



AACSD

1 [Overview](#)

2 [Install](#)

[Quick start](#)

3 [Inputs and outputs](#)

4 [Getting started](#)

[Help](#)

[System cutoff](#)

[Mixture system](#)

[EPE](#)

[CSP](#)

[CNA|a-CNA](#)

[CNP](#)

[BAA](#)

[NDA](#)

[OIM](#)

[LCO](#)

5 [Processing batch](#)

6 [Error](#)

7 [Color triangles](#)

Overview

AACSD (Atomistic Analyzer for Crystal Structure and Defects) is a command-line program for the post-analysis of atomic configurations generated by various atomistic simulation codes.

The functionalities of the program contain:

EPE (excess potential energy)

CSP (centrosymmetry parameter)

CNA (common neighbor analysis)

a-CNA (adaptive-common neighbor analysis)

CNP (common neighbor parameter)

NDA (neighbor distance analysis)

m-CSP (modified centrosymmetry parameter)

OIM (orientation imaging map)

LCO (local crystallographic orientation)

The program supports LAMMPS custom dump file and LAMMPS data file. Using AACSD one can get an LAMMPS custom dump formatted output file which contains extra property columns for each functionality.

Install

```
$tar -zxvf AACSD *.tar.gz
```

One may get the compiled AACSD program as executable file for three operating systems such as Linux, MAC and Windows. Four subfolders are attached in each compressed package, including exp for examples, doc for documents, pat for pattern files used by the NDA method, and col for high resolution color triangles used for the OIM and LCO methods. For instance, in linux platform,

```
$tar -zxvf AACSDver1.0.0_linux.tar.gz
```

After launching this command, one will get the uncompressed folder “AACSDver1.0.0_linux”, which includes the four sub-folders as mentioned above and the compiled AACSD.

Quick start

Usage in default mode,

```
AACSD <input> <output> <func>
```

Where <input> corresponds to one LAMMPS input data file or custom dump file to be analyzed, <output> is the generated output file in the format of LAMMPS custom dump file, and <func> is one keyword of functionality listed as follows: epe, csp, cna, cnp, nda, oim and lco. More usages in normal mode will be given in the latter sections.

Inputs and outputs

The AACSD program supports the input file in format of LAMMPS input data file or custom dump file including at least x y z position columns. One can get this with LAMMPS script like

```
dump 1 all custom 1000 dump.tensile *.dmp id type x y z
```

To be noted that if one need to compute EPE, an extra property column containing potential energy need to be present in the LAMMPS dump file. The box information in periodic boundary condition is read from LAMMPS dump file via the boundary keywords “pp pp pp”. One can get extra data saved by launching AACSD script:

```
AACSD* <input> <input>
```

One will get the input file with new data computed by AACSD and the older one will be also saved.

A general usage of AACSD program needs more parameters to be provided after the keyword of functionality by the potential user. For instance:

```
>>AACSD <input> <output> <epe> [col] [Er1 Er2...]
```

```
>>AACSD <input> <output> <cna> [rminc1 rmaxc1 rminc2 rmaxc2...]
```

```
>>AACSD <input> <output> <csp> [CN1 CN2...]
```

```
>>AACSD <input> <output> <cnp> [rc1 rc2...]
```

```
>>AACSD <input> <output> <baa>
```

```
>>AACSD <input> <output> <nda> [pattern1 pattern2...]
```

```
>>AACSD <input> <output> <oim> [cspc] [RD] [rc1 rc2...]
```

```
>> AACSD <input> <output> <leo> [cspc] [RD] [rc1 rc2...]
```

Note that for the keyword of functionality, only lower-case letter is identifiable.

Getting started

Help

Usage:

```
-h
```

Show the command usage of AACSD program.

System cutoff

Usage:

```
cutoff [cutoff]
```

Default:

$$\frac{1}{2} \frac{\sqrt{B_x^2 + B_y^2 + B_z^2}}{\sqrt[3]{N}}$$

Where B_x B_y B_z are the three dimensional lengths of the box and N gives the total number of atoms in the box.

This command is used to set the max searching distance of common neighbors that will be used by AACSD. The larger cutoff is chosen, the safer but slower is the analysis. To be noted that an adaptive mode would complain when too small cutoff is set. In general, a value larger than 3A is recommended for an appropriate choice of system cutoff.

Mixture system

Usage:

```
mix [type1 type2...]
```

To deal with some mixture system, a mixture mode needs to be activated before an analysis is performed by AACSD. It means that AACSD will treat each type of element separately in the analysis for a mixture system.

