

AtomViewer

Short manual

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1 About AtomViewer

AtomViewer is a visualization and analysis tool for atomistic simulations, primarily molecular dynamics simulations. By characterization of the atomic configuration it can display or filter certain atoms, making crystal structures or other properties visible. Plastic deformation in crystalline solids are mainly related to the creation and movement of dislocations. These entities are not directly part of atomistic simulations, but instead they need to be extracted from the atomistic configuration. The detection and characterization of dislocations and their Burgers vector is one of the main features of AtomViewer, since it includes reference implementations for the dislocation network detection and classification methods as published by Begau et al. [1, 2].

AtomViewer is open source software and is written in a way that it can be extended towards different materials and crystal structures as well as custom post-processing and rendering routines. Build-in features support functionality for crystals in FCC, BCC and B2 structures. However, the algorithms to detect and characterize dislocations are not limited to these structures and can be extended to other materials and polycrystalline materials as well.

AtomViewer is not intended as an replacement for other MD visualization tools as AtomEye¹, Ovito², VMD³ or many more, but as an addition to be used in certain applications.

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¹<http://li.mit.edu/Archive/Graphics/A/>

²<http://www.ovito.org/>

³<http://www.ks.uiuc.edu/Research/vmd/>

2 System requirements

AtomViewer requires

- an installed Java runtime environment version 6 or newer
- a graphic device supporting OpenGL version 2.0 or higher
- one of the supported operating systems: Microsoft Windows (XP-Win 7), Linux, MacOS, Solaris (each supported in 32- and 64-bit versions, not all platforms are tested)

Please start AtomViewer by starting the included scripts

- AtomViewer.sh – Linux, MacOS, Solaris
- AtomViewer.bat – Windows

Large atomistic data sets may require a large amount of memory. By default the maximum memory usage of AtomViewer is limited to about 1000 MB. If more memory is required, please modify the startup script. E.g. set the parameter “-Xmx4096M” to increase the maximum memory to 4 GB. The possible maximum of memory that can be acquired depends on operating system, physical memory in the computer and the installed java virtual machine.

3 Data format for import

AtomViewer supports files in the IMD-format as described in

<http://www.itap.physik.uni-stuttgart.de/~imd/userguide/config.html>

For easier import, the files can even be more simple, a minimal file looks as followed:

```
1 #F A
2 #C x y z
3 #X 3.520000 0 0
4 #Y 0 3.520000 0
5 #Z 0 0 3.520000
6 #E
7 2.636128 0.888096 0.891264
8 2.636128 2.648096 2.651264
9 0.876128 0.888096 2.651264
10 0.876128 2.648096 0.891264
```

Line 1 defines the file format (A=ASCII in this case), line 2 the type of each column (here x,y,z coordinate). Please note that only files with the order x y z are supported. Line 3-5 define the simulation box size. Currently only orthogonal simulation boxes are supported. The origin of the simulation box is always at (0.0, 0.0, 0.0). Atoms

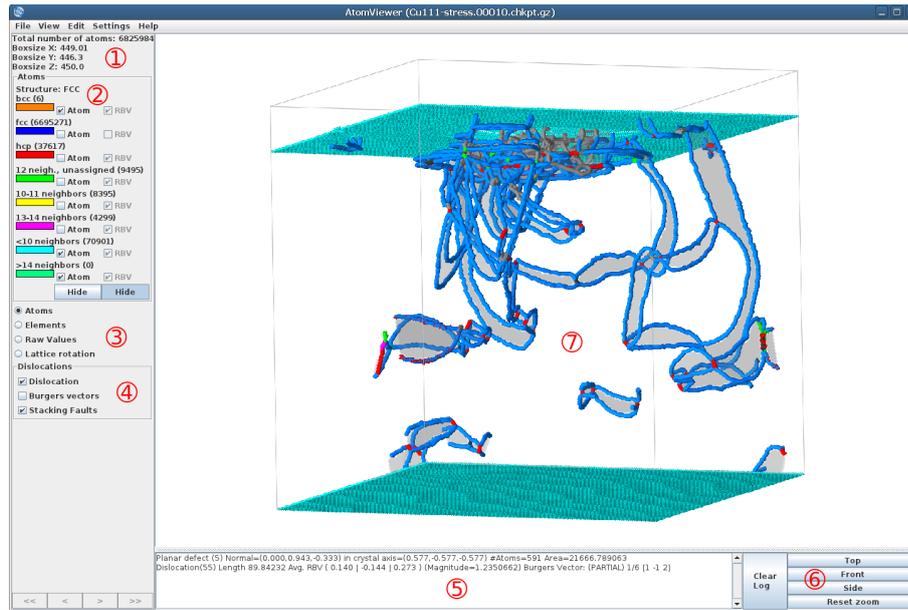


Figure 1: Atom Viewer main window

1. Information about the simulation volume and the number of imported atoms
2. Show/Hide the atoms assigned to certain classes and the resultant Burgers vector per atom (if available)
3. Different displaying styles for atomic information
4. Display the dislocation networks and (if available) stacking faults
5. Information for elements that are selected by clicking on them are printed to this log.
6. Select axis aligned perspectives. Holding down the Shift-key will clicking, results in selecting the opposite perspective.
7. Atoms and elements of microstructure are rendered here.

