Atomsk Cheat Sheet

For Atomsk version beta-0.11.2 - https://atomsk.univ-lille.fr/

Syntax

Convert a file into another file or format:
`atomsk <input> [<options>] <output>`

Use a mode:
`atomsk --mode <parameters>`

Basic examples

Convert a file:
`atomsk initial.xsf final.cfg`

Convert a file to several formats:
`atomsk initial.xsf cfg vesta lammps`

Duplicate a system:
`atomsk input.cfg -duplicate 3 3 4 final.cfg`

Create a unit cell of fcc aluminium:
`atomsk --create fcc 4.02 Al Al.cfg`

Display help:
`atomsk --help`

File for option -properties

```
auxiliary <property>
charge
displacement [function]
elastic [Voigt]
orientation
type
velocities
supercell
```

File for mode --polycrystal

box <H_x> <H_y> <H_z>
random <N>
lattice <sc|bcc|fcc|diamond|hcp>
node <x> <y> <z> <α> <β> <γ>

Options

Add new atom(s):
`-add-atom <species> at <x> <y> <z>`
`-add-atom <species> relative <index> <x> <y> <z>`
`-add-atom <species> near <index>`
`-add-atom <species> random <N>`

Add shells:
`-add-shells <species|all>`

Align first box vector along X:
`-alignx`

Re-associate shells with their matching core:
`-bind-shells`

Modify cell vectors:
`-cell <add|rm|set> <d>`
`<H1|H2|H3|x|y|z|xy|xz|yx|yz|zx|zy|xyz>`

Place atom of given index, or system's center of mass, at center of the box:
`-center <index|com>`

Insert a crack:
`-crack <I|II|III> <stress|strain> <$K_s$> <$p_1$> <$p_2$> <$\xi$> <n> <$\mu$> <$\nu$>`

Cut the system above or below the given plane:
`-cut <above|below> <d> <normal>`

Deform the system:
`-deform <direction> <$\epsilon$> <$\nu$>`

Insert a dislocation:
`-dislocation <$p_1$> <$p_2$> screw <$\xi$> <n> <b>`
`-dislocation <$p_1$> <$p_2$> <edge|edge_add|edge_rm> <$\xi$> <n> <b> <$\nu$>`
`-dislocation <$p_1$> <$p_2$> mixed <$\xi$> <n> <$b_1$> <$b_2$> <$b_3$>`
`-dislocation loop <x> <y> <z> <n> <radius> <$b_x$> <$b_y$> <$b_z$> <$\nu$>`

Options (continued)

Apply a random perturbation:
`-disturb <$d_{max}$>`
`-disturb <$d_x$> <$d_y$> <$d_z$>`

Duplicate the system:
`-duplicate <$N_x$> <$N_y$> <$N_z$>`

Fix the coordinates of some atoms:
`-fix <axis>`
`-fix <axis> <above|below> <d> <normal>`

Convert atom positions into reduced coordinates:
`-fractional`

Apply a mirror transformation:
`-mirror <d> <normal>`

Apply options from a file:
`-options <file>`

Change the crystal orientation:
`-orient <hkl>`$_x$ `<hkl>`$_y$ `<hkl>`$_z$ `<hkl'>`$_x$ `<hkl'>`$_y$ `<hkl'>`$_z$

Find a suitable equivalent orthogonal cell:
`-orthogonal-cell`

Read properties from a file (see Files):
`-properties <file>`

Auto-detect box dimensions:
`-rebox`

Reduce cell size, preserving periodicity:
`-reduce-cell [<x|y|z>]`

Remove atoms from the system:
`-remove-atom <index>`
`-remove-atom <species>`
`-remove-atom select`

Remove atoms that are too close to another one:
`-remove-doubles <distance>`

Options (continued)

Remove one or all per-atom property:
`-remove-property <property|all>`

Remove shells for one or all atom species:
`-remove-shells <species|all>`

Roll the system around an axis:
`-roll <direction> <θ> <axis>`

Rotate the system around an axis:
`-rotate [com] <axis> <θ>`

Round-off atom coordinates or a property to the given accuracy:
`-round-off <property> <accuracy>`

Select atoms according to given criteria:
`-select all`
`-select invert`
`-select <species>`
`-select <index>`
`-select <i1>,<i2>,<i3>:<i4>,...`
`-select list <file>`
`-select random <N> <species>`
`-select <above|below> <d> <dir>`
`-select <in|out> cell`
`-select <in|out> box <x> <y> <z> <x'> <y'> <z'>`
`-select <in|out> sphere <x> <y> <z> <R>`
`-select <in|out> cylinder <axis> <x1> <x2> <R>`
`-select <in|out> cone <axis> <x> <y> <z> <α>`
`-select <in|out> torus <axis> <x> <y> <z> <R> <r>`
`-select prop <property> <value1[:value2]>`
`-select <NNN> <species> neighbors <index>`
`-select grid <file>`
`-select stl [center] <file>`
`-select [add|rm|intersect|xor] <any of the above>`

Separate atoms that are too close to one another:
`-separate <distance> <shift>`

Options (continued)

Apply simple shear strain:
`-shear <n> <A> <s>`

Shift atoms:
`-shift <τx> <τy> <τz>`
`-shift <above|below> <d> <normal> <τx> <τy> <τz>`

Sort or pack atoms:
`-sort <property> <up|down|pack>`

Apply transformations of the given space group:
`-spacegroupe <group>`

Apply stress or read stress tensor from a file:
`-stress <xx|yy|zz|xy|xz|yz|p> <σ>`
`-stress <file>`

Substitute atoms:
`-substitute <sp1> <sp2>`

Swap two atoms or atom species, or Cartesian directions:
`-swap <id1> <id2>`
`-swap <sp1> <sp2>`
`-swap <x|y|z> <x|y|z>`

Apply torsion to the system:
`-torsion <axis> <θ>`

Change the unit of the given property:
`-unit <property> <factor>`
`-unit <unit1> <unit2>`

Change the box so that it appears less skewed:
`-unskew`

Generate random atom velocities:
`-velocity <T>`

Wrap atoms into the box:
`-wrap`

Modes

Average several systems:
`atomsk --average <listfile> <outputfile> [<formats>] [options]`

Create an atomic system from scratch:
`atomsk --create <lattice> <a0> [<c0>] <sp1> [<sp2> <sp3>...] [orient (hkl)x (hkl)y (hkl)z] [options] <outputfile> [<formats>]`
`atomsk --create nanotube <a0> <m> <n> <sp1> [<sp2>] [options] <outputfile> [<formats>]`

Read two files and write them in ddplot format:
`atomsk --ddplot <file1> <file2> [<outputfile>] [options]`

Read several files, write all systems into one:
`atomsk --gather <listfile> <outputfile> [<formats>] [options]`

Convert a list of files:
`atomsk --list <listfile> [<formats>] [options]`

Generate N systems by interpolation between two files:
`atomsk --interpolate <file1> <file2> <N> [<outputfile>] [formats] [options]`

Merge or stack N systems:
`atomsk --merge [x|y|z] <N> <file1>...<fileN> <outputfile> [<formats>] [options]`

Construct a polycrystal using Voronoï tesselation:
`atomsk --polycrystal <seed> <param_file> <outputfile> [<formats>] [options]`

Read a file containing several systems and write each of them in a separate file:
`atomsk --unfold <file> [<prefix>] <formats> [options]`

Unwrap atom coordinates:
`atomsk --unwrap <reference> <configuration> [<outputfile>] [<formats>] [options]`