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Characterizing structural features of two-dimensional particle systems through Voronoi topology

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Abstract

This paper introduces a new approach toward characterizing local structural features of two-dimensional particle systems. The approach can accurately identify and characterize defects in high-temperature crystals, distinguish a wide range of nominally disordered systems, and robustly describe complex structures such as grain boundaries. This paper also introduces two-dimensional functionality into the open-source software program *VoroTop* which automates this analysis. This software package is built on a recently-introduced multithreaded version of VORO++, enabling the analysis of systems with billions of particles on high-performance computer architectures.

Keywords: Voronoi cells, topology, local structure analysis, particle systems

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1. Introduction

Many two-dimensional physical systems can be studied as large sets of point-like particles, and the arrangement of these particles in space often determines many of these systems' chemical, electronic, and mechanical properties [1–6]. It is therefore important to have available precise, robust, and efficient tools that can automatically identify structural objects such as crystals and defects in large atomistic data sets. Figure 1 illustrates a pair of adjacent crystals, separated by a grain boundary and containing a vacancy. Although the rough contours of these defects can be observed visually, identifying them precisely enough for automated, quantitative analysis is challenging.

Recent decades have witnessed the development of powerful tools to automate the identification and analysis of structural objects in large atomistic data sets [7, 8]. Many of these approaches describe arrangements of particles by quantifying their similarity to an ideal reference arrangement with respect to some property. For example, some methods count the number of particles in a fixed range from each central particle [9], quantify the variation in distances to neighbors [10], or else the variation in angles between neighboring particles [11, 12]. Other methods quantify the degree to which the neighborhood is centrosymmetric [13], a defining feature of lattice crystals.

These approaches typically require carefully-chosen cutoffs for analyzing different kinds of systems. Moreover, such approaches are typically ineffective for characterizing particular kinds of defects. Perhaps most significantly, although these methods are typically well-suited for studying systems at low temperatures, they often perform poorly when applied to systems at high temperatures, or otherwise strongly perturbed from their ground state [7]. Topological approaches tend to be more effective, due to the method in which they segment data in a high-dimensional configuration space, instead of in an image of that space under a continuous mapping [14, 15]. Numerous methods based on machine learning have also been introduced in recent years [16–18], though these methods do not characterize crystalline structure directly.

This paper introduces a new, simple approach for classifying structure in two-dimensional particle systems. This approach is based on Voronoi topology and thus naturally ignores small fluctuations in particle positions associated with thermal vibrations and small strains, without the need for quenching, temporal averaging, or arbitrary order-parameter cutoffs. The method is further useful for studying both ordered and nominally disordered systems. Many ideas suggested here can be considered as adaptations and extensions of ideas introduced and developed previously for three-dimensional systems [15, 19, 20].

In addition to developing a new approach towards characterizing structure in two-dimensional particle systems, this paper also introduces two-dimensional functionality into the open-source command-line program called *VoroTop* to automate this analysis. The latest version of *VoroTop* is designed to utilize a recently-introduced, multithreaded version of the VORO++ library [21, 22] for computing Voronoi cells, enabling the study of large systems with billions of particles.

This paper is organized as follows. Section 2 describes the basics of Voronoi cells, and explains how their topology can be used to characterize and analyze structure in two-dimensional particle systems. Section 3 describes the two-dimensional *VoroTop* functionality and its core functions and features. Section 4 illustrates several example applications,

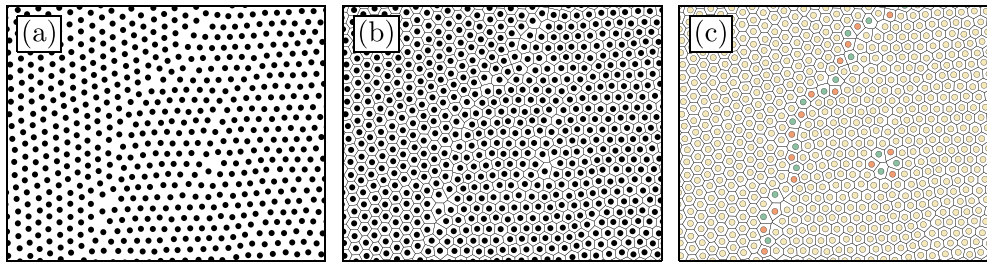


Figure 1. Two adjacent crystals separated by a grain boundary and containing a vacancy. The system was created using molecular dynamics through the cooling of a Lennard-Jones liquid: (a) particles, (b) particles and their Voronoi cells, (c) particles colored by the number of edges of their Voronoi cells.

including the identification of defects in crystals, the characterization of order in disordered systems, and the analysis of grain boundaries, including chiral features, in non-ideal systems.

2. Voronoi topology

2.1. Voronoi cells and their shapes

In a system of discrete particles, the *Voronoi cell* of each particle is the region of space closer to it than to any other particle [23–25]. Figure 1 illustrates a bicrystal and Voronoi cells of some of the particles. Geometric and topological features of a Voronoi cell can be used to characterize features of local ordering in the vicinity of each particle [26]. For example, particles can be defined as neighbors if they share a Voronoi edge, so that the number of Voronoi cell edges gives a count of neighbors. In a defect-free hexagonal crystal, even at temperatures above zero, the Voronoi cell of each particle has six edges. In crystals containing defects the Voronoi cells of some particles will have other numbers of edges. This can be vividly observed in figure 1(c), in which many Voronoi cells have five and seven edges.

The number of edges of a Voronoi cell, however, is a rather coarse description of local structure in particle arrangements. As can be seen in figure 1(c), five- and seven-sided Voronoi cells are associated with grain boundaries and vacancies, and so the number of edges alone provides only modest structural information. A more refined description of local arrangements of particles can provide a more nuanced, and useful, description. In particular, we characterize each particle according to its number of edges and the number of edges of its neighbors, ordered sequentially. Figure 2 illustrates three central particles and their Voronoi cells. Although each of the three central particles have Voronoi cells with five neighbors, these neighbors have different numbers of neighbors themselves, reflecting distinct local orderings. In figure 2(a), all neighbors have six neighbors except for one that has seven; this particle is associated to a dislocation. The two particles in figures 2(b) and (c) each have three six-sided neighbors and two five-sided ones. They are structurally distinct, however, in that the two five-sided neighbors are adjacent in figures 2(b) but not in (c); one belongs to a vacancy while the other belongs to a grain boundary.

