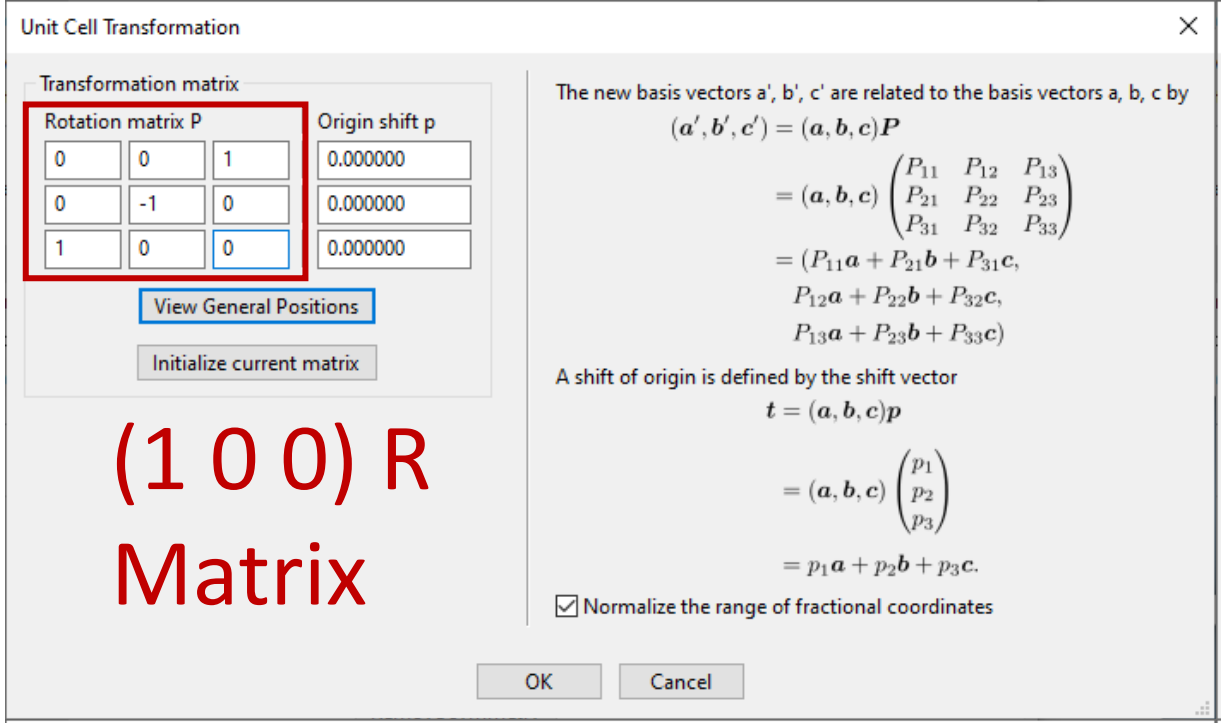
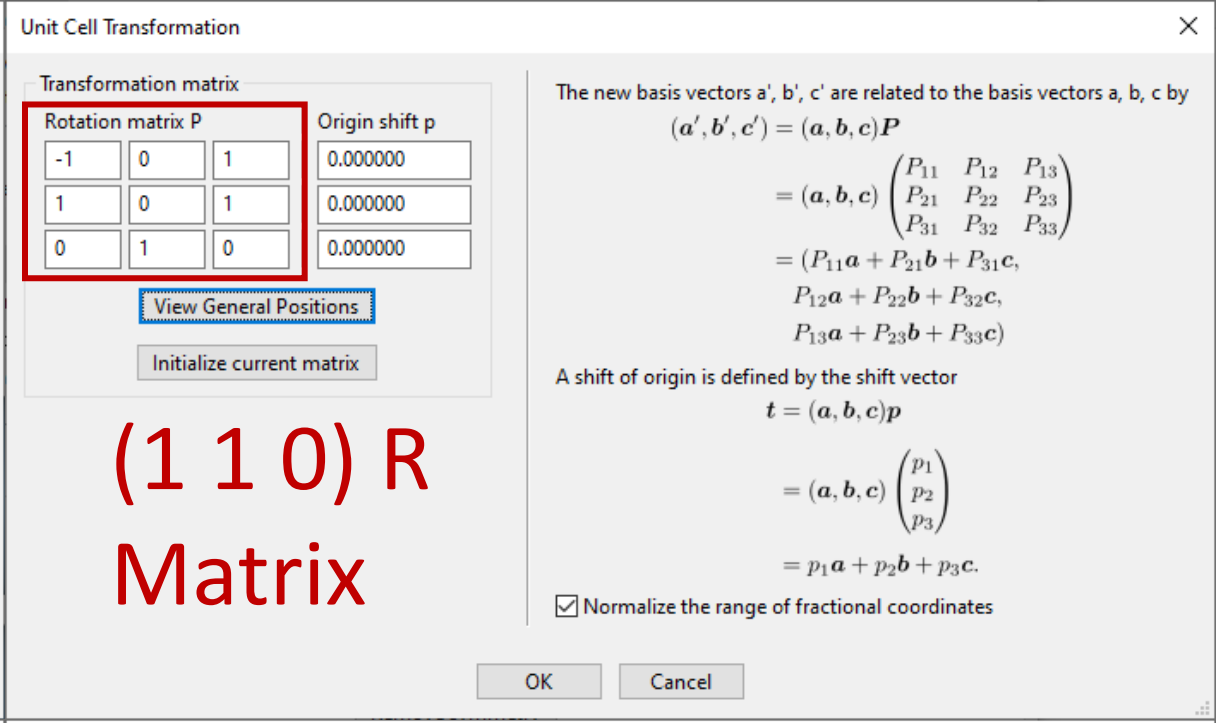
