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CellMuncher - A tool for super-cell manipulations

www.er-c.org

CellMuncher is a perl script that converts super-cell files and that manipulates the atom list in many ways. It uses an internal list representation. Super-cell data can be supplied in two different formats used by popular electron microscopy image simulation packages, namely MacTempas and EMS. The same formats are supported for export, besides CIF and VRML format and formats for the structure-viewer programs VESTA, CrystalMaker and JSV.

Installation

Unix flavoured machines

On a Unix flavour machine, determine the installation path of the perl binary by the shell command

$ which perl

The default installation path is /usr/local/bin. If your perl installation path deviates from the default one, open CellMuncher in an editor and edit the binary path for perl on the first line of the script. Finally, copy CellMuncher into a directory where binaries are looked for, e.g.

$ sudo cp CellMuncher /usr/local/bin

You probably need super user rights to do this.

Windows

There are two options to uses CellMuncher in Windows:

(1) Install the pre-compiled binary CellMuncher.exe. CellMuncher.exe can be executed in cmd.exe

(2) Install a Windows implementation of Perl, like Strawberry Perl. CellMuncher can then be executed in a perl shell.

Usage

CellMuncher is a command line driven program. To process a super-cell file called mycell.cel the command has the general form

$ CellMuncher [OPTIONS]

Important OPTIONS are

--input-file=<name of the input file>

--output-file=<name of the outputfile>

A complete listing of the available options is given below. A short help page is presented when the --help option is chosen:

$ CellMuncher --help

A simple example:

$ CellMuncher --input-file=mycell.cel --output-file=mycell_copy.cel

copies the Stadelmann EMS file mycell.cel into mycell_copy.cel. (Note that it is not an exact copy since the formatting of the file is checked upon copying!)

Options

Options can be given in a long form (--option[=value]) or (for almost all options) in a short form of a single character (-o [=value]). Only a few option are exclusively available in the long form. Note that the equal sign = is not mandatory, a space will do also.

Full list of options

Note: <> symbolize that the argument within the brackets is a mandatory argument.

--attach-cell=<value>

--align-z-axis-non-periodic|S=<value>

--align-z-axis-periodic|D=<value>

--cif

--centre-atoms=<value>

--centre-at-zero|N

--centre-rotate-axis|O=<value>

--correct-dimension|u=<value>

--create-block|b=<value>

--cut-above|c=<value>

--cut-above-plane|a=<value>

--cut-at-distance=<value>

--cut-below|C=<value>

--cut-below-plane|A=<value>

—cut-below-distance=<value>

--cut-cell-dimension=<value>

--decorate=<value>

--debug

--delete-duplicate|d

--delete-element|Y=<value>

--dice-pair-site-occupancy=<value>

--dice-site-occupancy

--expand-structure=<value>

--extend-cell|e=<value>

--extend-cell-centre|E=<value>

--extend-to-size=<value>

--frozen-lattice|F=<value>

--frozen-lattice-fix-margin=<value>

--help|h

--input-file|--input|f=<value>

--invert-axis|I=<value>

--merge-file|H=<value>

--mirror-atom|m=<value>

--mirror-axis|M=<value>

--output-file|--output|o=<value>

--override

--periodic|p=<value>

--point-defect-displacements=<value>

--preview=<value>

--preview-file=<value>

--prompt

--read-format|--input-format|r=<value>

--remove-close-atoms|v=<value>

--repeat|j=<value>

--repeat-to-size=<value>

--replace=<value>

--reverse

--rotate-axis|R=<value>

--rotate-non-periodic|Q=<value>

--set-dw-factor|B=<value>

--set-occupancy=<value>

--slice|L=<value>

--slice-by-list|l=<value>

--shuffle

--screw-dislocation=<value>

--sort|s=<value>

--swap-axes|x=<value>

--translate-atom|t=<value>

--translate-axis|T=<value>

--unformatted

--wedge-cut-above|k=<value>

--wedge-cut-below|K=<value>

--write-format|--output-format|w=<value>

Detailled Description

Values are given as a comma separated list. The following symbols are used:

s: string or character, e.g. x

i: integer value, e.g. 2

f: floating point value, e.g. 3.14159.