The number of edges of the Voronoi cells of a particle and its neighbors thus provides a simple description of particle arrangements that can distinguish particles associated with

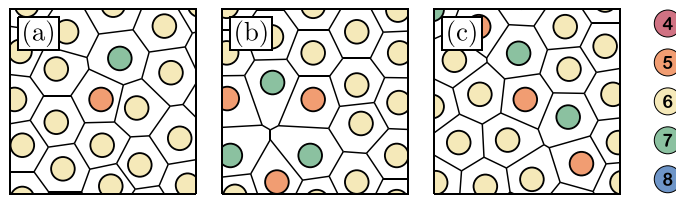


Figure 2. (a)–(c) Three central particles, each with five neighbors, associated to distinct structural defects. These structural differences are reflected in differences in the numbers of edges of neighboring Voronoi cells. Particle colors indicate numbers of Voronoi edges or neighbors.

different kinds of defects. Since topological features of Voronoi cells do not change under rotations, translations, or rescalings, this description is consistent with the intuition that such transformations do not impact structurally significant features of a system. Furthermore, since topological features of Voronoi cells do not generally change under small perturbations of particle coordinates, characterization will typically be insensitive to small measurement errors. Finally, even in special cases in which small perturbations will result in discrete shifts in topology, those shifts can be completely understood and the resulting topologies are fully described in statistically precise terms. All of this might be contrasted with approaches that rely on geometric features, such as Voronoi cell areas or perimeters. These quantities typically change under perturbations, and methods constructed based on them consequentially require choosing cutoffs, often somewhat arbitrary, for classification.

2.2. Canonical representations

We thus use the term *Voronoi topology* of a particle to refer to the number of edges of its Voronoi cell and those of its neighbors, ordered sequentially. For each particle whose Voronoi cell has n edges, this information is represented by an ordered list of $n + 1$ numbers. The first counts the neighbors of the central particle, equivalently the number of edges of its Voronoi cell; subsequent numbers count the numbers of neighbors of neighboring particles. This description might be considered a two-dimensional analogue of the Weinberg codes considered elsewhere for characterizing three-dimensional polyhedra [27–29]. We note that the first element of the p -vector is currently redundant, since the information can be inferred from the length of the vector. It is included to facilitate future generalizations, such as to multicomponent systems.

As an example, we consider the arrangement of particles in figure 2(c). The central particle has five neighbors. If we enumerate the number of edges of its neighbors in counterclockwise order beginning with the particle to its left, we arrive at the sequence (5, 6, 6, 7, 6, 7). If we had instead begun with the neighbor above, we would arrive at the sequence (5, 7, 6, 6, 7, 6); beginning with other neighbors can result in other sequences. Since all of these sequences describe the same structural information, we choose the lexicographically first one as the canonical representation of the Voronoi topology, and use the term p -vector to denote it. We say that two arrangements of particles have the same Voronoi topology if their p -vectors are identical.

A subtle issue arises when considering orientation. In some cases, had we enumerated the number of edges of neighbors in a clockwise manner instead of in a counter-clockwise manner, we would arrive at a different set of sequences and a different p -vector, indicating a chirality, or handedness, of the arrangement. In other cases, the two orientations generate the same sets of sequences, indicating a mirror symmetry in the arrangement.

Table 1. Lists of integer sequences associated with particle arrangements illustrated in figures 3(a) and (b). The sequences associated with the clockwise and counterclockwise orientations for figure 3(a) are identical, indicating a mirror symmetry and lack of handedness. In contrast, the sequences for the two orientations are different for the arrangement in figure 3(b), indicating a handedness. Since the lexicographically lowest sequence is in the counterclockwise list, we call the arrangement left-handed.

Orientation 1	Orientation 2	Orientation 1	Orientation 2
(5, 6, 6, 7, 6, 7)	(5, 6, 6, 7, 6, 7)	(6, 5, 6, 6, 6, 6, 7)	(6, 5, 7, 6, 6, 6, 6)
(5, 6, 7, 6, 6, 7)	(5, 6, 7, 6, 6, 7)	(6, 6, 6, 6, 6, 7, 5)	(6, 6, 5, 7, 6, 6, 6)
(5, 6, 7, 6, 7, 6)	(5, 6, 7, 6, 7, 6)	(6, 6, 6, 6, 7, 5, 6)	(6, 6, 6, 5, 7, 6, 6)
(5, 7, 6, 6, 7, 6)	(5, 7, 6, 6, 7, 6)	(6, 6, 6, 7, 5, 6, 6)	(6, 6, 6, 6, 5, 7, 6)
(5, 7, 6, 7, 6, 6)	(5, 7, 6, 7, 6, 6)	(6, 6, 7, 5, 6, 6, 6)	(6, 6, 6, 6, 6, 5, 7)
		(6, 7, 5, 6, 6, 6, 6)	(6, 7, 6, 6, 6, 6, 5)

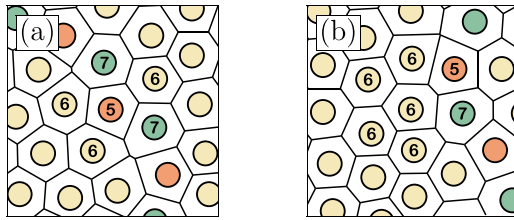


Figure 3. (a) In this arrangement of particles, p -vector descriptions of neighboring edges are identical whether we list neighbors sequentially in clockwise or counterclockwise fashion. (b) In this arrangement, p -vector descriptions will differ depending on whether we list neighbors in a clockwise or counterclockwise manner.

We thus establish the following convention. We calculate the sequences associated with both orientations and choose the lexicographically first one among all sequences as the *canonical* p -vector; we also store information about the chirality of the arrangement for further analysis. In particular, if the sequences for the two orientations are identical, then the arrangement is non-chiral. Otherwise, if the lexicographically-first sequence is in the counterclockwise list, we say that it is left-handed, and if the lexicographically-first sequence is in the clockwise list, we say that it is right-handed. Section 4.4 illustrates an example system in which Voronoi topology is able to detect chirality of a grain boundary.

To illustrate the procedure for constructing a canonical p -vector, table 1 lists the integer sequences that describe the Voronoi topology of the arrangements in figures 3(a) and (b) for each of two orientations, sorted in lexicographical order. The neighborhood illustrated in figure 3(a) is non-chiral and the two sets of sequences are identical. In contrast, the arrangement shown in figure 3(b) has a handedness, and the two sets of sequences are different. Since the lexicographically first sequence of numbers results from a counterclockwise enumeration of neighbor edges, this arrangement is considered left-handed.

2.3. Perturbation analysis

Small perturbations of particle coordinates do not always change their Voronoi topologies. For example, in the bicrystal illustrated in figure 1, the Voronoi cells of most particles are six-sided, even though the particles are slightly perturbed from ideal lattice positions as a result of thermal vibrations and small internal strains. Similarly, the Voronoi topologies of particles

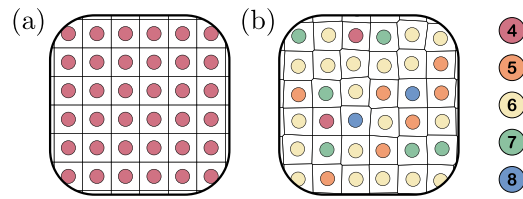


Figure 4. Particles colored according to the number of edges of their Voronoi cells in (a) an unperturbed square lattice and (b) a perturbed square lattice.