outside the box are either placed inside the box in case of periodic boundary conditions or are imported and displayed but are ignored during most analysis operations in case of free boundaries. The header must be closed with the sequence `#E`. Each following line defines the coordinate of an atom. Besides the mandatory xyz-coordinates, additional predefined parameters are possible as given in the following table:

Name	Format	Description
x y z	$3 \times \text{float}$	atomic coordinate
number	integer	unique number of the atom
type	integer	identifier for the (virtual) element of the atom

An example file including all these features looks like this.

```

1 #F A
2 #C number type x y z
3 #X 3.520000 0 0
4 #Y 0 3.520000 0
5 #Z 0 0 3.520000
6 #E
7 1 0 2.636128 0.888096 0.891264
8 2 0 2.636128 2.648096 2.651264
9 3 0 0.876128 0.888096 2.651264
10 4 0 0.876128 2.648096 0.891264

```

Additional custom columns can be imported using the editor under “Edit-;Edit configuration” and providing the custom column keywords, a name and an optional unit. The checkbox “Raw values” must be ticked when files to be opened are selected. Files should either have the ending “.chkpt” or “.ada” to be imported directly. If a sequence of multiple files is to be opened they should be ending with “.xxxxx.chkpt” or “.xxxxx.ada” where xxxxx is a continuous sequence of numbers. Files compressed with gzip can be opened directly. In this case the files need the additional suffix “.gz” at the end of the name.

Limited support for file from the Lammmps MD code is implemented as well.

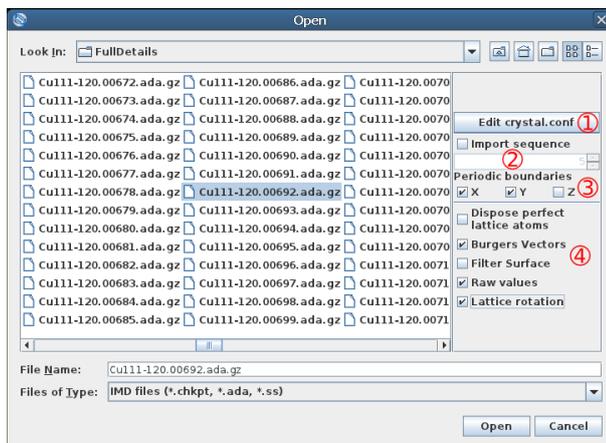


Figure 2: Open dialog: Different options can be enable and disabled before opening files

1. Edit the crystal configuration (see Figure 3).
2. If the files are properly number it is possible to open a sequence of files by selecting the first file and the number of files. Otherwise multiple files can be selected. This feature is not available for LAMMPS files.
3. Enable periodic boundaries conditions in selected directions. For LAMMPS files, this setting is ignored if the boundary conditions are given in the file header.
4. Enable and disable different features of analysis

Crystal parameters Besides the atomic configuration, additional information concerning the crystal is needed to analyze the crystal properly.

The following information must be provided:

- the crystal structure (e.g. BCC or FCC)
- the lattice constant
- the crystal orientation

Lattice constant and the crystal structure are required to identify defects correctly, where the crystal orientation is required to calculate Burgers vectors and lattice rotations correctly. If the configuration file “crystal.conf” is not found in the same folder as the data, AtomViewer will ask for these information.

Warning: Do not place simulations of different materials or orientations in the same folder. Each of these simulations has to be in its own subfolder together with a proper configuration file.

The screenshot shows a dialog box titled "Crystal configuration". It contains the following elements:

- Crystal orientation:** A table with three rows (X-Axis, Y-Axis, Z-Axis) and three columns. Values are: X-Axis (0, -1, 1), Y-Axis (2, -1, -1), Z-Axis (1, 1, 1). A red circled '1' is next to the Y-Axis label.
- Crystal structure:** A dropdown menu showing "FCC". A red circled '2' is next to it.
- Lattice constant:** A text input field containing "3.64".
- Import Raw Values:** A section with a table:

Name	ID in file	Unit	Active
Pot. Energy	EPot	eV	<input checked="" type="checkbox"/>

 A red circled '3' is next to the 'Active' column header. Below the table is an "add" button.
- Buttons:** "OK" and "cancel" buttons at the bottom.