Note: <> symbolize that the argument within the brackets is a mandatory argument. [] symbolizes optional arguments, multiple means that one command line may contain more than one of these options

option	description	value format/ choices	multiple	example/ explanation/ comment
--help	display a help page	-	✘	--help
--input-file=<value> --input=<value> -f <value>	file name of the input super-cell	s filename	✘	--input-file=mycell.cel input data will be read from mycell.cel
--output-file=<value> --output=<value> -o <value>	file name of the output super-cell	s filename	✘	--output-file=my2ndcell.cel

option	description	value format/ choices	multiple	example/ explanation/ comment
--read-format=<value> --input-format=<value> -r=<value>	file format of the input super-cell	s XMS=EMS format MT=MacTempas format XYZ=Ascii format	✘	--read-format=XMS input data is an EMS data file XYZ ascii data file format: line #1: comment line line #2: a b c alpha beta gamma line #3: number of atoms N line #4: Atom Symbol X Y Z line #N+3: - " - X,Y, and Z are in absolute coordinates (Angstrom)

option	description	value format/ choices	multiple	example/ explanation/ comment
--write-format=<value> --output-format=<value> -w=<value>	file format of the output super-cell	s XMS=EMS format (enhanced precsion 10F6, if --unformatted is not set) EMS=EMS format (standard precision 8F4, if --unformatted is not set) MT=MacTempas format CIF=CIF format VESTA=for Vesta structure viewer, identical with CIF format CM=Crystal Maker text format, also for Vesta ALI=Crystal Maker text format JSV=JSV structure viewer format WRL=VRML format	✘	--write-format=XMS output data is an EMS data file with enhanced accuracy (10F6 instead of 8F4 for the atom positions)

option	description	value format/ choices	multiple	example/ explanation/ comment
--attach-cell=<value>	attach a super cell file to the input file at the input cell upper face	s1,s2,s3 s1:filename s2:EMS,XMS,MT,XYZ,JSV s3: dimension along which the cell will be attached, i.e. x, y, or z	✔	--attach-cell=attachme.cel,XMS,x attaches the cell attachme.cel in EMS format to the super cell in the input file, the attached atoms will be placed at the upper face along the x dimension of the input cell Note: other cell dimensions have to match
--merge-file=<value> -H <value>	merges a super cell file to the input file	s1,s2[,f1,f2,f3] s1:filename s2:EMS,XMS,MT,XYZ,JSV f1,f2,f3: position in relative coordinates, optional	✔	--merge-file=mymerge.cel,XMS merges the cell mymerge,cel in EMS format to the super cell in the input file,the merged atoms will be centred in the middle of the cell --merge-file=mymerge.cel,XMS,0.2,0.3,0.6 same, but the atoms in mymerge.cel will be centred around the relative position 0.2,0.3,0.6 Note: so far the cell of the merge file needs to be smaller than the cell of the input file
--delete-element=<value> -Y <value>	delete an element from the list	s element symbol	✔	--delete-element=Mo delete all molybdenum atoms from the list
--set-dw-factor=<value> -B <value>	set the Debye-Waller factor for one element	s,f element symbol, DW factor in nm	✔	--set-dw-factor=Sr,0.0046 set the Debye-Waller factor of strontium atoms to 0.0046 nm - responds to 8*pi^2*u^2 where u^2 is the isotropic mean quadratic displacement
--set-occupancy=<value>	set the site occupancy for one element	s,f element symbol, site occupancy	✔	--set-occupancy=Ga,0.6 set the site occupancy of gallium atoms to 0.6