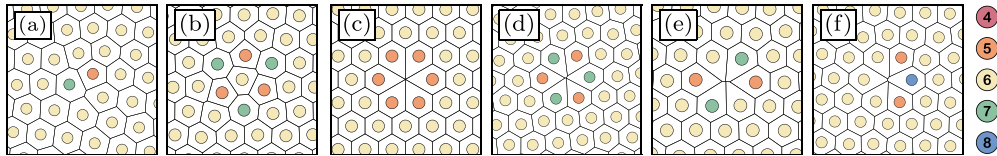


Figure 5. (a) An isolated dislocation and (b) interstitial with stable Voronoi topologies; (c) an unstable vacancy resolves under perturbations as either (d), (e) or (f).

associated with the grain boundary and vacancy are also stable under small perturbations of particle coordinates.

In some arrangements, however, especially those associated with perfect crystals and idealized defects, Voronoi topology can change under small perturbations such as those associated with thermal noise, small strains, or measurement error. As an example, figure 4 illustrates a square lattice; the p -vector of every particle is $(4, 4, 4, 4, 4)$. Under small perturbations, however, corners of Voronoi cells can resolve into edges and the resulting Voronoi cells can have between 4 and 8 edges each, resulting in many different p -vectors. Similarly, particles associated to the ‘ideal’ vacancy arrangement illustrated in figure 5(c) all have the p -vector $(5, 5, 5, 6, 6, 6)$. Small perturbations of the particle coordinates, however, can result in different Voronoi topologies of the associated particles, as illustrated in figures 5(d)–(f).

We therefore consider the possibility that a given structural object such as a crystal or defect can be associated with multiple Voronoi topologies, equivalently p -vectors, under infinitesimal perturbations. We use the term *family* to denote a set of Voronoi topologies that can be obtained from an ideal structure through infinitesimal perturbations of particle coordinates. Particles whose Voronoi topologies belong to a family of crystalline Voronoi topologies are classified as belonging to a bulk crystal, while those whose topologies belong to a family of defect topologies are classified as belonging to defects.

Families of Voronoi topologies associated with particular crystals and defects can sometimes be determined analytically by consideration of possible resolutions of individual unstable corners [15, 20, 30, 31]. However, this approach is often complicated by analytical and computational challenges.

2.4. Cluster analysis

The proposed approach characterizes the local ordering of individual particles. Analysis of contiguous groups of particles with particular local structural classification can be subsequently used to identify and analyze larger-scale structural objects. A defect-free hexagonal crystal, for example, can be defined as a set of contiguous particles all of which have p -vector $(6, 6, 6, 6, 6, 6)$. Likewise, interstitial defects can be identified with a particle with

p -vector (6, 5, 7, 5, 7, 5, 7) surrounded by six neighboring particles with alternating p -vectors (5, 6, 6, 7, 6, 7) and (7, 5, 6, 5, 6, 6, 6, 6), as illustrated in figure 5(b). This topological approach to characterizing defects is general in that it can be used to characterize and subsequently identify different kinds of crystals and defects. At the same time, this method is robust in that small perturbations of particle coordinates do not generally affect this structural classification.

In a similar manner we can also identify contiguous regions of unspecified non-crystalline order inside a crystalline system. In studying mechanisms such as melting, this approach provides a well-defined, robust method for characterizing different parts of a system as crystalline or not, facilitating quantitative analysis of growth and degradation of phases within a larger matrix such as those that occur under conditions suitable for phase transformations.

2.5. Indeterminate types and their resolutions

A complication that arises in enumerating families of Voronoi topologies is the possibility that a topology belongs to multiple structural families; we call such topologies *indeterminate*. As a concrete example, the Voronoi topology denoted by the p -vector (6, 6, 6, 6, 6, 6, 6) and that appears in hexagonal crystals also appears in perturbations of a square lattice [30, 31]. Likewise, the p -vector (5, 6, 6, 6, 6, 7) is associated with both an isolated dislocation, as illustrated in figure 5(a), as well as a vacancy, as illustrated in figure 5(e). To complicate the matter further, this topology can also appear at the end of a grain boundary.

These indeterminacies can be resolved in several ways. One approach involves consideration of probabilities of the indeterminate topologies appearing in various systems. For example, in a defect-free hexagonal crystal, all particles have the Voronoi topology given by the p -vector (6, 6, 6, 6, 6, 6, 6). In contrast, this topology appears in the perturbed square lattice and ideal gas with extremely small probabilities [31]. If we find such an arrangement in a general system, we might conclude that it more likely belongs to an hexagonal crystal than to a square one or to an ideal gas. This approach, however, is unsatisfactory since it suggests that every particle characterized by the p -vector (6, 6, 6, 6, 6, 6, 6) be classified as having hexagonal local structure, including those that appear in a square crystal or ideal gas. Large square lattice crystals with arbitrarily small random perturbations would then typically include particles classified as defects.

A second approach involves randomly perturbing particle positions and recomputing their topologies. We can repeat this process several times and classify the local structure according to whether the majority of resolutions result in a determinate topology of one kind or another. Such analysis was suggested in a paper describing an earlier version of *VoroTop* [19]. This approach, however, requires computing Voronoi cells multiple times per particle. Moreover, it also requires a default-case analysis so that (6, 6, 6, 6, 6, 6, 6) would be classified as hexagonal if no perturbations resulted in a determinate square lattice topology.

We thus suggest a third approach that builds on the analysis described in section 2.4. In particular, after classifying structure types of individual particles, we construct clusters of particles that are identified as non-crystalline and whose Voronoi cells are contiguous. To resolve indeterminate types, we then consider the Voronoi topologies of the particles that constitute the cluster. A dislocation, for example, consists of an adjacent pair of particles, one with Voronoi topology described by the p -vector (5, 6, 6, 6, 6, 7), and one by (7, 5, 6, 6, 6, 6, 6). Although such topologies can also appear individually at the ends of a grain boundary, knowing that they belong to a defect cluster with only one of each is sufficient to resolve them as constituting a dislocation. An example demonstrating this kind of analysis can be found in section 4.1. This approach might be contrasted with a mean-field approach developed and previously applied to disordered systems [32].

3. *VoroTop* software

The open-source *VoroTop* software package was developed to automate the analysis of structural features in particle systems using Voronoi topology [19]. The program was initially designed for three-dimensional systems. We now describe extensions to automate analysis of two-dimensional systems.