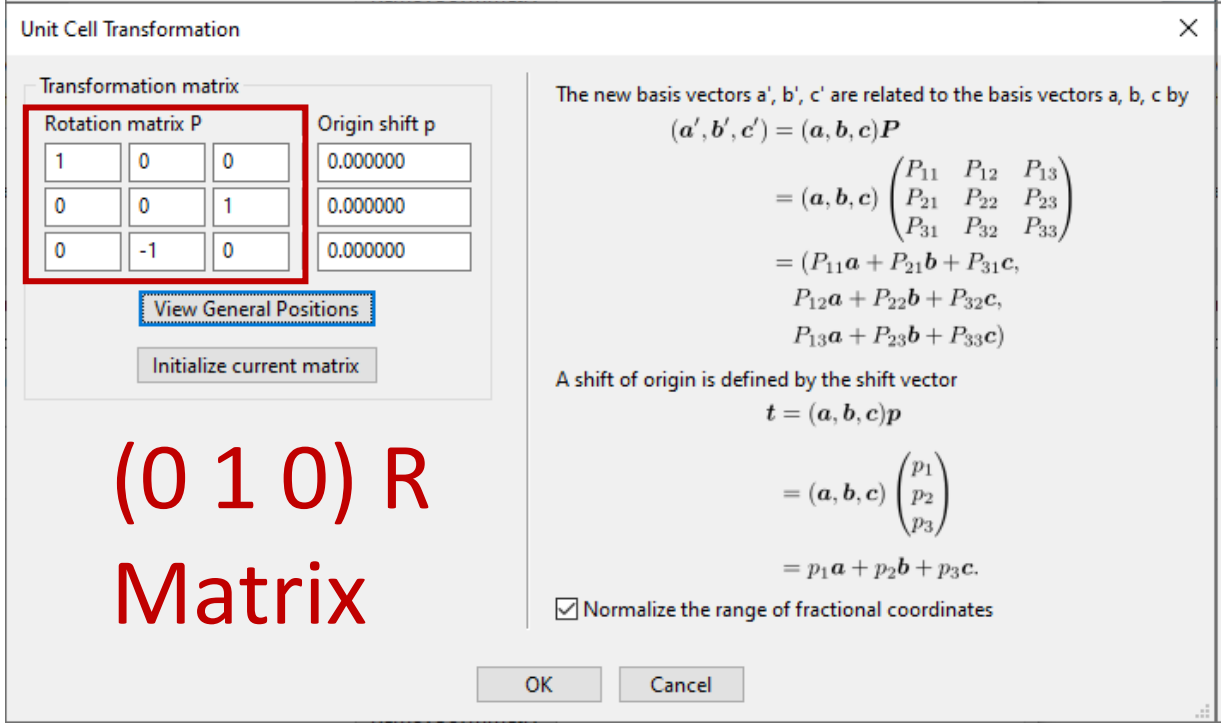