option	description	value format/ choices	multiple	example/ explanation/ comment
--dice-pair-site-occupancy=<value>	create a specific site occupancy configuration for a site that may be occupied by two elements A and B	s1,s2,f s1: element symbol for A s2: element symbol for B f: maximum distance between A and B sites in Angstrom	✔	--dice-pair-site-occupancy=Pd,Al,0.4 for each of the Pd and Al sites that are closer than 0.4 Å: set the occupancy of the Pd atom to 1 with a probability, that corresponds to the occupancy on that site, the occupancy of Al is set to 0 if the site is occupied by Pd and 1 otherwise note that vacant sites are deleted from the atom list!
--dice-site-occupancy	create a specific site occupancy configuration	-	✘	--dice-site-occupancy set the occupancy for each atom site to 1 or 0; the probability for site occupation corresponds to the occupancy parameter note that occupancies are either 1 or 0 afterwards, vacant sites are deleted from the atom list!
--repeat=<value> -j <value>	repeat the super cell along one direction	s,i direction: x,y or z, integer factor	✔	--repeat=x,2 repeat the super cell 2 times along x
--repeat-to-size=<value>	scale the super cell along one direction to a certain size in Ångstrom and fill with atoms	s,f direction: x,y or z, size in Ångstrom	✔	--repeat-to-size=x,200 scale the super cell in x-direction to 200 Ångstrom
--wedge-cut-above=<value> -k <value>	cut a wedge from the top of the super cell	s1,f1,f2 s1: x or y f1: angle in ° f2: offset in relative coordinates an atom is removed, when z > s1*tan(f1) + f2	✔	--wedge-cut-above=y,30,0 create a 30°-wedge in the yz-plane, top part of the cell is vacuum

option	description	value format/ choices	multiple	example/ explanation/ comment
--wedge-cut-below=<value> -K <value>	cut a wedge from the bottom of the super cell	s1,f1,f2 s1: x or y f1: angle in ° f2: offset in relative coordinates an atom is removed, when z < s1*tan(f1) + f2	✔	--wedge-cut-below=x,30,0 create a 30°-wedge in the xz-plane, bottom part of the cell is vacuum
--cif	Shortcut for converting an input EMS or XMS file to CIF	-	✘	--cif —input=mycell.cel creates CIF file with the name mycell.cif
--cut-above=<value> -c <value>	cut along one direction above a certain value	s1,f [,s2] s1: x or y f: cut coordinate [or atom index] s2: index, indicates that f is the number of atom from where to cut (optional)	✔	--cut-above=x,0.7 cut all atoms with x > 0 .7 --cut-above=x,123,index cut all atoms with index > 123 in the list sorted for x
--cut-below=<value> -C <value>	cut along one direction below a certain value	s1,f [,s2] s1: x or y f: cut coordinate [or atom index] s2: index, indicates that f is the number of atom from where to cut (optional)	✔	--cut-below=x,0.3 cut all atoms with x < 0 .3 --cut-below=x,12,index cut all atoms with index < 12 in the list sorted for x
--cut-above-plane=<value> -a <value>	cut atoms above a certain plane in a distance from the origin	f1,f2,f3,f4 f1,f2,f3: plane indices f4: distance from origin in Angstrom	✔	--cut-above-plane=1,1,1,25 cut all atoms above the 111-plane in a distance of 25 Angstrom

option	description	value format/ choices	multiple	example/ explanation/ comment
--cut-below-plane=<value> -A <value>	cut atoms below a certain plane in a distance from the origin	f1,f2,f3,f4 f1,f2,f3: plane indices f4: distance from origin in Angstrom	✔	--cut-below-plane=-1,-1,-1,25 cut all atoms below the 111-plane in a distance of 25 Angstrom
--cut-at-distance=<value>	cut atoms beyond a certain distance from the origin	s,f s: axis, x,y or z or xy,yz or xz or xyz f: distance from origin in Angstrom	✔	--cut-at-distance=xy,25 cut a cylinder with the z-axis as the cylinder axis and a radius of 25 Angstrom --cut-at-distance=xyz,25 cut a sphere with a radius of 25 Angstrom Note: Only for orthogonal lattices
--cut-below-distance=<value>	cut atoms below a certain distance from the origin	s,f s: axis, x,y or z or xy,yz or xz or xyz f: distance from origin in Angstrom	✔	--cut-below-distance=xyz,15 cut atoms within a a sphere with a radius of 15 Angstrom Note: Only for orthogonal lattices
--cut-cell-dimension=<value>	cut cell along one direction below and above a certain relative coordinate	s1,f1,f2 s1: x or y or z f1, f2: relative cut coordinate, lower bound and upper bound	✔	--cut-cell-dimension=x,0.2,0.8 cut all atoms with x < 0 .2 and x > 0.8 and correct unit cell dimension
--decorate=<value>	decorates the positions in a super cell with a point group from a file	s1,s2[,s3] s1: filename s2: file format: EMS,XMS,MT, XYZ,JSV s3: orientation, optional values: "rndrot"	✔	--decorate=molecule.cel,XMS,rndrot decorates all the positions in the input file with the molecule data in molecule.cel. The molecule will be rotated in a random fashion. Note that the centre of the molecule in molecule.cel should be at 0,0,0.