3.1. Language, license, and availability

The *VoroTop* software package is written in C++11 and is compatible with all major operating systems. *VoroTop* is released under an OpenSource BSD 3-Clause license, which permits redistribution and use of source and binaries, with or without modification, to both academic and for-profit groups. *VoroTop* is available online in a Git repository at <https://gitlab.com/mLazar/VoroTop/>.

3.2. Performance, optimization, and runtime

The latest version of *VoroTop* is built using a new version of VORO++ [21, 22] that incorporates multithreading with OpenMP [33]. The VORO++ library computes Voronoi cells individually, and the total computation time scales approximately linearly for typical, dense particle arrangements. Since each Voronoi cell can be computed independently of others, the multithreaded version has near-optimal parallel efficiency, in both two and three dimensions [22]. The computation of the p -vectors in *VoroTop* is also multithreaded, and typically takes a constant amount of additional work per particle. Running with a single thread on an Intel Xeon Gold 6240 CPU running at 2.60 GHz, *VoroTop* can currently compute about 160 000 Voronoi cells and p -vectors per second, or roughly ten million particles per minute.

3.3. Filters

We use the term *filter* to refer to a list of one or more families of Voronoi topologies used by *VoroTop* to identify crystalline and defect structure. As a simple example, a filter can enumerate only the unique p -vector (6, 6, 6, 6, 6, 6) associated with the ideal hexagonal lattice, or else also list families associated with defects such as dislocations, vacancies, and grain boundaries.

File format. Filter files are divided into three parts. The first part consists of optional comments about the filter, such as its source, statistical analysis, or other notes; all lines that begin with a '#' are treated as comments. Lines in the second part begin with a '*' and specify user-defined structure types. Each such line, after the '*', includes an index and a name for the structure type. Indices of structure types are listed in increasing order and begin with 1. The third part consists of lines that record Voronoi cell topologies, represented by p -vectors, and their associated structure types. Each line begins with a structure type index and an associated p -vector, as described above. Topologies listed as belonging to multiple structure types are indeterminate. Filter files for several common structure types, included those considered in this paper, can be found at www.vorotop.org.

VoroTop begins by reading in information about a system represented in the LAMMPS dump file format [34]; if specified, a filter file is also read. Next, the VORO++ library [21, 22] is used to compute the Voronoi cell of each particle, and *VoroTop* computes the Voronoi cell topologies. Finally, the system is analyzed using features specified by the user and output is saved to disk; all output is saved in plain-text format.

3.4. Command-line options

Features of the *VoroTop* program are controlled through command-line options. Some features described previously in [19] are omitted.

-2 two-dimensional system. Interpret the data as describing a two-dimensional system. If x , y , and z coordinates are all specified, then only the x and y coordinates are considered.

-f load filter file. Specifies a filter file to use for analysis. If this option is used, then a new LAMMPS dump output file will be created that includes the original data plus the structure types as determined by the given filter.

-p p -vectors. The Voronoi topology of each particle in the system is computed and saved to disk. The following information is recorded for the Voronoi cell of each particle: its number of edges, its number of neighbors with 3, 4, 5, etc edges, its canonical p -vector, the order of its symmetry group, and its chirality. Left-handed chirality is indicated by -1 , right-handed chirality is indicated by 1 , and a non-chiral Voronoi topology is indicated by 0 .

-d distribution of p -vectors. This option calculates the distribution of Voronoi topologies in a system, and records it as a histogram of p -vectors.

-c cluster analysis. This feature implements the cluster analysis described in section 2.4. Each defect and crystal cluster is assigned a unique index, ordered by size. Positive indices indicate crystal clusters; negative indices indicate defect clusters. Also recorded for each particle is the size of the cluster to which it belongs. Particles with structure types listed in the specified filter are treated as crystalline, and defect clusters are built from particles whose structure types are not listed.

-r resolve indeterminate topologies. This feature implements the analysis described in section 2.5; it is currently in testing form. Particles with indeterminate types are resolved by consideration of other particles in the same defect cluster.

-v Voronoi pair correlation function. Computes the Voronoi pair correlation function for the system as described in [35]. This is the average number of Voronoi neighbors at each Voronoi distance from a central particle, averaged over all particles and normalized by data from the ideal gas. If an integer is specified, then the program computes the Voronoi pair correlation function up to that maximum Voronoi distance k ; if left unspecified, data will be computed up to $k = 50$.

The $-u$ option outputs the unnormalized version of the Voronoi pair correlation function. This is the average number of Voronoi neighbors at each Voronoi distance from a central particle, averaged over all particles.

-e Encapsulated postscript. Outputs an encapsulated PostScript (eps) image of the system's particles and Voronoi cells. Table 2 lists different coloring scheme options. If no color scheme is specified then particles are colored according to the number of edges of their Voronoi

Table 2. Color schemes for the `-e` option.

Flag value	Particle coloring
0	do not draw particles
1	color all particles black
2	color by number of edges
3	color by filter index
4	color by Voronoi distance from center

cells. The `-n` flag can be added to specify that only the particles themselves be drawn, and not the Voronoi cells.

Drawing all particles may be undesirable for large systems. If the `-e` flag is followed by two numbers, then the first specifies the coloring scheme and the second specifies the number of particles that should be drawn; a window centered at the middle of the system and whose area is proportional to the number of particles specified is drawn.

3.5. Limitations

At present, *VoroTop* cannot distinguish between particles of different sizes or chemical types. A future version of *VoroTop* will handle particles of different sizes using the radical Voronoi tessellation, a generalization of the standard Voronoi tessellation; computation of the radical Voronoi tessellation is already available in VORO++. Analysis of multicomponent systems will require generalizing the canonical representation introduced in section 2.2; implementation of this analysis in *VoroTop* will require new data structures and algorithms.

4. Application examples

4.1. Identifying defects in polycrystalline systems

To illustrate the effectiveness of Voronoi topology in characterizing and visualizing defects in crystalline systems, figures 6 and 7 illustrate part of a two-dimensional polycrystal using several standard methods, and with Voronoi topology. The simulated system was constructed using a molecular dynamics simulation of a Lennard-Jones liquid, which was cooled until it crystallized and then annealed at half of its bulk melting temperature. Although it is possible to identify visually the rough contours of grain boundaries, dislocations, and vacancies from the particles themselves, automating further analysis requires an algorithmic approach.

Standard methods. Particles in figure 6(a) are colored according to the areas of their Voronoi cells. Particles whose Voronoi cells have smaller than average areas are colored yellow, while those with larger than average areas are colored red. Figure 6(b) shows the same system but with particles colored according to centrosymmetry [13]; darker shades indicate higher values. Particles in figure 6(c) are colored according to a bond-angle order parameter, in particular the sample variation of the angles formed by adjacent pairs of Voronoi neighbors. Finally, the particles in figure 6(d) are colored according to the sample variation of the distances to Voronoi neighbors. Generally speaking, particles belonging to defects have order parameter values that are different from those associated to particles belonging to bulk crystals. Thus, with each approach, defects can be detected through the presence of particles colored in darker shades.