For example:

```
mix1 2
```

Taken Cu_3Ag system as example, Cu and Ag is computed as fcc. If they are defined as mixture system, they will be analyzed as unknown structure.

EPE

Usage:

```
epe
```

```
epe [col] [Er1 Er2...]
```

Default:

```
epe 6 0
```

Where [col] determines which column contains the values of actual potential energy in the LAMMPS custom dump file, and [Er1 Er2...] give the reference potential energies of each elements to be subtracted from the actual potential energies via AACSD.

In default mode, the reference energies of all elements will be set to be equal to zero.

CSP

Usage:

```
csp
```

```
csp [CN1 CN2...]
```

This command needs the number of common neighbors for structure analysis.

If there are more elements present than that provided in setting, AACSD will apply the same

setting as the first element for the unset.

Default:

`csp 12`

After analysis, two extra data columns will be saved into the output file. The larger csp is, the more possible structure is the defect. In addition, if -1 occurs in csp, it means that too small system cutoff is used. In such case, it needs to be changed by cutoff command.

CNA|a-CNA

Usage:

`cna`

`cna [0 rc1 0 rc2...]`

`cna [rminc1 rmaxc1 rminc2 rmaxc2...]`

The first command is used to start a-CNA analysis, the second command corresponds to the normal CNA with simple cutoff, and the third command is used to start normal CNA with settings of double cutoffs. rc is defined as a cutoff within which 12 neighbors are included for fcc and hcp, while 14 neighbors for bcc. AACSD allows two cutoff parameters to define a range between [rminc1 rmaxc1]. The estimations of rc or rmax can be made based on the following equations,

$$r_{fcc/hcp} = \frac{\sqrt{2}+1}{2} \left(\frac{\sqrt{2}}{2} a \right)$$

$$r_{bcc} = \frac{\sqrt{2}+1}{2} a$$

These definitions can also be used in the CNP, OIM and LCO methods. This command will generate one extra data column in the output file.

The values of <1|2|3> in CNA correspond to the structure types of <fcc|bcc|hcp>, while the values of <1.5|2.5|3.5> mean the mixture substance with the structure types of <fcc|bcc|hcp>. The value <0.75> means how many neighbors this atom has.

In case of unknown structure,

$$P = a + b \cdot CN$$

Where P means it returns a value for unknown, a and b stands for two defined parameters with a default of 0.75 and -0.125. CN is the coordination number defined by rc.

CNP

Usage:

`cnp`

`cnp [rc1 rc2...]`

Default:

`cnp rc`

$$rc = \frac{1}{12} \frac{\sqrt{2}+1}{2} \left(\sum_{n=1}^4 \frac{2}{\sqrt{3}} R_i + \sum_{n=5}^{12} R_i \right)$$

In default, an average value of local cutoff is used for each atom in a similar manner for a-CNA analysis.

Because CNP combines the properties of CSP and CNA methods, the CNP method needs the same input parameters as CNA method, while its dump data looks similar to that of the CSP method. A large value of `cnp` corresponds to the appearance of defects.

BAA

Usage:

```
baa
```

BAA will run in an adaptive mode and does not need any setting parameters.

This command will generate one extra data column in the output file.

The values of `<1|2|3>` in BAA correspond to the structure types of `<fcc|bcc|hcp>`, while the values of `<1.5|2.5|3.5>` mean the mixture substance with the structure types of `<fcc|bcc|hcp>`. The value `<0.75>` means how many neighbors this atom has.

In case of unknown structure,

$$P = a + b \cdot CN$$

Where P means it returns a value for unknown, a and b stands for two defined parameters with a default of 0.75 and -0.125. CN is the coordination number defined by BAA. (r1 in definition of BAA is used).

NDA

Usage:

```
nda
```

```
nda [pattern1 pattern2...]
```

Using the NDA analysis method, one needs to provide pattern file. NDA will print the message how many times a pattern file is loaded by AACSD program. For example, Return 1 for the first pattern appeared in command line.

A pattern contains:

- 1) How many neighbors are necessary to identify the structure.
- 2) $NDA = \delta * R_0$. R_0 is the nearest neighbors. δ is the deviation, and 21% is recommended in previous work.
- 3) Atomic position with respect to the central atom.

For example:

For a diamond structure :

```
# this is a diamond pattern data  
16 0.21  
0.5 0.5 0  
0.5 -0.5 0
```

```

-0.5 0.5 0
-0.5 -0.5 0
0 0.5 0.5
0 -0.5 0.5
0 0.5 -0.5
0 -0.5 -0.5
0.5 0 0.5
0.5 0 -0.5
-0.5 0 0.5
-0.5 0 -0.5
0.25 0.25 0.25
0.25 -0.25 -0.25
-0.25 0.25 -0.25
-0.25 -0.25 0.25

```

In default, NDA will use the build-in patterns in fcc and bcc structure.