option	description	value format/ choices	multiple	example/ explanation/ comment
--extend-cell=<value> -e <value>	extend unit cell without translating elements	s,f s: axis, x,y or z f: scaling factor	✔	--extend-cell=x,1.15 extends the unit cell along x by a factor of 1.15
--extend-cell-centre=<value> -E <value>	extend unit cell, translate atoms so that the old cell is centred in the new cell	s,f s: axis, x,y or z f: scaling factor	✔	--extend-cell-centre=y,1.2 extends the unit cell along y by a factor of 1.2, then translates along y by 0.1
--extend-to-size=<value>	extend unit cell to a certain size in Ångstrom, translate atoms so that the old cell is centred in the new cell	s,f s: axis, x,y or z f: size in Å	✔	--extend-to-size=z,100 extends the unit cell along z to a size of 100 Ångstrom and translates the atoms into the centre around z=50 Ångstrom
--expand-structure=<value>	expand a non-periodic structure e.g. a nanoparticle by a factor	f f: factor	✘	--expand-structure=1.05 expands a structure by 5 %
--align-z-axis-periodic=<value> -D <value> BROKEN!	align the z axis to a direction uvw for a periodic object, tries to find new period	f1,f2,f3 f1,f2,f3: uvw indices	✘	--align-z-axis-periodic=1,2,1 Aligns the z-axis to the 121 viewing direction Works only for orthogonal lattices! Use the --periodic option to fold the cell periodic. Use the --remove-close-atoms option to remove close atoms
--align-z-axis-non-periodic=<value> -S <value>	align the z axis to a direction uvw for a periodic object	f1,f2,f3 f1,f2,f3: uvw indices	✘	--align-z-axis-non-periodic=1,2,1 Aligns the z-axis to the 121 viewing direction. Works only for orthogonal lattices!

option	description	value format/ choices	multiple	example/ explanation/ comment
--rotate-non-periodic=<value> -Q <value>	rotate a non-periodic object around an axis uvw through the centre of a super-cell	f1,f2,f3,f4 f1,f2,f3: uvw indices f4: angle in °	✔	--rotate-non-periodic=1,2,2,14 Rotates by 14° around the 122 direction, the rotation axis goes through the centre of the super-cell. Works only for orthogonal lattices!
--rotate-axis=<value> -R <value>	rotate around an axis uvw through 0,0,0	f1,f2,f3,f4 f1,f2,f3: uvw indices f4: angle in °	✔	--rotate-axis=2,1,0,10 Rotates by 10° around the 210 direction, the rotation axis goes through the 000 corner of the super-cell. Works only for orthogonal lattices!
--centre-rotate-axis=<value> -O <value>	rotate around an axis uvw through the centre of the super-cell	f1,f2,f3,f4 f1,f2,f3: uvw indices f4: angle in °	✔	--centre-rotate-axis=2,1,0,10 Rotates by 10° around the 210 direction, the rotation axis goes through centre of the super-cell. Works only for orthogonal lattices!
--orthogonalize-plane=<value> -g <value>	orthogonalize a plane with non-orthogonal base vectors	s,i s: xy, xz or yz i: maximum increase in cell volume	✘	--orthogonalize-plane=xz,10 Orthogonalize xz-plane, maximum increase in cell volume is 10. The algorithm tries to find a new periodic supercell. Works only for xz so far (beta is not 90°), xy and yz are not implemented yet! Note: it depends on the angle and base vector lengths whether a solution can be found. The program will stop if there is no exact solution within the given bound. In that case it is better to create a non-periodic orthogonal cell using the --create-block option.