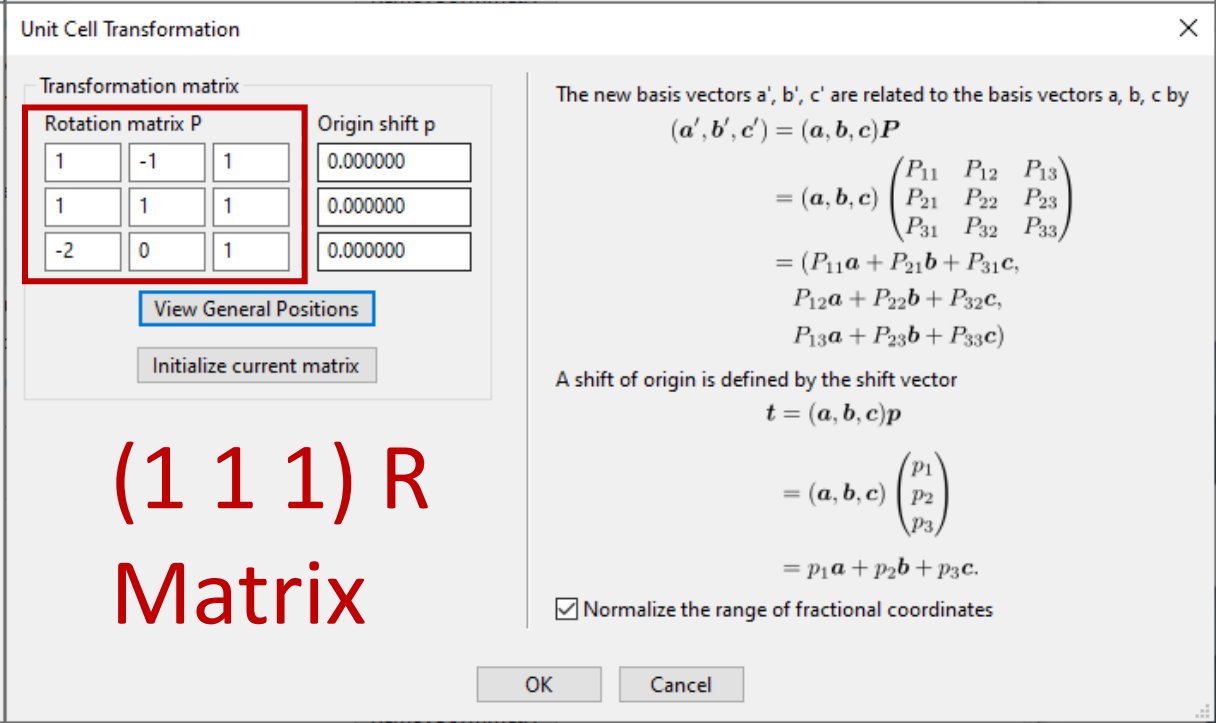
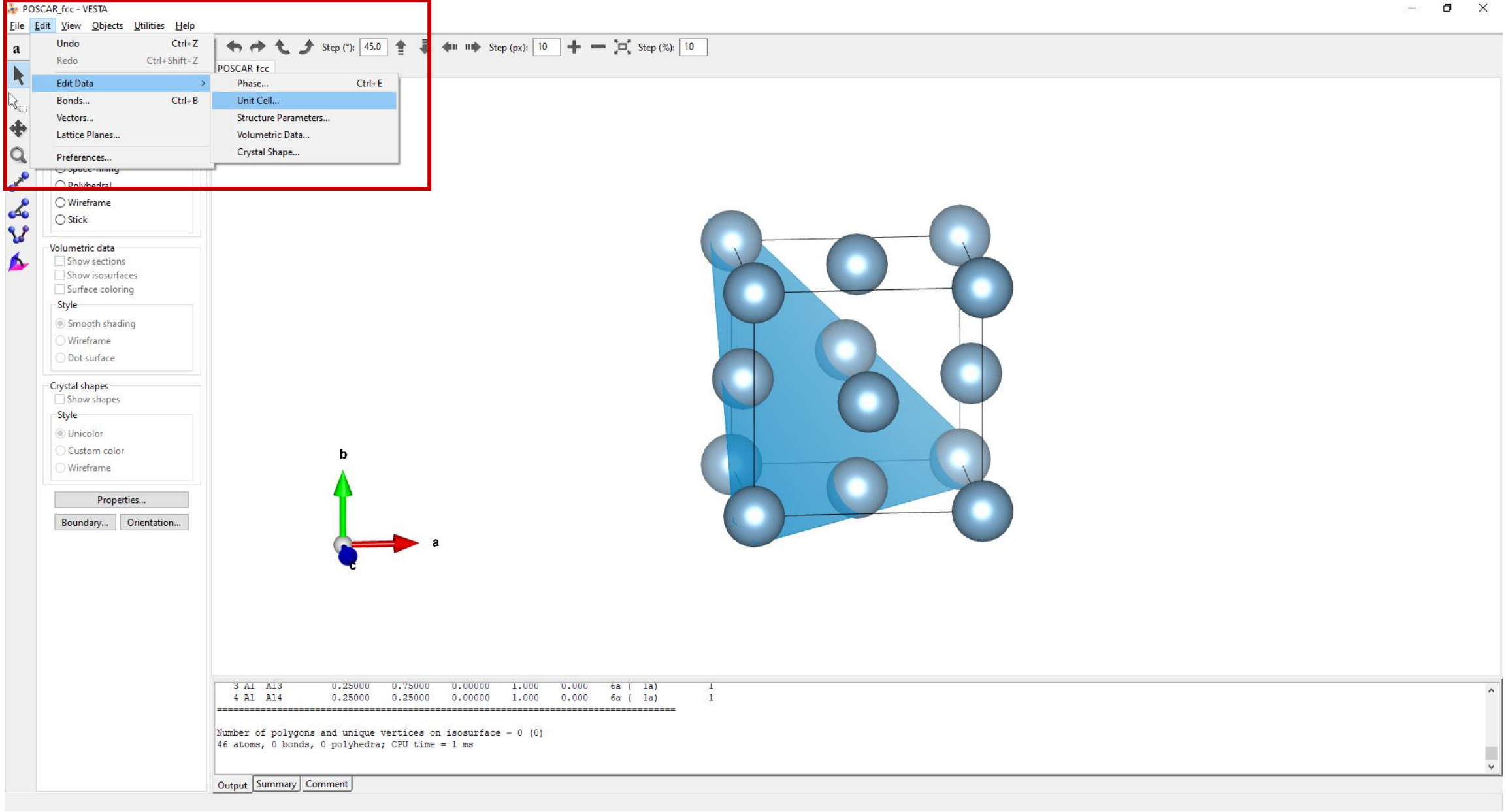