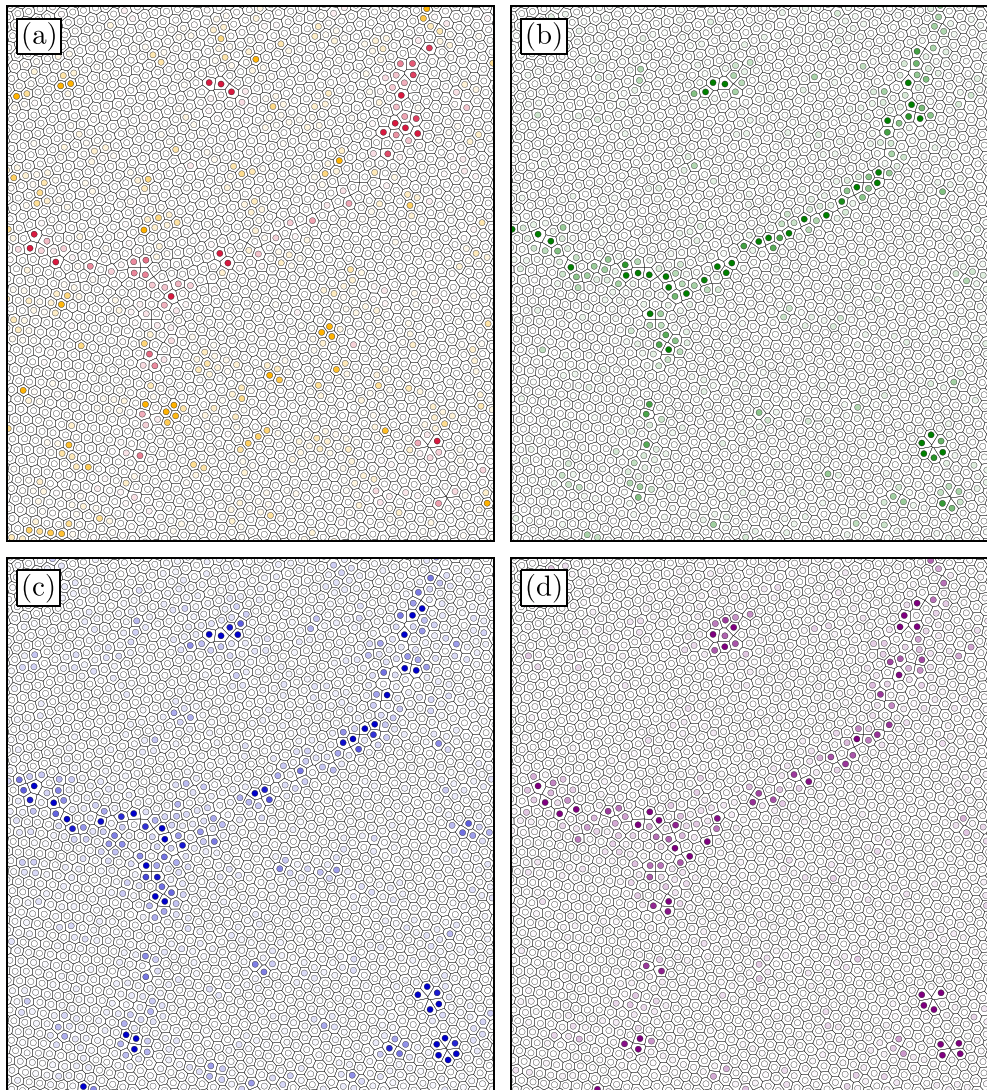


Figure 6. A polycrystal with vacancies, dislocations, and grain boundaries created using molecular dynamics through the cooling of a Lennard-Jones liquid. Particles colored according to (a) Voronoi cells areas, with larger ones colored red, and smaller ones colored yellow; (b) centrosymmetry, (c) bond-angle analysis, and (d) the variance in distances to Voronoi neighbors.

Classifying particles as belonging to either a bulk crystal or else to a defect requires choosing an order-parameter cutoff. At low temperatures, there exists a gap between order-parameter values associated with the bulk crystal and those associated with defects. Any choice of cutoff in that gap will thus result in the same binary classification of particles. At finite temperatures, however, and especially at high temperatures, thermal fluctuations result in bulk crystal particles that have order parameter values associated with defects. Consequently, any choice of order parameter cutoff will result in bulk crystal particles that are misidentified as belonging

to defects, defect particles misidentified as belonging to a bulk crystal, or both. Consequently, the particle-level details of defects are often difficult to discern.

Moreover, even when conventional order parameters can reliably detect the presence of a defect, they typically cannot distinguish between defects of different kinds. Order-parameter values associated with a vacancy, for example, might coincide with those associated with a dislocation or grain boundary. Thus, even at low temperatures, when the distinction between locally crystalline particles and those associated to defects is clear, distinguishing different kinds of defects is still challenging.

Voronoi topology. Figure 7 uses Voronoi topology to characterize and visualize individual particles. Particles in figure 7(a) are colored according to the number of edges of their Voronoi cells. This basic approach highlights the efficacy of using topological features of the Voronoi cells—particles belonging to crystals have hexagonal Voronoi cells, while those belonging to structural defects have Voronoi cells with other numbers of edges.

Particles in figure 7(b) are colored using a filter of Voronoi topologies associated with bulk crystals, grain boundaries, dislocations, and vacancies. The list of Voronoi topologies, denoted by p -vectors, used to color this figure can be found in table 3. Note that certain topologies are associated with multiple defects, and are hence called indeterminate and colored multiple colors, corresponding to their multiple associated structures. Particles with other Voronoi topologies are colored light grey. This visualization provides a clear picture of the bulk crystals as well as vacancies, interstitials, and grain boundaries.

Finally, figure 7(c) shows the result of a post-processing cluster analysis to resolve indeterminate types and to identify structural defects such as dislocations, vacancies, and grain boundaries. In particular, we considered contiguous sets of particles with non-crystalline Voronoi topologies. A cluster containing one of each of the topologies associated with a dislocation, and none of the other topologies in table 3, is identified as a dislocation. Defect clusters with exactly three or six particles with topologies associated with vacancies are identified as vacancies. Finally, contiguous sets of particles all of whose topologies are associated with grain boundaries are identified as grain boundaries.

