

On the concept of long range order in solids: the use of algorithmic complexity

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Abstract. The paper focus on the ongoing discussion on how to better define the notion of crystallinity. We suggest that the use of algorithmic complexity captures, from a mathematical point of view, the notion of long range order in solids without the need of referring to the nature of the diffraction pattern. The possibility to compare different degrees of “crystallinity” by means of the corresponding algorithmic complexity is discussed. The diffraction space is studied from the same perspective, and it is proven that zero algorithmic complexity of the diffraction pattern does not imply the same result for the arrangement of atoms.

1. Introduction

The discovery of quasicrystals [1] rendered the definition of crystalline state as a periodic solid too narrow [2–4]. Consequently, a discussion on how to better define the notion of crystalline order has been going on for more than ten years (see for example Refs. [5–14]), and it is still open. A good concept of crystal should be rigorous from the mathematical point of view, flexible to accommodate future advancements, conceptually clear and useful. These points are fundamental for the definition to be valid as a working tool in scientific research and communication.

The International Union of Crystallography defines a crystal as a solid with essentially a discrete diffraction pattern [2]. As it stands, the notion of long range order is not explicitly included. The argument has been explained by Lifshitz [12] as follows:

1. *A Crystal is a solid that has long range positional order.*
2. *Long-range positional order can be inferred from the existence of Bragg peaks in the Fourier spectrum of the solid.*

The association between long range positional order of crystals and certain features of its diffraction pattern, does not seem mandatory. Indeed, as compelling as it may seem, it has a strong, if not decisive, historical component.

As successful as diffraction crystallography has been in the XX century, and will certainly continue to be, from the conceptual point of view there is no reason why there should not be a history of crystal “beyond” diffraction. The need to shift focus from the diffraction view to a more “structural” approach also follows from the phase problem in diffraction analysis, which makes the information contained in the diffraction pattern incomplete.

Much has been clarified in the last years regarding the mathematical connections between positional arrangement of atoms and diffraction [15–22]. Bragg diffraction or essentially discrete diffraction pattern is the fingerprint of long-range order resulting from the correlations between the interatomic vectors [15]. Yet, if this is the only type of positional order valid for a solid remains to be answered. In addition, as discovered by Höffe and Baake [17, 18], there is also an homometric issue: The same Fourier power spectrum can be associated with a one dimensional Rudin-Shapiro sequence with deterministic long-range order, and a statistically disordered Bernoulli sequence. Hence, Bragg diffraction does not only characterize order, but also certain types of disorder. The difficulty to disassociate positional long-range order from diffraction lays in how to grasp the former in mathematical terms. In the words of Baake: *the meaning of ‘long-range order’ need further explanation-as it stands, it is as vague as the original one* [11].

In spite of the claims that long range order is ‘vague’, the concept, in terms of predictability, can be mathematically and therefore rigorously formalized by means of algorithmic information or Kolmogorov complexity theory [23, 24]. This is a so general definition to leave enough room for future developments. The algorithmic complexity also allows discussing disorder in a unified manner. The relation between diffraction space and real structure can be seen as an irreversible process of information reduction with an unknown loss of entropy. Even more, Kolmogorov complexity can also be closely tied up with recent developments in the treatment of crystal as realizations of certain Delone sets.

The present work advances a simple approach to the crystal problem: *Perfect long range order in solids is characterized by zero algorithmic entropy per atom.* This argument is analyzed and discussed with two threads:

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1) A finer classification of perfect crystals can be achieved by resorting to the algorithmic complexity of the solid description, 2) the discrete portion of the diffraction pattern seems to grasp the zero entropy rate portion of the atomic description.

Before continuing a note is advisable. This work is intended as a contribution to the ongoing discussion of how to better describe a crystal [8–14]. It must be understood as thoughts thrown into the current “storm” of ideas been discussed. As the material here presented seems, at first sight, to be “outside” the main current views, we prefer to present it as a regular article to make the presentation as complete as possible. In what follows, we try to avoid as much as possible being mathematically formal, and just advance ideas which can be easily proven or are at least intuitively plausible for the reader, and could inspire further research.