Unit Cell Transformation
Transformation matrix
Rotation matrix P
Origin shift p
0 0 1
0 -1 0
1 0 0
0.000000
0.000000
0.000000
View General Positions
Initialize current matrix
(1 0 0) R Matrix
The new basis vectors a', b', c' are related to the basis vectors a, b, c by
$(a', b', c') = (a, b, c)P$
$= (a, b, c)\begin{pmatrix} P_{11} & P_{12} & P_{13} \\ P_{21} & P_{22} & P_{23} \\ P_{31} & P_{32} & P_{33} \end{pmatrix}$
$= (P_{11}a + P_{21}b + P_{31}c,$
$P_{12}a + P_{22}b + P_{32}c,$
$P_{13}a + P_{23}b + P_{33}c)$
A shift of origin is defined by the shift vector
$t = (a, b, c)p$
$= (a, b, c)\begin{pmatrix} p_1 \\ p_2 \\ p_3 \end{pmatrix}$
$= p_1a + p_2b + p_3c.$
Normalize the range of fractional coordinates
OK
Cancel


Unit Cell Transformation
Transformation matrix
Rotation matrix P
Origin shift p
-1 0 1
1 0 1
0 1 0
0.000000
0.000000
0.000000
View General Positions
Initialize current matrix
(1 1 0) R Matrix
The new basis vectors a', b', c' are related to the basis vectors a, b, c by
$(a', b', c') = (a, b, c)P$
$= (a, b, c)\begin{pmatrix} P_{11} & P_{12} & P_{13} \\ P_{21} & P_{22} & P_{23} \\ P_{31} & P_{32} & P_{33} \end{pmatrix}$
$= (P_{11}a + P_{21}b + P_{31}c,$
$P_{12}a + P_{22}b + P_{32}c,$
$P_{13}a + P_{23}b + P_{33}c)$
A shift of origin is defined by the shift vector
$t = (a, b, c)p$
$= (a, b, c)\begin{pmatrix} p_1 \\ p_2 \\ p_3 \end{pmatrix}$
$= p_1a + p_2b + p_3c.$
Normalize the range of fractional coordinates
OK
Cancel