4.2. Characterizing order in disordered systems

Voronoi topology analysis can also be used to characterize and analyze nominally disordered systems. In crystalline systems, local arrangements of particles are all of the same kind, or else of a small number of kinds. This order is reflected in the relatively small number of Voronoi topologies observed in such systems. In the hexagonal crystal, for example, all Voronoi cells are hexagons and have the p -vector $(6, 6, 6, 6, 6, 6)$, even after particle coordinates are perturbed. Systems with multiple particles in a repeating unit cell may be associated with several Voronoi topologies, though this number is always finite.

In contrast, nominally disordered systems can have an infinite number of possible arrangements of particles due to their lack of long-range periodic order. A statistical description of the relative frequencies of distinct particle arrangements, as classified through Voronoi topology, is one way to describe local structural features in these systems. We thus consider the distribution of Voronoi topologies in several disordered systems.

We consider three examples: an ideal gas, a Lennard-Jones liquid heated to 150% of its bulk melting temperature, and a hyperuniform system constructed using a Vicsek model of collective motion [36]. To sample the ideal gas, we generated 80 systems, each containing 4 million points, randomly distributed in the unit square with periodic boundary conditions. To sample from the Lennard-Jones liquid, we constructed 1600 systems, each containing 17 280

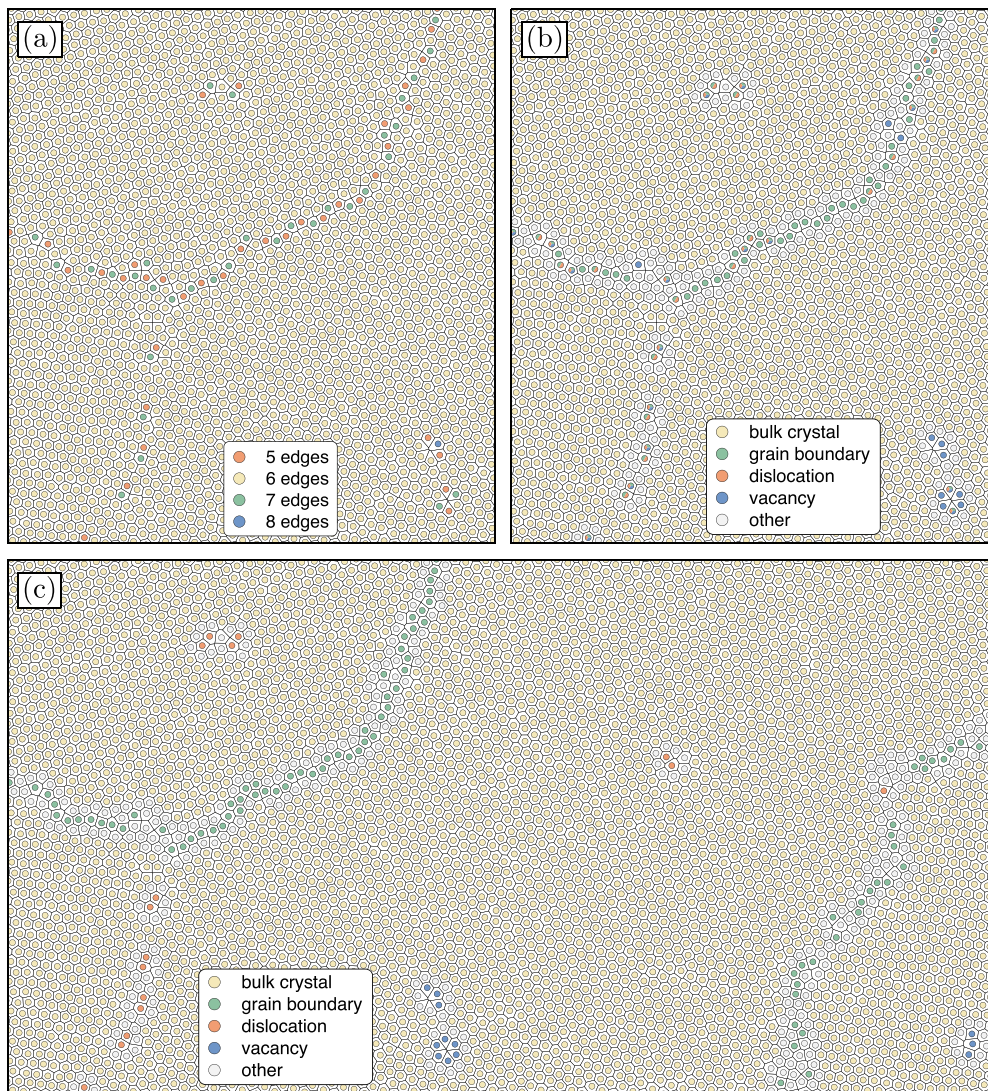


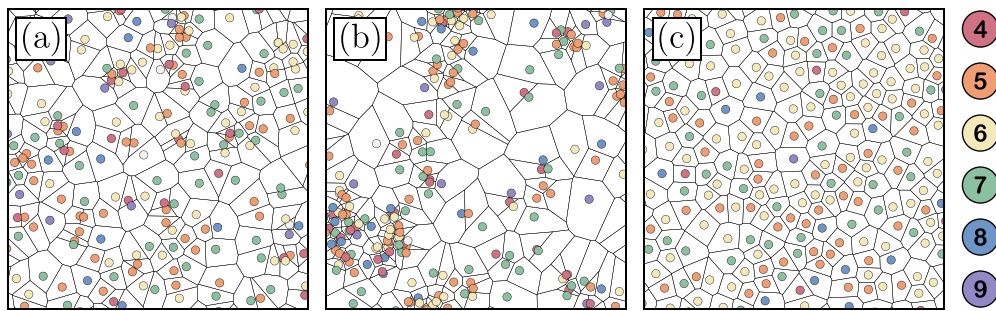
Figure 7. A polycrystal with vacancies, dislocations, and grain boundaries created using molecular dynamics through the cooling of a Lennard-Jones liquid. Particles colored according to (a) the number of edges of each particle; (b) Voronoi topology using a simple filter; indeterminate types are colored using multiple colors; (c) Voronoi topology after indeterminate types are resolved using cluster analysis.

particles. We used a Vicsek model with one million particles, unit density, and uniform noise in $[-0.6\pi, 0.6\pi]$; simulations were run for 50 000 time steps. Particles in the three systems are illustrated in figure 8.

Table 4 shows the frequencies of particles with different numbers of Voronoi cell edges or neighbors in the three systems. Although the average number of Voronoi cell edges must be six in all of them, the distribution of number of edges differs. Notice in particular that this distribution appears narrowest in the Lennard-Jones liquid, reflecting what appears to be a more regular kind of disorder as compared with that in the other systems.

Table 3. A list of structural defects and associated Voronoi topologies, denoted by their p -vectors. Note that some topologies are associated with multiple defects.

