_i$  is a subgroup of the group  $G := \text{Sym}(X)$  (i.e.,  $(G_i \subseteq G)$ ).

Let us take now any  $f \in \text{Sym}(X)$ , and any point  $x \in X_i$ . Since  $f$  maps  $X$  onto  $X$ . It is clear that  $f$  establishes  $(\rho_0 + t)$ -equivalence of points  $x$  and  $f(x)$ , therefore  $f \in G_i$ . Hence, we proved that for any  $i \in [1, m]$   $G_i = \text{Sym}(X)$ .  $\square$

To complete the proof of Theorem 4.2 we need to make two observations.

First, by definitions of a subset  $X_i$  and of a group  $G_i$ ,  $G_i$  acts transitively on  $X_i$ . Therefore,  $X_i = G \cdot x_i$ . Since  $G_i = \text{Sym}(X)$  we have  $X_i = \text{Sym}(X) \cdot x_i$  for any  $i \in [1, m]$ .

Let  $X_0$  denote a set that consists of one point from each subset  $X_i$ :  $X_0 = \{x_1, x_2, \dots, x_m\}$ . Then we obtain

$$X = \bigcup_{x_i \in X_0} \text{Sym}(X) \cdot x_i.$$

This concludes the proof of Theorem 4.2.  $\square$

## 5. Concluding Remarks

In the paper we give criteria for regular and multi-regular  $t$ -bonded sets. The significance of this generalization of well known criteria for regular and multi-regular Delone sets is that the terms of  $t$ -bonded sets seem to be more appropriate for describing the chemical bonds existing between atoms in real structures. In many respects this theory follows in the tracks of the local theory of regular Delone systems. However, the  $t$ -bonded sets essentially extend the limits of the family of Delone sets, and therefore it is no surprise that in spite of the similarity of the theories, there are essentially new features in the behavior of  $t$ -bonded sets that are not Delone sets.

From our point of view the studies of  $t$ -bonded sets should be continued in two directions. First, to get the upper bound for radius  $\rho_0$  of a cluster such that the condition  $N(\rho_0) = 1$  implies regularity of a  $t$ -bonded set in the 3D space. Second, regarding potential application of the theory, it makes sense to extend the above mentioned theory of regular sets for clusters defined by other metrics.

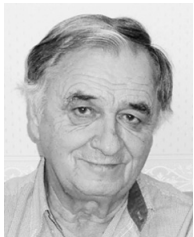
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**Mikhail Bouniaev** Prof. Dr. is Professor of School of Mathematical and Statistical Sciences, University of Texas Rio Grande Valley, Brownsville-Edinburg-Harlingen, USA.



**Nikolay Dolbilin** Prof. Dr. is Leading scientific fellow of Mathematical Steklov Institute of Russian Academy of Sciences, Professor of Moscow State University, Moscow, Russia.