option	description	value format/ choices	multiple	example/ explanation/ comment
--create-block=<value> -b <value>	repeat a unit cell to an orthogonal block of a certain size and with a certain viewing direction	f1,f2,f3,f4,f5,f6,f7,f8,f9 f1-f3: x,y,z components of the viewing direction relative to the unit cell axes; this direction will be the new z direction f4-f6: x,y,z components relative to the unit cell axes of a direction that has an orthogonal component to the viewing direction; this direction defines the new b axis of the resulting super-cell f7-f9: the dimensions x,y, and z of the new cell in nm	✘	--create-block=1,1,0,-1,1,0,5,5,3 create a block with a size of 5x5x3 nm3 and a z-direction that corresponds to 110, the new y-direction is parallel to -1,1,0
--invert-axis=<value> -I <value>	invert atom positions on an axis	s s: x,y or z	✔	--invert-axis=z Invert atom positions on the z-axis.
--mirror-axis=<value> -M <value>	mirror atom positions on an axis	s,f s: x,y or z f: mirror position in relative coordinates	✔	--mirror-axis=x,0.3 Mirror atom positions on the x-axis, mirror point is the relative coordinate 0.3

option	description	value format/ choices	multiple	example/ explanation/ comment
--mirror-atom=<value> -m <value>	mirror single atom on an axis	s,i,f s: x,y or z i: atom index f: mirror position in relative coordinates	✔	--mirror-atom=y,121,0.6 Mirror atom 121 on the y-axis, mirror point is the relative coordinate 0.6
--translate-axis=<value> -T <value>	tranlate atom positions on an axis	s,f s: x,y or z f: translation in relative coordinates	✔	--translate-axis=x,0.3 Translate all the atoms on the x-axis by value 0.3 in relative coordinates
--translate-atom=<value> -t <value>	translate single atom on an axis	s,i,f s: x,y or z i: atom index f: translation in relative coordinates	✔	--translate-atom=z,12,0.1 Translate atom 12 on the z-axis by 0.1 relative to the z-dimension of the unit cell.
--frozen-lattice=<value> -F <value>	generate a frozen lattice configuration	s s: x,y or z or a combination like x,y or x,z or x,y,z	✔	--frozen-lattice=x,y create a frozen lattice configuration takes for each atom the DW factor and creates a random displacement in x,y displacements along one crystallographic direction follow a normal distribution with standard deviation Sqrt(1/(3*8Pi^2)*DW) and are usually about 4-6 pm on average

option	description	value format/ choices	multiple	example/ explanation/ comment
--frozen-lattice-fix-margin=<value>	generate a frozen lattice configuration, keep atoms at the boundary fixed	s,f1,f2,f3 s: x,y or z f1,f2,f3: margin width in x,y and z respectively in relative supercell size	✔	--frozen-lattice-fix-margin=x,0.1,0.2,0.0 create a frozen lattice configuration for atoms in 0.1 <= x <= 0.9 and 0.2 <= y <= 0.8 and 0 <= z <=1 takes for each atom the DW factor and creates a random displacement in x,y displacements along one crystallographic direction follow a normal distribution with standard deviation Sqrt(1/(3*8Pi^2)*DW) and are usually about 4-6 pm on average
--sort=<value> -s <value>	sort atom list	s s: x, y, z, e, all	✔	--sort=x --sort=e first sort according to the x-coordinate then according to the element
--correct-dimension=<value> -u <value>	correct unit cell dimensions (deletes vacuum space)	s s: x,y or z or a combination like x,y or x,z or x,y,z	✔	--correct-dimension=x,y correct dimensions in x and y, after correction, the minimum (maximum) x ynd y relative atom coordinate is 0 (1)
--centre-atoms=<value>	centre atoms within the volume of the unit cell	s s: x,y or z or a combination like x,y or x,z or x,y,z	✔	--centre-atoms=x,y centre atoms in x and y hint: use the --periodic option before!
--centre-at-zero	centre atoms around the origin (0,0,0) of the coordinate system		✘	--centre-at-zero centre atoms around x=0, y=0, z=0 hint: use the --periodic option before!