Crystal	Vacancy	Dislocation
(6,6,6,6,6,6)	(5,6,6,6,6,7)	(5,6,6,6,6,7)
	(5,6,6,6,6,8)	(7,5,6,6,6,6,6,6)
Grain boundary	(5,6,6,6,7,7)	
(5,6,6,6,6,7)	(6,5,6,6,6,6,8)	Interstitial
(5,6,6,7,6,7)	(6,5,6,6,6,7,7)	(5,6,6,7,6,7)
(6,5,6,6,6,7,6)	(6,6,6,6,6,6,8)	(6,5,7,5,7,5,7)
(6,5,6,6,7,6,6)	(7,5,6,6,6,5,7,7)	(7,5,6,5,6,6,6,6)
(7,5,6,6,5,6,6,6)	(7,5,6,6,6,6,7,6)	
(7,5,6,6,6,6,6,6)	(8,5,6,6,6,5,6,6,6)	

**Figure 8.** Images of particles in (a) an ideal gas, (b) a Vicsek model of collective motion, and (c) a Lennard-Jones liquid heated to 150% of its bulk melting temperature; each figure has roughly 200 particles. Colors indicate numbers of Voronoi edges or neighbors.**Table 4.** The fraction of particles (%) in each system with a given number of Voronoi sides or neighbors in the ideal gas, a Vicsek model of collective motion, and a Lennard-Jones liquid.

Distribution of Voronoi cell sides			
Sides	Ideal gas	Vicsek	LJ liquid
3	1.12	1.47	0.05
4	10.69	12.11	4.94
5	25.94	26.12	27.69
6	29.47	27.48	38.42
7	19.88	18.42	21.46
8	9.01	9.10	6.22
9	2.97	3.63	1.09
10	0.74	1.20	0.13
11	0.15	0.35	0.01
12	0.02	0.08	0.00

Table 5 tabulates the frequencies of the most common Voronoi topologies observed in these systems. Despite their different origins, the ideal gas and Vicsek model system appear most structurally similar, judging by frequencies of Voronoi topologies in the systems. In contrast,

Table 5. Lists of the ten most common p -vectors and their frequencies f in three nominally disordered systems: the ideal gas, a Vicsek model, and a Lennard-Jones liquid heated to 150% of its bulk melting temperature.

Ideal gas		Vicsek model		Lennard-Jones liquid	
p -vector	$f(\%)$	p -vector	$f(\%)$	p -vector	$f(\%)$
(4, 6, 6, 7, 8)	0.3502	(4, 5, 6, 6, 7)	0.3691	(5, 6, 6, 6, 6, 7)	1.1139
(5, 5, 6, 7, 6, 7)	0.3372	(4, 5, 6, 7, 7)	0.3480	(6, 5, 6, 6, 6, 6, 7)	0.9264
(5, 5, 6, 6, 6, 7)	0.3371	(5, 5, 6, 6, 6, 7)	0.3276	(5, 6, 6, 7, 6, 7)	0.9088
(5, 5, 6, 6, 7, 7)	0.3141	(4, 6, 6, 6, 7)	0.3095	(5, 5, 6, 7, 6, 7)	0.8961
(5, 5, 6, 6, 7, 6)	0.3123	(5, 5, 6, 6, 7, 6)	0.3091	(5, 5, 6, 6, 6, 7)	0.8342
(5, 5, 7, 6, 7, 7)	0.3110	(4, 6, 6, 7, 8)	0.2921	(5, 5, 7, 6, 7, 7)	0.8190
(4, 5, 6, 7, 7)	0.3000	(4, 5, 7, 6, 8)	0.2761	(6, 5, 6, 6, 6, 7, 6)	0.7879
(4, 6, 7, 7, 8)	0.2978	(4, 5, 6, 6, 8)	0.2732	(5, 6, 6, 6, 7, 7)	0.7838
(4, 6, 6, 7, 7)	0.2954	(5, 5, 6, 7, 6, 7)	0.2659	(5, 5, 6, 6, 7, 7)	0.7608
(4, 6, 6, 6, 7)	0.2887	(4, 6, 6, 7, 7)	0.2586	(5, 5, 6, 6, 7, 6)	0.6780

the distribution of Voronoi topologies appears qualitatively different in the Lennard-Jones liquid. In particular, the most common types in the Lennard-Jones liquid appear roughly three times more frequently than the most common types in the other systems. These differences in particle arrangements in the different systems likely reflect different energetic and entropic forces that govern their behavior.

In all systems, the relatively high frequencies of Voronoi topologies whose central particle have only four or five edges might appear puzzling, given that six-sided Voronoi cells are the most common in all systems. This can be understood as a combinatorial result of the increasing number of possible Voronoi topologies as the number of neighbors of a central particle increases. Since there are many more ways of arranging 6 neighbors, for example, than only 5, the relative frequency of many arrangements with five neighbors will be greater than those with 6.

4.3. Characterizing real grain boundaries

A significant challenge that arises in studying grain boundaries in realistic systems is their structural complexity as compared with grain boundaries in ideal systems. Thus, while perfect symmetric tilt grain boundaries, for example, can be described in the language of bicrystallography [37] and structural unit models [38–41], those in realistic ones typically cannot. Figures 9(a) and (b) illustrate high- and low-angle symmetric tilt grain boundaries in a two-dimensional, Lennard Jones bicrystal annealed at half of its bulk melting temperature. The irregular nature of these grain boundaries complicate their description.

Voronoi topology can be used to provide a statistical characterization of order in local structural terms. Figure 9(c) illustrates the frequencies of different Voronoi topologies in realistic symmetric tilt grain boundaries as a function of misorientation angle. This approach provides a robust characterization of grain boundary structure that is largely independent of micro-degrees of freedom [42]. Moreover, this characterization can be useful in solving a related inverse problem—given a set of particle positions can we determine the misorientation angle? Figure 9(c) suggests that knowledge of the distribution of Voronoi topologies, or even just the relative frequencies of several common types, is sufficient to identify the misorientation

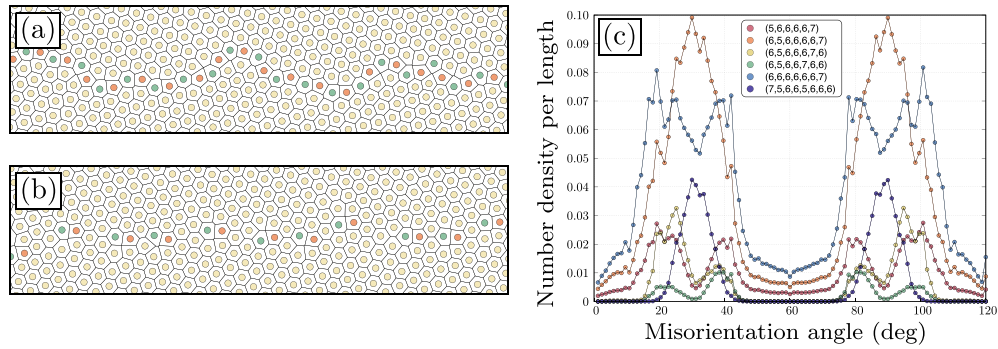


Figure 9. (a) High- and (b) low-angle real symmetric tilt grain boundaries in two-dimensional bicrystals; particles colored according to the number of edges of their Voronoi cells. (c) The number density of various Voronoi topologies per unit length as a function of misorientation angle; each color indicates a different Voronoi topology.

between the two grains. Voronoi topology thus provides a method to robustly characterize complex structure in statistical-structural terms. Analysis of energetic features of particle arrangements might provide insight into energetic aspects of realistic grain boundaries.