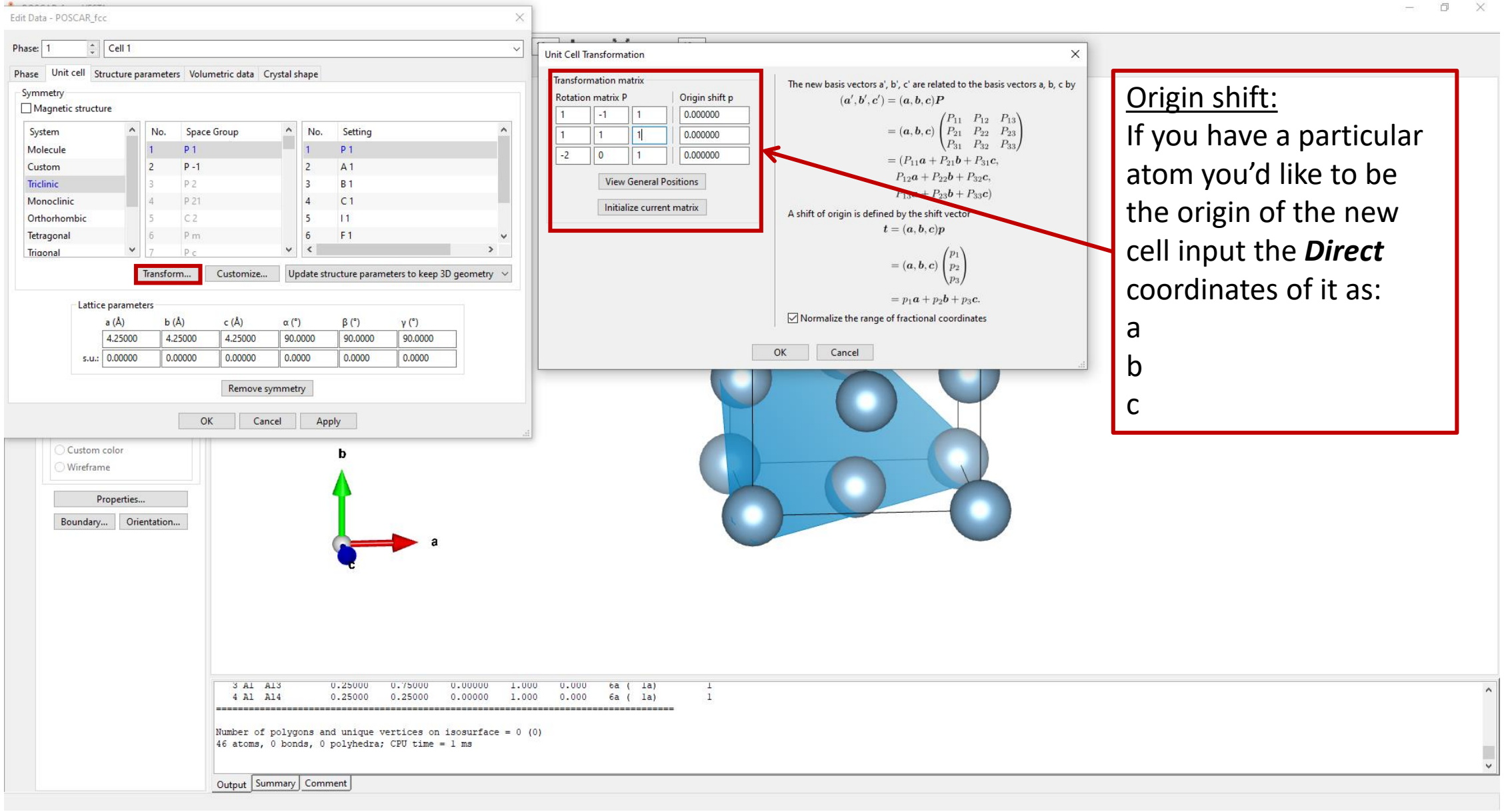

Unit Cell Transformation
Transformation matrix
Rotation matrix P
Origin shift p
1 0 0
0 0 1
0 -1 0
0.000000
0.000000
0.000000
View General Positions
Initialize current matrix
(0 1 0) R Matrix
The new basis vectors a', b', c' are related to the basis vectors a, b, c by
$(a', b', c') = (a, b, c)P$
$= (a, b, c)\begin{pmatrix} P_{11} & P_{12} & P_{13} \\ P_{21} & P_{22} & P_{23} \\ P_{31} & P_{32} & P_{33} \end{pmatrix}$
$= (P_{11}a + P_{21}b + P_{31}c,$
$P_{12}a + P_{22}b + P_{32}c,$
$P_{13}a + P_{23}b + P_{33}c)$
A shift of origin is defined by the shift vector
$t = (a, b, c)p$
$= (a, b, c)\begin{pmatrix} p_1 \\ p_2 \\ p_3 \end{pmatrix}$
$= p_1a + p_2b + p_3c.$
Normalize the range of fractional coordinates
OK
Cancel


Unit Cell Transformation
Transformation matrix
Rotation matrix P
Origin shift p
1 -1 1
1 1 1
-2 0 1
0.000000
0.000000
0.000000
View General Positions
Initialize current matrix
(1 1 1) R Matrix
The new basis vectors a', b', c' are related to the basis vectors a, b, c by
$(a', b', c') = (a, b, c)P$
$= (a, b, c)\begin{pmatrix} P_{11} & P_{12} & P_{13} \\ P_{21} & P_{22} & P_{23} \\ P_{31} & P_{32} & P_{33} \end{pmatrix}$
$= (P_{11}a + P_{21}b + P_{31}c,$
$P_{12}a + P_{22}b + P_{32}c,$
$P_{13}a + P_{23}b + P_{33}c)$
A shift of origin is defined by the shift vector
$t = (a, b, c)p$
$= (a, b, c)\begin{pmatrix} p_1 \\ p_2 \\ p_3 \end{pmatrix}$
$= p_1a + p_2b + p_3c.$
Normalize the range of fractional coordinates
OK
Cancel



1. Drag and drop the POSCAR file into VESTA window

2. Edit > Edit Data > Unit Cell…



Origin shift:

If you have a particular atom you'd like to be the origin of the new cell input the ***Direct*** coordinates of it as:

