VoroTop: Voronoi Cell Topology Visualization & Analysis Toolkit

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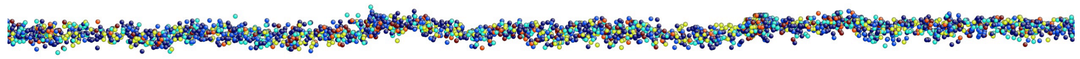


INTRODUCTION

Increasingly powerful computational resources have made possible large-scale studies of an enormously broad range of physical systems and mechanisms using atomistic simulation techniques. A central challenge in large-scale atomistic simulation is the automated characterization, analysis, and visualization of structure, so that meaningful results can be extracted from massive sets of raw data. Given only a set of atomic coordinates, what can we say about the underlying structure of the sample?

VoroTop is a set of open-source tools for characterizing, analyzing, and visualizing structure in three-dimensional atomistic data sets. These tools are built on a complete topological description of the Voronoi cell of each atom or particle in a system. *VoroTop* provides a robust alternative to conventional order-parameter methods for studying atomic systems. In particular, *VoroTop* can correctly analyze defect structure in high-temperature systems, up to the melting temperature and beyond [1].

THEORY

Local structure in atomic systems is frequently characterized using continuous "order parameters" such as bond-angle and centrosymmetry analysis. A critical limitation of such approaches is exhibited by degeneracies that arise when describing atomic arrangements that are assigned identical order-parameter values but which are structurally dissimilar. For example, a large centrosymmetry value can indicate the presence of a small local strain, a structural defect, or a thermal vibration.

This degeneracy can be understood by considering how different order-parameters divide the space of all possible configurations into regions of constant order-parameter value. In particular, the following theorem [2] shows that all continuous order-parameters have very large "level sets":

Theorem. *Let $f : \mathbb{R}^n \to \mathbb{R}^m$ be a continuous map where $n > m$. Then for any $M > 0$, there exists a $y \in \mathbb{R}^m$ such that $f^{-1}(y)$ has diameter greater than M.*

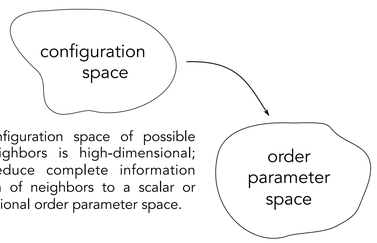
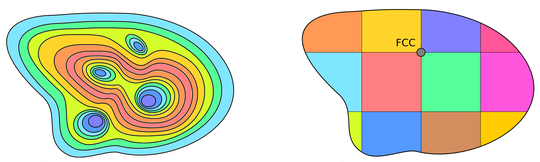


Figure 1. The configuration space of possible arrangements of neighbors is high-dimensional; order parameters reduce complete information about a configuration of neighbors to a scalar or vector in a low-dimensional order parameter space.

Figure 2. Order parameters divide the configuration space into "level sets" of constant order-parameter value. (a) Level sets of continuous order-parameters tend to be low-dimensional and arbitrarily "large", whereas (b) those of discrete order parameters tend to be high-dimensional but small.

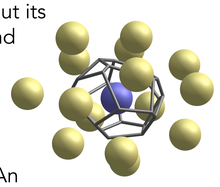


(a) Continuous order parameters (b) Discrete order parameters

A consequence of this theorem is that for any continuous order parameter, there will exist arrangements of neighbors represented by points arbitrarily far apart in configuration space but which are assigned identical order-parameter values. Discrete order parameters, such as Voronoi topology, can avoid this degeneracy.

VORONOI TOPOLOGY

The Voronoi cell of a particle is the region of space closer to it than to any other particle. A complete description of its topology includes information about its number of faces, its types of faces, and the way in which they are arranged.



The topology of the Voronoi cell is important for understanding local structure because it describes how neighboring particles are arranged. An *n*-sided face, for example, indicates a neighbor with which a particle shares *n* other neighbors.

Voronoi topologies associated with small perturbations of crystal structures can be computed *a priori* by considering the many ways in which unstable topologies can resolve.

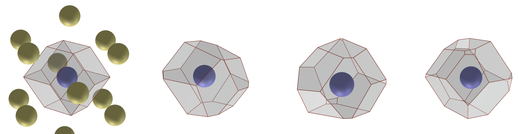


Figure 3. The topology of the Voronoi cell associated with FCC is unstable, and changes under small perturbations of the atomic coordinates, such as those associated with small strains or thermal vibrations.

The Voronoi cell of a particle in an FCC crystal is an example of a topologically unstable Voronoi cell. Figure 3 illustrates several ways in which this Voronoi cell can resolve under small perturbations. The topologies of the resulting cells correspond to regions meeting at the FCC point in the configuration space as illustrated in Figure 2(b).

SOFTWARE

VoroTop reads data files with *xyz*-coordinates of a system of particles and uses the Voro++ library [3] to construct the Voronoi cell of each particle. An algorithm described in [1] is then used to compute the topology of each Voronoi cell and store it as an integer code. This code is then checked against a database of codes known to be associated with crystal structures such as FCC, HCP, and BCC crystals, or other defect structures.

Outputted data can then be saved in data formats that can be further analyzed or visualized using software such as AtomEye and OVITO.

RUN TIME AND SCALING

Runtime scales linearly with the number of particles in a system; *VoroTop* can analyze roughly 15,000 particles per second on a single-core 2.53GHz processor.

DATA FORMATS

VoroTop can read LAMMPS dump and AtomEye cfg file formats, and can save into either format. Support for additional file formats is expected.

APPLICATIONS

DEFECT IDENTIFICATION

Most continuous order parameters require the choice of a somewhat arbitrary threshold such that particles with order-parameter values on one side of the threshold are identified as belonging to the bulk structure, while those on the other side are identified as belonging to defect structure. Such thresholding invariably results in incorrectly identifying many atoms as having bulk or defect structure.