4.4. Chirality in grain boundaries

A unique strength of the present approach towards structure characterization is its ability to identify chiral features of particle arrangements. As described in section 2.2, certain arrangements of particles lack a mirror symmetry, and hence can be distinguished from their mirror images. Although the canonical representation of Voronoi topology via the p -vector ignores differences in orientations, this information is recorded while computing the p -vector.

Figure 10 illustrates a circular grain boundary in a two-dimensional hexagonal Lennard-Jones bicrystal heated to 50% of its bulk melting temperature. For some misorientation angles, we expect that right-handed and left-handed versions of particle arrangements, as classified through Voronoi topology, appear in the same proportions. Even if thermal vibrations result in local differences, these differences should be negligible for large samples. However, for other misorientation angles, grain boundaries, even in two dimensions, can exhibit an orientation. This can be examined through Voronoi topology analysis.

Particles in figure 10 are colored according to their Voronoi topology and orientation, as indicated in the key. In addition, particles with oriented p -vectors are further labeled with directed arrows, to indicate whether they are right- or left-handed. Notice that all right-handed forms of the p -vector (6,5,6,6,6,6,7), colored red, and all left-handed forms of (6,5,6,6,6,7,6), colored green, appear on the inside part of the circular grain boundary, whereas particles with identical topologies but opposite orientations appear on the outside of the grain boundary. The appearance of chiral features on the single-particle scale results from a chirality of the grain boundary itself. Automating the analysis of chiral features in particle systems might aid in the study of grain rotation and its impact on grain growth in two-dimensional polycrystals [43].

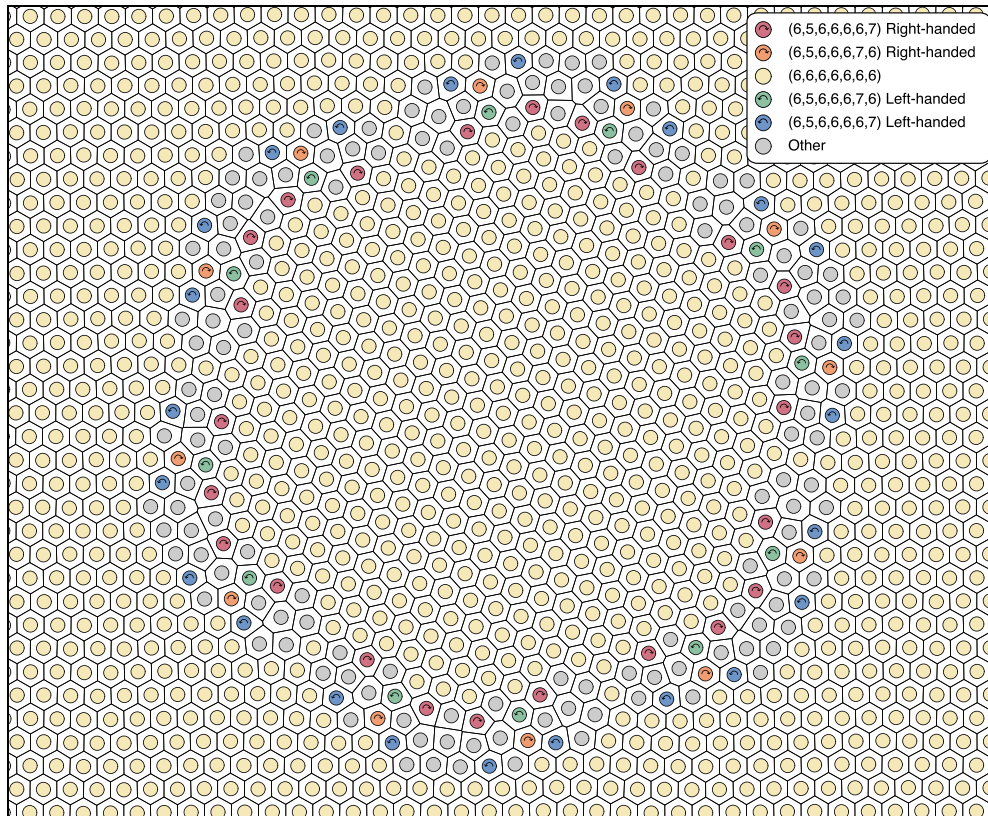


Figure 10. A circular grain boundary in a two-dimensional hexagonal Lennard-Jones bicrystal. The inside grain was constructed by rotating a circular region by 16° and then annealing the system at 50% of its bulk melting temperature. The orientation of the grain boundary can be observed in Voronoi topologies of the particles.

5. Discussion

Voronoi topology provides an effective approach to characterizing structural features of two-dimensional particle systems. As a topological method, it is generally insensitive to small perturbations of particle coordinates, making it particularly useful for analyzing imperfect systems, including finite-temperature crystals, and systems otherwise perturbed from their ground states. Similarly, it is effective for analyzing experimental data, which is often characterized by some measurement error. This robustness in the face of uncertainty is consistent with the intuition that structural features of particle systems do not change under small local perturbations.

The effectiveness of the proposed approach in a broad range of applications—identifying crystals and defects in high-temperature systems, characterizing disordered systems, non-ideal grain boundaries, and even chiral features of particle systems—highlights its general utility. Any one of these tasks can be challenging, and the ability to approach all of them with a single set of tools is noteworthy.

The proposed method is limited in certain respects. Voronoi topology is naturally insensitive to questions of scale, and also cannot capture local density fluctuations. To some degree, these limitations could be remedied by consideration of Voronoi cell areas and perimeters, or other

geometric features of the particle positions. The development of hybrid methods, integrating Voronoi topology with geometric information, might provide a more powerful approach with more general applications [44].

Another current limitation of Voronoi topology as described above is its identical treatment of all particles. The methods described above, as well as the p -vector notation, however, can be extended so to generalize the analysis for multicomponent systems such as those consisting of particles of different chemical types. We leave these extensions to future work.

Data availability statement

The paper is about an algorithm and software; any data described is incidental. The data that support the findings of this study are available upon reasonable request from the authors.


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