2. Algorithmic complexity and positional long-range order

Algorithmic information $K(s)$ of a string s , is the length of the smallest program s^* that when given as input to a Universal Turing Machine (UTM), will give as output the string [23]:

$$K(s) = \{|s^*|: s^* \text{ is the shortest description of } s\}. \quad (1)$$

According to the definition, the maximum complexity that a string can achieve is its length $|s|$. Conditional complexity $K(s|p)$ is the size of the smallest program that computes s given the information stored in p . The use of a UTM guarantees that this notion is an objective (up to a constant only depending on the UTM) measure of information content.

Algorithmic complexity is mathematically sound and well defined [23, 24], and has been applied in dissimilar subjects [25], *e.g.* neural networks computing [26], financial markets [27, 28], biological systems [29, 30] and physical systems [31]. In spite of its name, algorithmic entropy actually quantifies randomness in contrast to modern views of complexity.

To have a well behaved complexity function $K(s)$, it is easier to consider only prefix free programs, so that the UTM knows when the program has finished [23, 24]. There is no algorithmic way of constructing the smallest program s^* , or a systematic way of finding out if a given one is the shortest possible. This is perhaps the strongest limitation to the use of algorithmic complexity. However, Zurek [31] has shown that upper bounds of $K(s)$ can be nevertheless estimated for physical systems if enough information is known.

Even if the absolute algorithmic complexity can not be systematically constructed, a related function $h(s)$, known as entropy rate or entropy density [32–35], has been introduced and calculated as

$$h(s) = \lim_{N \rightarrow \infty} h(s, N) = \lim_{N \rightarrow \infty} \frac{K(s|N)}{N} \quad (2)$$

with N being the “size” of the system. In an infinite string of symbols, $h(s)$ is the randomness that persist as larger

and larger blocks are considered, *i.e.*, knowing all previous symbols how uncertain are you (on average) about the next one [33]. This quantity can be computed because any program with the same scaling behavior as the shortest one s^* will suffice in Eq. (2), even if $K(s|N)$ is not available.

A full description of a solid of N atoms is provided by the list s of their time average coordinates. For a completely random disordered state, $K(s|N)$ should increase roughly at the same rate as N , and it holds that $h(s) \neq 0$. As the system grows, no recipe exists to accommodate the information of the additional atoms into the existing program: If the knowledge regarding any part of the disordered solid is lost, it is impossible to recover it from the remaining part. In contrast, in a perfect crystal the length $K(s|N) = |s^*|$ of the shortest program s^* does not increase, or it does slowly, as N grows, *i.e.*, in the limit $N \rightarrow \infty$ the algorithmic entropy per atom vanish. No new information is added as the size of the system increases beyond some minimal finite volume. A solid with perfect long range order, from the point of view of the information that it conveys, can be regarded as an extremely redundant message. *Hence, the concept of perfect positional long-range order surmounts to saying that the entropy rate is zero.*

The structure of certain solids could naturally lead, to the split of the describing algorithm s^* into several parts, $s^* = s_0^* + s_1^* + s_2^* + \dots$, each one grasping different aspects which helps to understand the contributions to the total entropy rate. From the Kolmogorov complexity definition (1) it is clear that the additive property holds. These parts could be classified according to the type of description they supply: (i) identical for all crystals of the same type, *e.g.* periodic crystals, quasicrystals, incommensurate crystals; (ii) specific for subsets of a certain crystal type, *i.e.*, crystals of the same space group, and (iii) the “initial” data which are characteristic for each individual crystal, such as atom type, lattice parameter or atomic position in the asymmetry cell.

3. Algorithmic complexity and crystals

The advantage of Kolmogorov complexity to analyze structure of any type rest on its general nature that allows to accommodate any redundant information regarding the positional order of the atoms in such a way that it implies a reduction of $K(s|N)$.