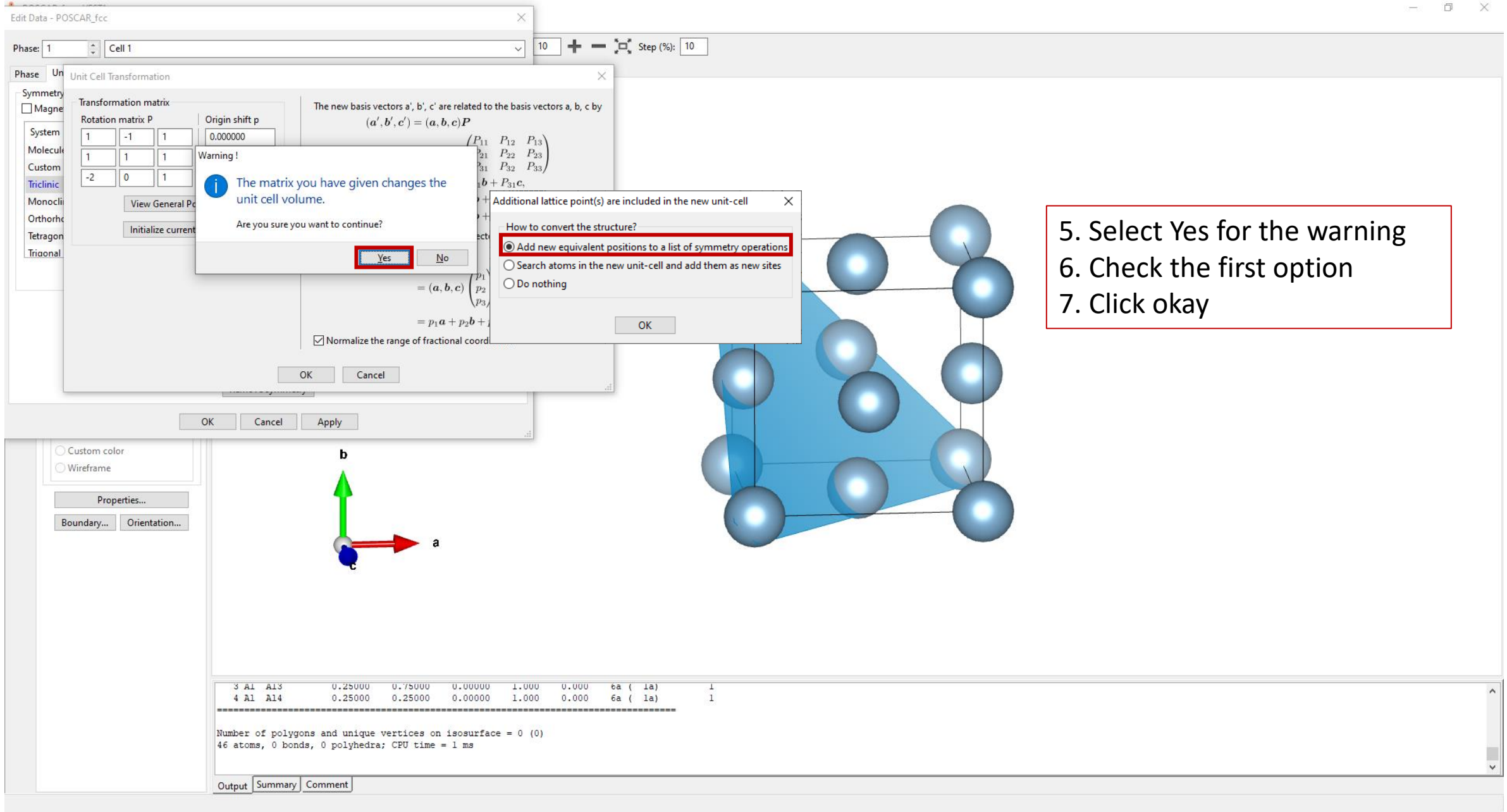
a

b

c

3. Select Transform…

4. Input rotation matrix (see first page for reference)



5. Select Yes for the warning
6. Check the first option
7. Click okay

Edit Data - POSCAR_fcc

Phase: 1 Cell 1

Phase | Unit cell | Structure parameters | Volumetric data | Crystal shape

Symmetry

Magnetic structure

System
Molecule
Custom
Triclinic
Monoclinic
Orthorhombic
Tetragonal
Trigonal

No.	Space Group
1	P 1
2	P -1
3	P 2
4	P 21
5	C 2
6	P m
7	P c

No.	Setting
1	P 1
2	A 1
3	B 1
4	C 1
5	I 1
6	F 1

Transform... Customize... Update structure parameters to keep 3D geometry

Lattice parameters

	a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)
	10.41033	6.01041	7.36122	90.0000	90.0000	90.0000
s.u.:	0.00000	0.00000	0.00000	0.0000	0.0000	0.0000

Remove symmetry

OK Cancel Apply

Custom color

Wireframe

Properties...

Boundary... Orientation...

