

diOPA – A Database Implementation for Orders Parameter Analysis

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Background

The local order on a specific atomic or molecular site within an agglomerate or ordered compound such as a crystal can be quantified with reference to a given coordination symmetry. For instance, nearest neighbor bond vectors can be compared to those in a perfect crystal. A single atom/molecule site with index i in the bulk of a bcc (or fcc) crystal is expected to have 8 (or 12 for fcc) nearest neighbors j in a cubic (cuboctahedral) coordination. An unscaled order parameter ζ can be calculated based on the difference between the actual position of neighbors j relative to a central atom/molecule i , r_{ij} , and the reference positions R_j in a perfect crystal (K. G. F. Janssens et al., Computing the mobility of grain boundaries. *Nat. Mater.* **5**, 124 (2006)). For each of the atoms/molecules forming the agglomerate, ζ_i is then defined as the distance measure

$$\zeta_i = \min_{k \in S^3} \sum_{j=1}^N \|r_{ij} - R_j^k\|$$

where N is the coordination number, $\| \dots \|$ is the distance norm and S^3 the unit sphere in three dimensions. The index k represents a polar orientation of the reference coordination as a point on the unit sphere S^3 . The minimization is carried out over all possible orientations of the reference coordination. A second minimization not explicitly stated here includes all permutations of the neighbors j .

diOPA Implementation and Notebooks

diOPA is a collection of Mathematica (www.wolfram.com) notebooks that implement the computation of ζ_i for a given data set of atomic/molecular coordinates.

For efficient computation the minimization over all possible orientations of the reference coordination was implemented as a data base comparison between bond vectors r_{ij} with pre-calculated reference vectors R_j^k . A database item with index k corresponds to a vector R_j^k representing a discretized orientation (θ_k, ϕ_k) of the reference coordination on the unit sphere.

For comparability between different symmetries, the order parameter ζ_i in diOPA is normalized to the number of nearest neighbors.

diOPA contains the following notebooks:

- create_db.nb
- test_db.nb
- evaluate_order.nb
- evaluate_density.nb
- evaluate_pdf.nb

create_db is a program to create a database that contains rotation variants of a predefined coordination polyhedron. The database is used for the local order parameter determination on a dataset of "atoms" that can e.g. represent a crystalline condensate or a less ordered cluster.

test_db is a consistency check to evaluate database match, i.e. the match of a given coordination polyhedron with the rotation variants of the database.

evaluate_order.nb calculates for a data set with xyz "atom" coordinates for each "atom" the best match, i.e. the minimum distance norm against all rotation variants in a database file of a given coordination. evaluate_order.nb creates a three dimensional temperature map for this best match of each "atom" in the xyz data.

evaluate_density.nb calculates for a data set with xyz "atom" coordinates for each "atom" the local density of "atoms" around this centre "atom". evaluate_density.nb creates a three dimensional temperature map for the local density.

evaluate_pdf.nb is a helper tool that calculates the pair correlation function for a data set with xyz "atom" coordinates.

Software Requirements

Mathematica version 7.0.1 or higher is required, available from www.wolfram.com.

Installation

Copy the full directory tree into a program folder of your choice. The top directory contains the notebooks. You can run the notebooks from the installation directory. The subfolder 'db' is an output folder where create_db.nb stores by default its database files. The subfolder 'data' contains exemplary xyz atomic cluster files, together with a description of the file format. The subfolder 'out' is used by evaluate_order.nb and evaluate_density.nb for data and graphics file output. The subfolder 'extra' contains the pdf output of exemplary notebook evaluations.

Usage

Each notebook contains header information about input, output and usage. Open a notebook in Mathematica and follow the instructions in the header information. In general each notebook requires a minimum input of parameter values in a marked section that starts with 'BEGIN USER INPUT' and ends with 'END USER INPUT'. Afterwards you simply delete all cell output and evaluate the notebook.

test_db.nb and evaluate_order.nb require a database file as input. This should be created with create_db.nb beforehand. evaluate_order.nb, evaluate_density.nb and evaluate_pdf.nb further require a file with xyz "atomic" coordinates for input.

Input file format

A super-cell structure file is used as input file for the xyz atom/molecule coordinates. The super-cell has the most simple symmetry P1. The following description details the format of the super-cell file. The common suffix for this format is .cel.

Format specification

Use ANSI character encoding when saving the .cel file, separate the values by at least one space character, use the "period" (.) as decimal delimiter.

```
line 01: # comment or structure name, no relevant structure data
line 02: <zero> <x cell size> <y cell size> <z cell size> <alpha cell angle in deg> <beta cell angle in deg>
<gamma cell angle in deg> (currently only 90 degree cell angles!)
line 03: <Atom symbol> <x fractional coordinate> <y fractional coordinate> <z fractional coordinate>
<occupancy> <vibration parameter for Debye-Waller factor in nm^2> <zero> <zero> <zero> (Example: " Ge
0.00000 0.00000 0.00000 1.0000 0.60000 0.00000 0.00000 0.00000")
line 04: <Atom symbol> <x fractional coordinate> <y fractional coordinate> <z fractional coordinate>
<occupancy> <vibration parameter for Debye-Waller factor in nm^2> <zero> <zero> <zero> (Example: " Ge
0.50000 0.50000 0.50000 1.0000 0.55000 0.00000 0.00000 0.00000")
line 05: ... ( more atomic data as in line 03 and 04)
....
line XX: * (final line, the "*" signalises the end of atomic data)
```

Note that for the order parameter analysis notebooks

- (1) The nearest neighbour distance is required to be 1. You need to scale the cell dimensions x y z appropriately!
Example: In Germanium the unit cell dimensions (x cell size, y cell size and z cell size) are 0.5657 nm. The nearest neighbour distance between two Germanium atoms is 0.244944. In order to scale the nearest neighbour spacing to 1 the cell dimensions need to be multiplied by the factor $1/0.244944$.
- (2) Atom symbol, occupancy, Debye-Waller factors and absorption parameters are ignored. You can safely choose any two-character symbol label and set occupancy, Debye-Waller factors and absorption parameters to zero.

Example .cel file

```
# Germanium super cell file
0 2.3094 2.3094 2.3094 90.0000 90.0000 90.0000
Ge 0.750000 0.750000 0.250000 1.000000 0.005000 0.100000 0.100000 0.100000
Ge 0.750000 0.250000 0.750000 1.000000 0.005000 0.100000 0.100000 0.100000
Ge 0.500000 0.500000 0.000000 1.000000 0.005000 0.100000 0.100000 0.100000
Ge 0.500000 0.000000 0.500000 1.000000 0.005000 0.100000 0.100000 0.100000
Ge 0.250000 0.750000 0.750000 1.000000 0.005000 0.100000 0.100000 0.100000
Ge 0.250000 0.250000 0.250000 1.000000 0.005000 0.100000 0.100000 0.100000
Ge 0.000000 0.500000 0.500000 1.000000 0.005000 0.100000 0.100000 0.100000
Ge 0.000000 0.000000 0.000000 1.000000 0.005000 0.100000 0.100000 0.100000
*
```

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