As no consideration of the atomic arrangement is made in the entropy rate definition (2), it can be used to compare solids in terms of their degree of long range order. This can be done without regard of the type of atomic organization: perfect periodic crystals, perfect aperiodic crystals, disordered crystals, glasses, polymers, amorphous or any other kind of atomic structure.

3.1 The ideal crystal

In the case of the periodic perfect crystal the input program s^* can be split in three distinctive parts. The first one is composed by a finite set of rules r^* . They are noth-

ing else than the minimal information needed to generate the symmetry operations of the corresponding space groups. Such information is contained in the generators of the space group [36]. The second part v^* includes the “initial data” of the structure, which consists in the coordinates of the atoms in a fixed finite volume v_1^* , *i.e.* the asymmetric unit cell, and the metric of the lattice v_2^* , *i.e.* the lattice parameters. Finally, the third component a^* is the algorithm to compute all the atomic positions from r^* and v^* . Note, that a^* should be more or less constant for all periodic crystals. The algorithmic complexity up to a constant value takes the form

$$K(s | N) = |r^*| + |v^*| + |a^*|.$$

Since, the three contributions have a fixed size and do not increase with the number of atoms, the entropy rate is zero.

A complete physical description of the system must take into consideration not only the positions of the atoms, but also their momenta and the corresponding interaction potential. Notice that if \hat{S} is a symmetry operator of the crystal, the Hamiltonian must fulfill $H(\hat{S}\mathbf{r}) = H(\mathbf{r})$. This in turn implies that it will suffice to know the Hamiltonian in a definite minimal volume in order to describe the function in the whole crystalline space. In the momenta space the minimum volume has to do with the Brillouin zone. The result is that, even when considering all the other terms, the complexity rate will be zero.

The entropy rate does not allow to classify perfect periodic crystals according to their complexity. Instead, a comparison of their periodic structure can be performed in terms of the complexity of the programs needed to describe them: the rules r^* and the information contained in the ‘initial’ data v^* . The amount of generators (excluding the translational symmetry), and the number of lattice parameters for each ideal crystal system are given in Table 1.

Roughly speaking for the periodic crystals, the complexity of the 230 space groups should not show large variations. The space group which needs fewer rules is the triclinic $P1$ with no rule apart from the three translations which adds to six cell parameters. On the other extreme, some cubic space groups for example $Fm\bar{3}m$, needs seven generators to build the whole group operations and only one cell parameter. In general, each generator can be de-

Table 1. The maximal and minimal number of generators (excluding the translational symmetry) together with the number of different lattice parameters for each crystal system.

Crystal System	Max. No. Generators	Min. No. Generators	No. Latt. Param.
Triclinic	1	0	6
Monoclinic	3	1	4
Orthorhombic	5	2	3
Tetragonal	5	2	2
Trigonal	3	1	2
Hexagonal	4	2	2
Cubic	7	3	1

scribed by Seitz operator represented by a 3×3 matrix of ones and zeros and a three dimensional vector. The matrix part results in a 9 bits long string. Each component of the vector is a rational number which can be coded in 4 bits. The total length of each generator description is approximately 13 bits long. The description could be further compressed but this adds up length to the generating algorithm.

The lattice parameter is in general a real number. Consider the lattice parameter l specified with a precision of $\pm\Delta u$. The number of bits needed to specify one lattice parameter is then $\log_2 \left[\frac{l}{\Delta u} + 1 \right]$, with $[z]$ being the integer value of z . Without loss of generality numbers are taken in its binary representation.

Based on the complexity of the minimal local volume, algorithmic information also complies with the intuitive notion of crystal complexity. Hence, structures with fewer atoms in the asymmetric unit cell (*e.g.* Copper) are less complex than those with dozen or even hundreds of atoms in the same volume (*e.g.* Hemoglobin).