option	description	value format/ choices	multiple	example/ explanation/ comment
--screw-dislocation=<value>	create a displacement field of a srew islocation, including Eshelby twist	f1,f2,f3 f1,f2: x position in relative coordinates f3:magnitude of Burgers vector in Ångstrom	✘	--screw-dislocation=0.5,0.5,1.5 creates a screw dislocation in the centre of the super cell Burgers vector has a magnitude of +1.5 Angstrom atoms are shifted according to the Eshelby equation hint: expand unit cell before in order to avoid wrap-arounds
--swap-axes=<value> -x <value>	swap two axes	s s: xy or xz or yz	✔	--swap-axes=xy swap x-axis with y-axis
--periodic=<value> -p <value>	fold periodic	s s: x or y or z	✔	--periodic=x fold x axis periodic, that means all relative x-coordinates will be translated to the interval [0,1[, presuming that the structure is periodic
--delete-duplicate -d	delete duplicate atoms	-	✘	--delete-duplicate delete duplicate atoms in the list
--remove-close-atoms=<value> -v <value>	removes atoms that are closer than a certain distance to an atom that appeared earlier in the list	f f: distance in Angstrom	✘	--remove-close-atoms=0.8 removes atoms that are closer than 0.8 Angstrom: the atom wit the lower index in the list will remain, use together with the --sort, --shuffle, --reverse options on elements to re-arrange the list and determine which atom or element will be first and remain
--debug	switch on debugging code	-	✘	--debug
--override	don't ask if output-file exists, just override it	-	✘	--override

option	description	value format/ choices	multiple	example/ explanation/ comment
--point-defect-displace-ments=<value>	calculate an exponentially decaying displacement with the distance around a given centre, including a cosine modulation of the radial displacement	f1,f2,f3,f4,f5,f6,f7,f8 f1: point defect centre x, relative coordinates f2: point defect centre y, relative coordinates f3: point defect centre z, relative coordinates f4: displacement amplitude (A) f5: sigma width (A) f6: cosine amplitude, fraction of f4 as a relative number between 0 and 1, 0 means pure exponential, 1 means cosine with exponentially dampened amplitude f7: cosine period width (A) f8: cut-off radius (A)	✘	
--preview=<value>	generate a preview file and display the preview in CrystalMaker or Vesta (Mac OS X so far)	s s: CM or VESTA or Safari	✘	--preview=VESTA sends output to Vesta, choose CM for CrystalMaker preview and Safari for a Safari preview

option	description	value format/ choices	multiple	example/ explanation/ comment
--preview-file=<value>	generate a preview file and for CrystalMaker or Vesta or Safari	s s: CM or VESTA or Safari	✘	--preview-to-file=VESTA sends output to a Vesta file, choose CM for CrystalMaker preview
--prompt	wait for user input after each preview output	-	✘	--prompt
--reverse	put atom list in reverse order	-	✘	--sort=x --reverse first sort according to ascending x-coordinate, then reverse output
--shuffle	shuffle atom list	-	✘	—shuffle
--unformatted	write unformatted output in combination with EMS or XMS output	-	✘	--unformatted
--slice=<value> -L <value>	slice the supercell in z direction	i i: number of slices	✘	--slice=10 create 10 slices in z direction with the thickness dz=0.1 in relative coordinates,slices are labelled by a running counter starting from 001, specify only the prefix for the output, e.g. -o slc will lead to the output of slc001.cel, slc002.cel ... for --output-format=XMS or the output of slc001.at, slc002.at ... for --output-format=MT or the output of slc001.cif, slc002.cif ... for --output-format=CIF

Further Notes

CellMuncher does not rely on strictly formatted input. Since most operations do not commute, it is safe to perform them one by one in a sequential manner.