This command will generate one extra data column in the output file.

The type of crystal structure identified by NDA method corresponds to the loaded one. Return n for the nth structure appear in command line, n+0.5 for the nth mixture structure appear in command line. The value of -1.25 is for unknown.

OIM

OIM needs a preliminary analysis done by the m-CSP method to identify the crystal structure, and then the orientation of the related structure is calculated for each atom. A cutoff is needed for m-CSP method to determine the type of crystal structure. To get an orientation, a reference direction is generally defined for projection operation and color coding.

Usage:

```

oim
oim [cspc] <RD> [rc1 rc2...]

```

Where, <cspc> gives the cutoff used for the m-CSP method. A value less than $3a^2$ is allowed when fcc structure will be analyzed in the system. RD is the reference direction that is defined by 3-indexes, e.g. 0 0 1. The values for rc are the same as those for the CNA method.

Default:

```

oim 3 0 0 1 rc

```

$$rc = \frac{1}{12} \frac{\sqrt{2}+1}{2} \left(\sum_{n=1}^4 \frac{2}{\sqrt{3}} R_i + \sum_{n=5}^{12} R_i \right)$$

In default, an average value of local cutoff is used for each atom in a similar manner for the a-CNA analysis

After analysis, four extra data columns will be saved into the output file. Using these data, one may visualize the color-coded atomic structure based on the calculated crystallographic

orientation.

data	color	Direction(fcc&bcc)	Direction(hcp)
<code>oim</code>	None(structure)		
<code>o r</code>	red	[001]	[100]
<code>o g</code>	green	[011]	[210]
<code>o b</code>	blue	[111]	[001]

In oim analysis, the structure is determined by the m-CSP method, in which the values of $\langle 1|2|3 \rangle$ correspond to the crystal structures of $\langle \text{fcc}|\text{bcc}|\text{hcp} \rangle$, and the values of $\langle 1.5|2.5|3.5 \rangle$ indicate the mixed crystal structures of $\langle \text{fcc}|\text{bcc}|\text{hcp} \rangle$. The value $\langle 0.75 \rangle$ means how many neighbors this atom has.

In case of unknown structure,

$$P = a + b \cdot CN$$

Where P means it returns a value for unknown, a and b stands for two defined parameter with a default of 0.75 and -0.125. CN is the coordination number defined by the m-CSP method.

LCO

LCO provides another way to color code the atoms by local crystallographic orientation in a similar manner to the OIM method.

Usage:

`lco`

`lco [cspc] <RD> [rc1 rc2...]`

Default:

`lco 3 0 0 1 rc`

$$rc = \frac{1}{12} \frac{\sqrt{2}+1}{2} \left(\sum_{n=1}^4 \frac{2}{\sqrt{3}} R_i + \sum_{n=5}^{12} R_i \right)$$

In default, an average local cutoff is used for each atom in a similar manner for the a-CNA analysis. After analysis, four extra data columns will be saved into the output file. Using these data, one may visualize the color-coded atomic structure based on the calculated crystallographic orientation.

data	color	Direction(fcc&bcc)	Direction(hcp)
<code>lco</code>	None(structure)		
<code>l r</code>	red	[001]	[100]
<code>l g</code>	green	[011]	[210]
<code>l b</code>	blue	[111]	[001]

Processing batch

This is one way to run AACSD with processing batch.

```
dump="dump tensile "
mp=".lmp"
```

```
color="color"  
for((i=0;i<=20000;i+=1000))  
do  
./AACSD $dump$i$mp $color$i$mp cna 2.1 3.1 csp 12 oim 1.5 0 0 1 3.1  
Done
```

Error

This page shows errors will occur in AACSD program. The following errors are not bug. However if an error occurs without ERROR: symbol, please connect the author with input file by e-mail immediately. We'll get it fixed as soon as receiving the report.

ERROR: error data type * should be float or int type**

When this occurs, please check the input file. AACSD can only load LAMMPS custom dump file or data file. Please check file first.*** is the error character in the number. If the problem can't be solved, please contact the authors.

ERROR: input file not found

ERROR: this program can't open in this way at this time

Run without input file or a wrong name or no command is received.

ERROR: LAMMPS dump file doesn't contain enough data

LAMMPS custom dump file errors because the index doesn't fix with AACSD. Please prepare x y z in order in the input file.

Color triangles