Figure 3: Crystal.conf dialog: Define the crystal properties and imported fields here

1. Define the crystal orientation in the Cartesian system. Axis x and y must be orthogonal, z is automatically computed.
2. Set crystal structure and lattice constant
3. Define additional values that are imported directly from the input file. “Name” defines the label that will be used for displaying the value. “ID in file” must match the values ID used in the files to be imported. The unit is optional, if provided it will be added to values in the color bars. Remove a value by unticking the “Active” checkbox. Add another value by clicking “add”.

4 Analysis features

Defect state Defects are automatically detected with a modified bond angle analysis method (see [3] and [1] for the modified version) if the column “defectType” is

FCC characterization

ID	Description	Burgers vectors calculated
0	BCC	no
1	FCC	yes
2	HCP	yes
3	14 neighbors atoms, distorted order	yes
4	12-13 neighbors	yes
5	15 neighbors	yes
6	Free surface, <11 neighbors	no
7	Unknown	yes

BCC characterization

ID	Description	Burgers vectors calculated
0	BCC	yes
1	FCC	no
2	HCP	no
3	12 neighbor atoms, distorted order	yes
4	<12 neighbors	yes
5	>12 neighbors	yes
6	Free surface, <10 neighbors	no
7	Unknown	yes

not found in the input files. Depending on the configuration of the nearest neighbor atoms are assigned.

Resultant burgers vectors & dislocation network Dislocation networks including Burgers vectors are computed if the option “Burgers vectors” is enabled during import. Burgers vectors are computed via a modified version of the Nye-tensor analysis by Hartley&Mishin ([4, 5]). The derived resultant burgers vectors are combined into dislocation networks ([1]). Resultant burgers vectors are computed for each atom identified as certain defect types. If the crystal orientation is given correctly, the results of the dislocation network analysis are in most cases fairly accurate, but are prone to wrong classifications in the vicinity of free surfaces or defects like cracks.

Lattice rotations Per atom lattice rotations can be calculated in full atomic simulations. The rotations can be displayed either in degrees of rotation around the x-axis, y-axis or z-axis or as an absolute deviation angle. For very severely distorted atoms the calculation can fail. In this case a rotation of zero is assigned.

5 Output Formats

Dislocation networks can be saved to be processed in other applications. The output file consists of two sections. The first defines the number of nodes and their position. The second section defines a dislocation per line as a sequence of nodes and the Burgers vector. The three components of the Burgers vector are in crystal coordinates. If the Burgers vector has been identified, the line terminates with “y”. If no Burgers vector has been identified the line terminates with “n”. In this case either no Burgers vector has been identified at all or the numerical averaged resultant Burgers vector could not be mapped to a crystallographic possible one. The numerical value is then printed instead of the true burgers vector.

```
1 #total number of nodes
2 209
3 #number x y z
4 0 155.61615 185.73717 219.36273
5 1 124.12319 162.65952 380.88416
6 2 126.55689 162.48555 380.7972
7 3 128.97746 162.46237 380.71375
8 4 135.29456 201.71378 382.6585
9 5 135.15097 207.23106 384.94006
10 ....
11 #total number of dislocations
12 406
13 #number numberOfNodes n_1 n_2 ... n_n BV_x BV_y BV_z BV_identified
14 #BV_identified: (y) if Burgers vector is identified,
15 #(n) if just a numerical average is known
16 0 6 17528 17601 17695 17685 15752 17539 0.1667 -0.6667 0.1667 y
17 1 2 17840 17842 0.0000 0.0000 0.0000 n
18 3 2 17824 17833 0.0000 0.0000 0.0000 n
19 ...
```

6 Known limitations

Dislocations in pseudo 3D simulation and infinitely long dislocations Dislocations are not properly identified in case the simulation box is very small and dislocations are infinite due to periodic boundaries. However, resultant Burgers vectors are correctly identified.

Rendering performance Default settings are fairly stable but slow. Improvements can be made by enabling “instanced rendering” in the settings menu. However, some AMD graphic cards produce a rather strange behavior with this option.

Enabling more features in AtomViewer AtomViewer contains several features that are either not well tested, are not usable in all crystal structures or rely on

special data structures as for example grain- and phaseboundary approximations in its current state. These features are included in AtomViewer, but are not available by default. Additional functionality becomes available by unchecking “Basic features only” in the settings menu. Beware, additional features are likely not working in the way it is expected.

7 License

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References

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