From a thermodynamic perspective, any system that process information in an irreversible manner must dissipate energy. Landauer [37, 38] formulates this idea taking into account that losing information is essentially an irreversible process that reduces the degrees of freedom, and, therefore, according to the second law of thermodynamics, this loss of entropy should be compensated for [39]. Landauer’s principle gives to the information conveyed by a system, a physical existence as a negative contribution to free energy.

A periodic perfect crystal does not retain much information regarding the melt disordered state from which it can be considered to evolve from. Thus, in the infinite limit the dissipation of energy per atom due to (irreversible) information loss, when going from the melt to the crystalline state, is much larger than for any other disordered solid. The difference of the entropy rate between the melt and the crystalline state (zero in the last case) can be used as a measure of this information loss.

3.1.1 Disordered crystalline states

The algorithmic complexity of different type of disorder can also be estimated. For example, the Kolmogorov complexity of a periodic crystal with vacancies has two contributions

$$K(s | N) = |\text{perfect crystal}| + |\text{vacancies}|.$$

The entropy rate of the perfect crystal description is, as already argued, zero. Whereas, it is larger than zero for the stochastic process of removing atoms. Indeed, generalizing a run length encoding procedure used in layer structure [40], the periodic crystal with vacancies can be shown to have entropy rate

$$h(s) = -p(1-p) \log_2 p(1-p)$$

where p is the defect probability.

Analogously, other types of disorder can be incorporated into the algorithmic description of the crystal. Furthermore, as been discussed by Varn et al. [41], dif-

ferent models of disorder in solids can be described by the underlying stochastic state machine which describes the process. The reconstruction of the dynamics leading to the disorder can be optimized by the use of a so called ϵ -machine which directly leads to the determination of the entropy rate of the process and the disorder [32, 33, 35, 42]. A related approach was recently used to describe the random single faulting model in close packed structures [43].

3.2 Quasicrystals and incommensurate structures

In the case of quasicrystals and incommensurate structures, one way of specifying the set of rules is to describe their structure in a higher dimensional periodic space and then, add to the algorithm the projection procedure to the three dimensional space [44]. Both procedures are of fixed size and do not contribute to the entropy rate.

A large number of quasicrystals can be described by a cut-and-project procedure [45]. The cut-and-project scheme starts from a full rank lattice Λ in some higher dimensional space $\mathbb{R}^n = \mathbb{R}^3 \times \mathbb{R}^k$, where a window Ω bounded in \mathbb{R}^k is cut and the resulting subset of Λ is then projected into the final three dimensional space \mathbb{R}^3 . Figure 1 shows a often used example of a cut-and-project scheme from a two dimensional space to a one dimensional space. A strip in a square lattice in two dimensions is projected onto a straight line, making an irrational slope with the basis vector of the square lattice.

Thus, the Kolmogorov complexity of the quasicrystal, described by the cut-and-project scheme, is given, up to a constant value, by

$$K(s | N) = |\Lambda^*| + |\Omega^*| + |P^*| + |v^*|,$$

with $|\Lambda^*|$, $|\Omega^*|$ and $|P^*|$ being the lengths of the descriptions of the full rank lattice, the cut window, and the projection algorithm, respectively. v^* is equivalent to the asymmetric cell describing the atom decoration associated to the obtained tiling. Compared to the periodic crystal in