10 Step (%): 10

b

a

c

8. Click Apply & the new unit cell will appear with the surface of your choice directed in the ĉ direction

```
   3 Al  Al3          0.25000    0.75000    0.00000    1.000    0.000    6a (  1a)         1
   4 Al  Al4          0.25000    0.25000    0.00000    1.000    0.000    6a (  1a)         1
================================================================================

Number of polygons and unique vertices on isosurface = 0 (0)
46 atoms, 0 bonds, 0 polyhedra; CPU time = 1 ms
```

Output | Summary | Comment

POSCAR_fcc - VESTA

File Edit View Objects Utilities Help

a b c a* b* c* Step (°): 45.0 Step (px): 10 Step (%): 10

Tools Style Objects

Structural models
- Show models
- Show dot surface

Style
- Ball-and-stick
- Space-filling
- Polyhedral
- Wireframe
- Stick

Volumetric data
- Show sections
- Show isosurfaces
- Surface coloring

Style
- Smooth shading
- Wireframe
- Dot surface

Crystal shapes
- Show shapes

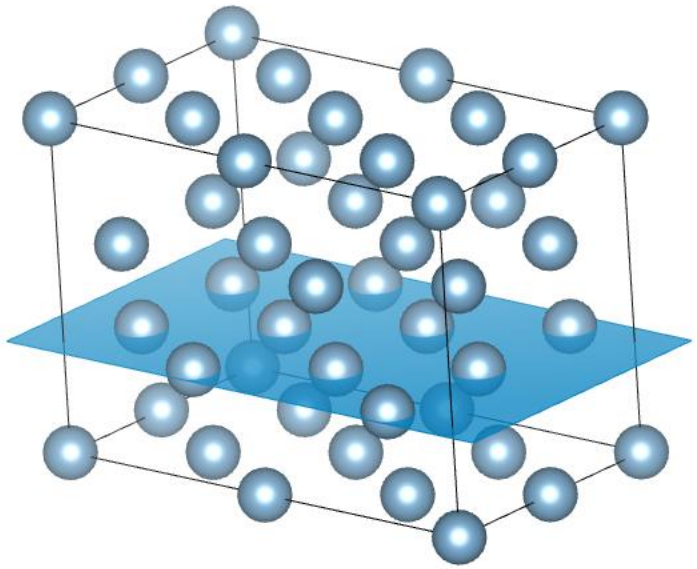
Style
- Unicolor
- Custom color
- Wireframe

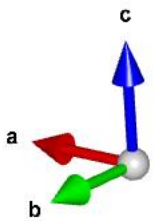
Properties...

Boundary... Orientation...

POSCAR_fcc

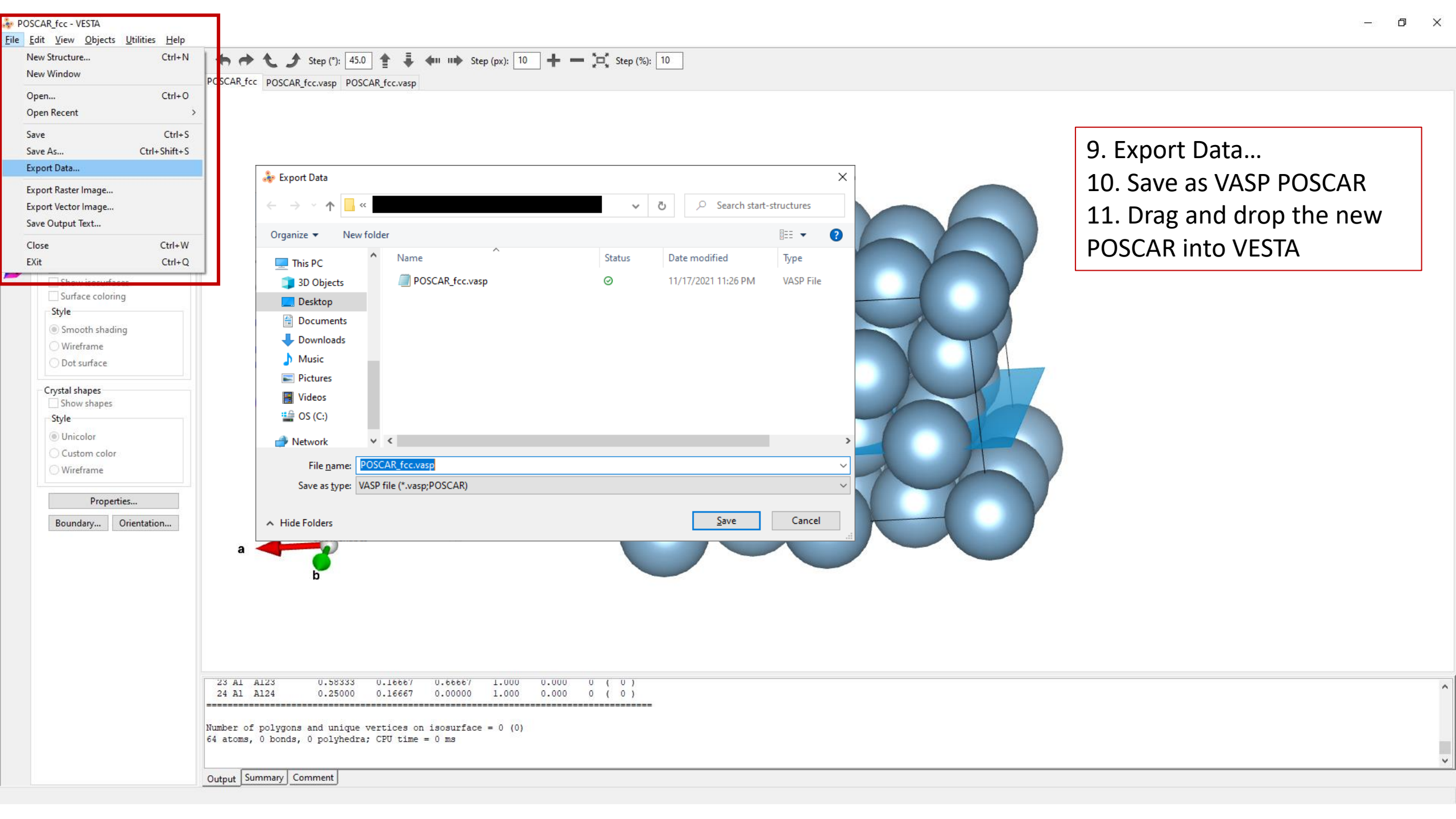
FCC (111) surface unit cell






```
   3 Al  Al3         0.91667    0.75000    0.33333    1.000    0.000    6a (  1a)         1
   4 Al  Al4         0.91667    0.25000    0.33333    1.000    0.000    6a (  1a)         1
================================================================================

Number of polygons and unique vertices on isosurface = 0 (0)
46 atoms, 0 bonds, 0 polyhedra; CPU time = 0 ms
```