Examples

Example 1: Create a rectangular cell of Hübnerite ($MnWO_4$) in two steps.

Download an ICSD structure file from the ICSD database and convert it to an EMS super cell using BuildCell. Note: You may need to check the occupancy values and the Debye-Waller factors in the EMS file after conversion!

```
BuildCell --cif=MnWO467906.cif --output=MnWO467906.cel
```

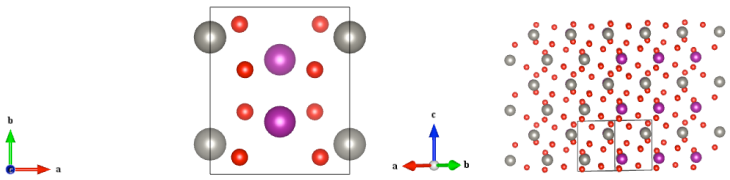


Fig.: P2/c unit cell of $MnWO_4$ (converted from ICSD file No. 467906 using BuildCell) and a repeated cell in <110> viewing direction. The monoclinic unit cell dimensions are a=4.83000, b=5.76030, c=4.99400, alpha=90.0000, beta=91.1420, gamma=90.0000.

Then use the --create-block option to make a rectangular super-cell of a size of 3x3x6 nm^3 with the <110> direction parallel to the z direction of the unit CellMuncher. Note that a, b, and c are all different and that beta is not 90°! To construct a rectangular cell you need the new z-direction, <110> in this case, and one orthogonal direction. One possible direction is $<|a||c|/|a|^2\cos(a,c),0,1>$ = <0.020607064,0,1>, which is parallel the plane normal to the ab-plane. CellMuncher will suggest a direction close to the chosen one in case it is not orthogonal. In fact, any direction which is not parallel to the new z-direction will do. Therefore, we can choose <0,0,1> and let CellMuncher do the rest:

```
CellMuncher --preview-file=VESTA --create-block=1,1,0,0,0,1,3,3,6 --input=MnWO467906.cel --output=Mn-
WO467906-110-super-cell.cel
```

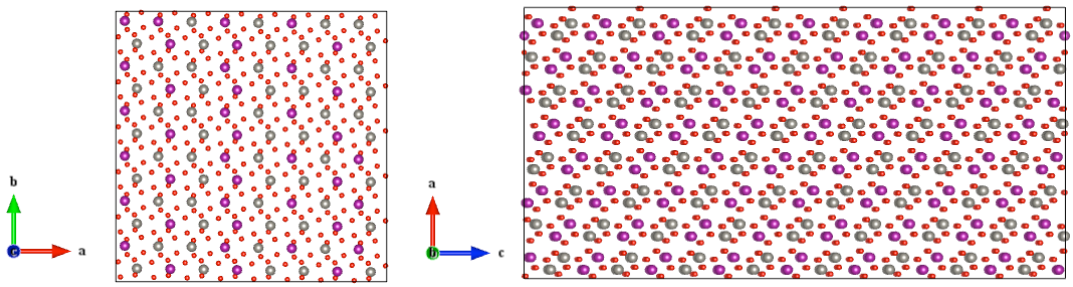


Fig.: Super-cell of $MnWO_4$ with the z-direction parallel to the <110> viewing direction of the original unit cell.

Example 2: A rectangular cell of hexagonal GaAs in more steps

Create an EMS super cell containing a unit cell of hexagonal GaAS and name the file GaAs_wurtzite_unitcell.cel