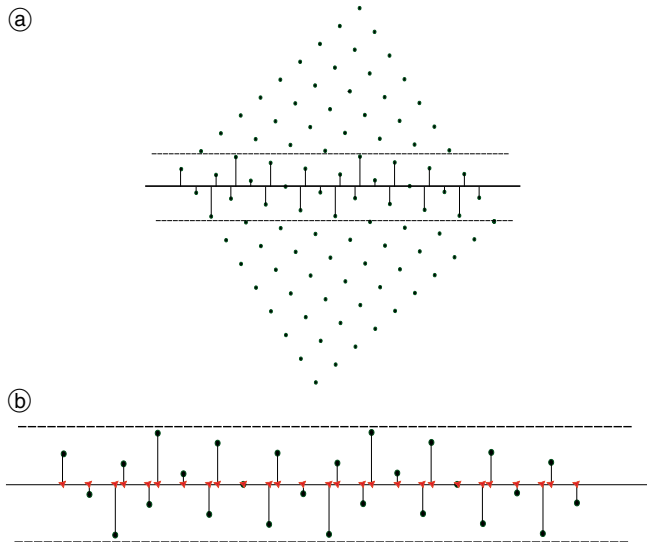


Fig. 1. A cut-and-project set. The slice in the two dimensional lattice (a) is orthogonally projected over the straight horizontal line. (b) The set resulting from the projection.

the three dimensional space, the complexity of the quasicrystal description is in general larger. If the complexity of the remaining terms is taken to be the same, the description of the higher dimensional lattice Λ needs of at least $n > 3$ lattice base vectors, compared to the 3 lattice vectors needed for the ideal crystal. This construction scheme has algorithmic complexity rate equal to zero: the full rank lattice Λ is specified by a fixed size program, and the projection operators and the strip Ω are also specified by a finite fixed number of rules.

For the incommensurate structures, the description of the lattice or chemical modulation must be added to the description of the underlying periodic structure. This can be done by describing the structure in a $(3 + d)$ -dimensional space [46]. A similar analysis, as the previously done for quasicrystals and ideal crystals, gives a vanishing entropy rate for these systems; whereas, in general, their algorithmic complexity also is larger than the corresponding value for periodic crystals.

Finally, let us remark the important implications associated with the fact that a crystal, *i.e.*, a ideal crystal, a quasicrystal or an incommensurate structure, has zero complexity entropy per point. In periodic crystals, a Brillouin zone can be constructed from the real space description. The Brillouin zone carries the same information on the crystal properties (those depending on the atomic arrangement) and is of the same “type” as the real space description. We define a fixed minimal volume unit and a fixed finite set of (translational invariant) rules in reciprocal or momentum space. The Bloch theorem is a statement about the finite amount of information needed to describe the solid with periodic translational symmetry, which can be rephrase in terms of the constant character of algorithmic complexity rate when going from one description to the other. For more general types of crystals defined through $h(s) = 0$ the same is true. We can not say if a Brillouin zone can be defined or not, but the constant character of the algorithmic complexity rate allows us to assert that, in reciprocal or momentum space, a suitable complete description can be found that requires the same amount of information density as the real space description. The procedure does not change the “quality” of the description.

4. Algorithmic complexity and diffraction pattern

From the mathematical point of view, the diffraction pattern is given by the Fourier transform of the autocorrelation function of the distribution of scatterer [18].

Let \mathcal{D} be a set describing the atoms positions on the solid, then the distribution of scatterer can be described by a Dirac comb [17]:

$$w_{\mathcal{D}} = \sum_{x \in \mathcal{D}} w(x) \delta(x), \quad (3)$$

with $w(x)$ being a bounded complex weight function. The autocorrelation function g , if it exist, is given by

$$g = \sum_{x \in \mathcal{D} - \mathcal{D}} \nu(z) \delta(z) \quad (4)$$

where $\nu(z)$ is the frequency of having two scatterer at a distance z .

The derivation of the autocorrelation function (4) from expression (3) can be done without adding any further algorithmic complexity density. In addition, the Fourier transform is also a computable function, and algorithms independent of the solid size, which perform the transform, are well known [47]. Therefore, in going from the atomic distribution to the diffraction pattern description, no additional complexity rate is added.

Yet, in the calculation of the autocorrelation function, information of the absolute atomic arrangement is lost, only remaining the information on the relative displacements (this is at the root of the so called phase problem [48]). This also implies that going from Eq. (4) to (3) there is no unique solution, *i.e.*, different atomic configurations can give rise to the same diffraction pattern (homometric set).