Voronoi topology, in contrast, allows for the identification of structure type without the need for arbitrary thresholds. Instead, the set of Voronoi topologies associated with a bulk structure, and defects of various kinds, can be determined *a priori*. After a particle's Voronoi topology is determined, that particle can be easily identified as belonging to the bulk or to a defect of various kinds. The strength of this approach is especially evident in studying high-temperature systems.

Figure 4 illustrates a thin cross-section of polycrystalline FCC nickel, heated to 85% of its bulk melting temperature and visualized using centrosymmetry and Voronoi topology. Centrosymmetry requires the choice of a threshold, below which an atom is identified with the bulk structure, and above which an atom is identified with a defect; visualizations using two different thresholds are shown. Although it is possible to make out the grain-boundary network using centrosymmetry, it is difficult to precisely locate twin boundaries, stacking faults, dislocations, and vacancies. These defect structures are clearly visible using Voronoi topology, as determined by *VoroTop*.

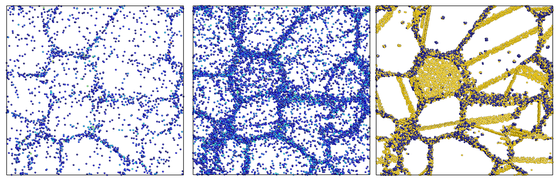
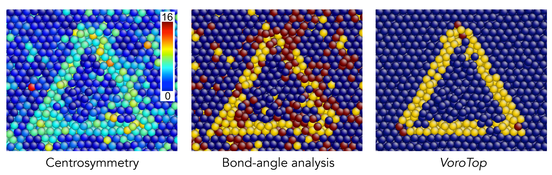


Figure 4. An FCC nickel polycrystal heated to 85% of its bulk melting temperature, visualized using two centrosymmetry thresholds and *VoroTop*. Voronoi topology enables the clear identification of grain-boundary microstructure, as well as twin-boundaries, dislocations, and vacancies.

Figure 5 illustrates a cross-section of an FCC copper crystal containing a stacking-fault tetrahedron (SFT). This sample is heated to 80% of its bulk melting temperature and then visualized using centrosymmetry, bond-angle analysis, and Voronoi topology. Atoms identified as having FCC structure are colored blue, while those with HCP structure are colored gold; remaining atoms are colored red. Although the general outline of the SFT can be observed in all three images, *VoroTop* provides the clearest picture, and the one most amenable to automated analysis.



Centrosymmetry Bond-angle analysis *VoroTop*

Figure 5. Cross-section of a stacking-fault tetrahedron in FCC copper, heated to 80% of its melting temperature, visualized using centrosymmetry, bond-angle analysis, and Voronoi topology. In the second and third images, dark blue atoms are those identified as belonging to the bulk, yellow atoms are those identified as having HCP local structure, and red atoms are those with alternate structures.

GRAIN BOUNDARY CHARACHTERIZATION

VoroTop enables quantitative analysis of grain boundary transformation. Figure 6 shows three ∑5 symmetric tilt boundaries in a BCC tungsten bicrystal. These metastable grain boundaries share five macroscopic degrees of freedom, but differ in the relative alignment of neighboring crystals. Voronoi topology provides a simple method for characterizing these distinct grain boundary structures.

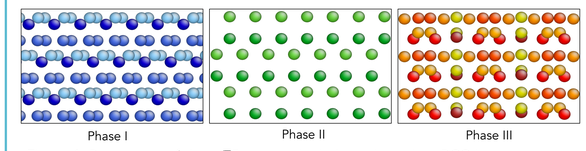
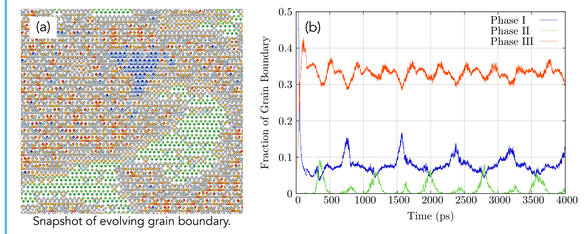


Figure 6. Planar view of three ∑5 symmetric tilt boundaries in a BCC bicrystal; atoms are colored by topological type.

In one simulation experiment, a ∑5 symmetric tilt boundary is constructed in Phase I. The sample is heated and interstitial defects are randomly inserted inside the grain boundary to mimic the effects of irradiation damage. Figure 7(a) shows a snapshot in time of the evolved grain boundary; each of the phases can be identified. Figure 7(b) shows the fraction of the grain boundary of each phase.



Snapshot of evolving grain boundary.

Figure 7. **(a)** Planar view of a ∑5 symmetric tilt boundary after it has mostly transformed from Phase I into Phases II and III structures. (b) Fraction of each phase over time.

MELTING

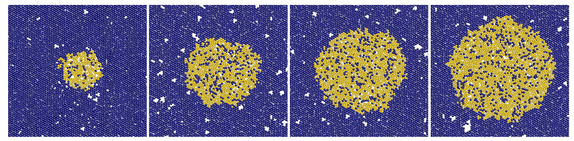


Figure 8. A single (111) plane inside an FCC copper crystal, heated to 110% of its bulk melting temperature. Atoms colored dark blue belong to the bulk crystal. A single supercritical liquid nucleus, colored gold, grows with time; atoms belonging to subcritical liquid nuclei are not shown.

MISC

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[3] C. H. Rycroft, Voro++: A three-dimensional Voronoi cell library in C++, *Chaos* 19, 041111 (2009).

ACKNOWLEDGEMENTS

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visit **WWW.VOROTOP.ORG** for code, examples, and documentation