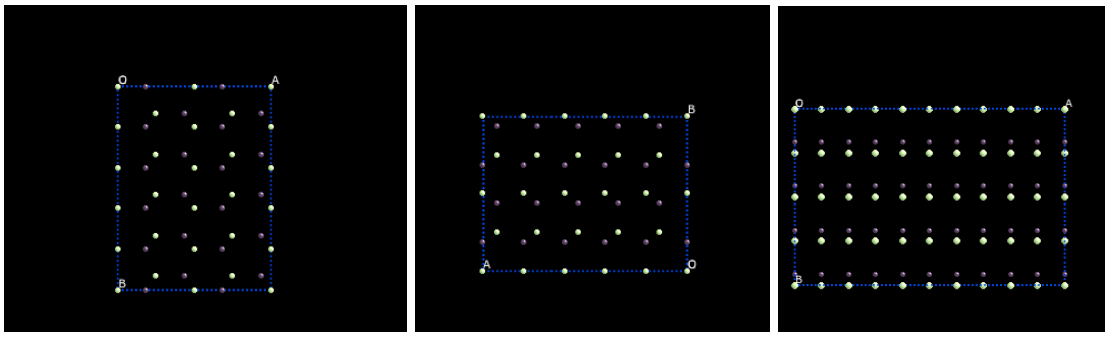
```
# GaAs wurtzite unit cell data
 0 0.624 0.382 0.382 120 90 90
Ga 0.0    0.0      0.0     1.0   0.006  0.0   0.0   0.0
Ga 0.5    0.666667 0.33333 1.0   0.006  0.0   0.0   0.0
As 0.375  0.0      0.0     1.0   0.0055 0.0   0.0   0.0
As 0.875  0.666667 0.33333 1.0   0.0055 0.0   0.0   0.0
*
```

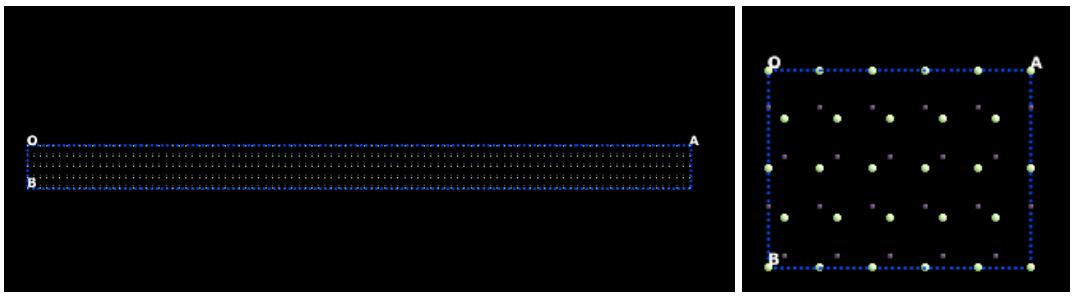
Now create a shell script with the CellMuncher commands

```
#!/bin/bash

# repeat hexagonal cell, open preview in CrystalMaker and prompt user to continue
CellMuncher --repeat=x,2 --repeat=y,5 --repeat=z,5 --override  --prompt --preview=CM --input-file=GaAs_wurtzite_unitcell.cel --output-file=tmp001.cel

# swap axes, preparation for orthogonalisation, only beta can be orthogonalized,
# open preview in CrystalMaker and prompt user to continue
CellMuncher --swap-axes=xy --override  --prompt --preview=CM --input-file=tmp001.cel --output-file=tmp002.cel

# orthogonalisation, only beta can be orthogonalized
# open preview in CrystalMaker and prompt user to continue
CellMuncher --orthogonalize-plane=xz,10 --override  --prompt --preview=CM --input-file=tmp002.cel --output-file=tmp003.cel

# repeat in x-direction, make 20 nm thick, y and z are periodicm
# open preview in CrystalMaker and prompt user to continue
CellMuncher --debug --delete-duplicate --repeat=x,10  --override  --prompt --preview=CM --input-file=tmp003.cel --output-file=tmp004.cel

# swap axes, so that z is the large dimension and x > y,
# open preview in CrystalMaker and prompt user to continue
CellMuncher --swap-axes=xz --override  --prompt --preview=CM --input-file=tmp004.cel --output-file=tmp005.cel
```

then execute the script file. You may need to change the path to the bash shell in the first line of the script according to your installation path.

CrystalMaker will show the preview of the 5 steps:





Known Bugs

Option processing is order sensitive! It is wise to do only one operation at a time.
Leave a blank between option specifier and argument for the single character short option.

Author/Contact

mail to the author