Höffe and Baake [17] described a homometric one dimensional pair of sequences with a pure point discrete diffraction pattern, superimposed over a constant background. One sequence is built from a Bernoulli stochastic process (a flip of coin), and the other one from a deterministic set of rules. Surprisingly, for the first sequence the complexity per symbol of the corresponding atomic arrangement is 0.5, whereas it is zero for the second case. In contrast, the diffraction patterns of both systems have a complexity per diffraction spot of zero. This is an evident example that zero complexity per diffraction spot does not imply zero complexity per structural unit in the atomic arrangement. This fact can be traced down to the non unique solution of the inverse problem (going from Eq. (4) to (3)). Several algorithms can be built to convert the same diffraction pattern to different atomic arrangements. We then say that the direct computation is irreversible [31]. In order to get a unique solution of the inverse problem additional input is needed, and there is no way to assert the complexity per atom of the missing information.

The “essential” discrete part of the diffraction pattern of the vacancy crystal, or its equivalent Bernoulli sequence in one dimension, is not grasping the long range order of the involved structure. Instead, it provides information of the underlying template over which the structure is constructed. In the two cases discussed above the template is periodic and therefore, with an infinite correlation length. *What the discrete portion of the diffraction pattern seems to grasp, is the part of the positional order of the solid which has an algorithmic entropy rate of zero.* If this information is not completely lost by disorder, then it seems to give rise to a discrete diffraction pattern. Hence, defining the actual long range order of the real structure using the discrete nature of the diffraction patterns is an ill defined concept.

We remark that the algorithmic complexity approach does not answer the question of how long range order and discrete diffraction pattern are related. Instead, it focus on the “economy of resources” needed to describe the diffraction pattern as a function of the amount of information required for the solid description. We can conclusively affirm that as the diffraction pattern description does not add complexity rate to the description of the solid, then the

former is, at most, as short as the latter. Furthermore, as the process from the Dirac comb to the autocorrelation function does not create complexity, *if in the description of the solid there is no part with entropy rate zero, then no feature of the diffraction pattern can be represented by means of a zero entropy rate description, and that includes the usual type of discrete component found on diffraction patterns.*

A question still open is if it exist a solid with such positional (dis)order as to give rise to a discrete diffraction pattern, that nevertheless has algorithmic entropy per diffraction “spot” larger than zero. The question is just a rephrasing of the diffraction problem: which type of solids diffracts? Although the answer seems to be negative, a demonstration from the algorithmic complexity point of view could perhaps give headway to the solution of the diffraction question.

5. Conclusion

The main idea of this work is that looking at solids from the perspective of algorithmic complexity gives a deeper physical insight into the rules that governs solid organization. This perspective allows to define long range order in a rigorous way, which could be used to describe what a crystal is without resorting to the diffraction pattern of the solid. Kolmogorov complexity rate also allows to compare disorder in a unifying manner without regard of the different type of positional disorder present in a solid. Zero complexity of the diffraction pattern does not imply the same result for the arrangement of scatterer.

Essentially, discrete diffraction pattern is not a well defined measure of the actual long range order, but, instead, of the underlying template of the structure which carries zero algorithmic entropy rate. Furthermore, any physical property derived algorithmically from the atomic arrangement can not have a higher complexity rate than the arrangement itself. This in turn means, for example, that if zero complexity per structural unit exists in the atomic configuration then, in the momentum space, a description must exist with the same complexity rate. In a periodic crystal it can be recognized that the zero complexity description has to do with the definition of the Brillouin zone. Even if it were the case that such zero complexity description is not known for another type of ideal crystal-line order, Kolmogorov complexity theory assures nevertheless that it exist.

A rather natural extension to the present work would be the investigation of Delone sets and associate concepts in terms of their entropy rate. Entropy rate allows to classify Delone sets according to the nature of the underlying description giving a link to other approaches. This analysis will be carried out in a second article.

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