Output Summary Comment



9. Export Data…
10. Save as VASP POSCAR
11. Drag and drop the new POSCAR into VESTA

POSCAR fcc.vasp

File Edit View Objects Utilities Help

Undo Ctrl+Z
Redo Ctrl+Shift+Z
Edit Data
Bonds... Ctrl+B
Vectors...
Lattice Planes...
Preferences...

Phase... Ctrl+E
Unit Cell...
Structure Parameters...
Volumetric Data...
Crystal Shape...

Step (°): 45.0 Step (px): 10 Step (%): 10

POSCAR fcc.vasp POSCAR fcc.vasp

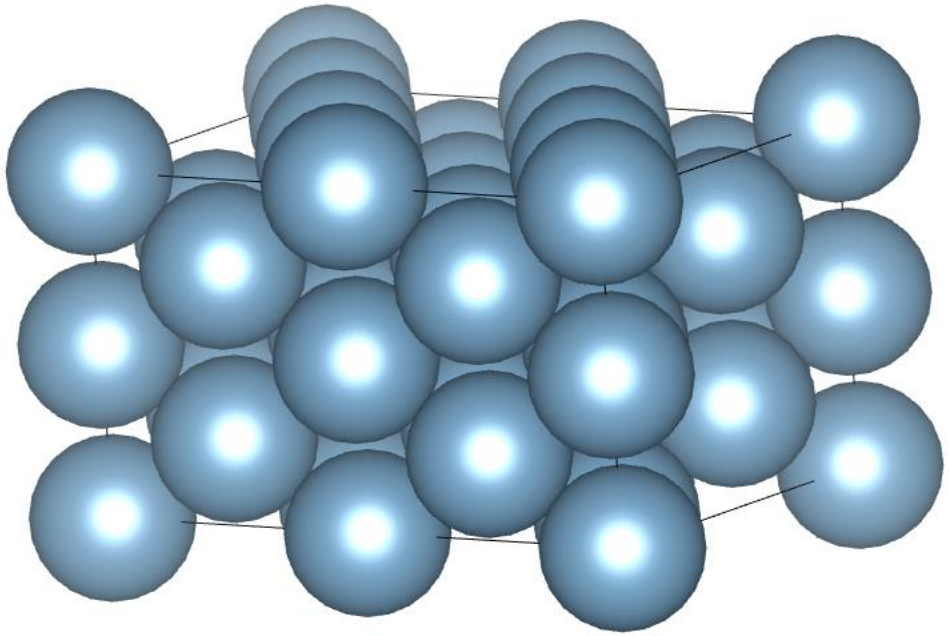
12. Edit > Edit Data > Unit Cell
13. Click Transform

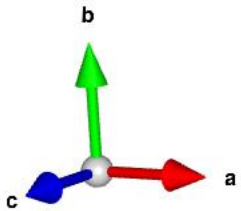
Wireframe
Stick

Volumetric data
Show sections
Show isosurfaces
Surface coloring
Style
Smooth shading
Wireframe
Dot surface

Crystal shapes
Show shapes
Style
Unicolor
Custom color
Wireframe

Properties...
Boundary... Orientation...






```
Atom:  1   All  Al   0.00000   0.00000   1.00000  ( 0, 0, 1)+ x, y, z
          (x,y,z):   0.00000   0.00000   7.36122
              Occ. = 1.000         Ueq = 0.00000      1a       1
Atom: 10  All0  Al   0.00000   0.50000   1.00000  ( 0, 0, 1)+ x, y, z
          (x,y,z):   0.00000   3.00520   7.36122
              Occ. = 1.000         Ueq = 0.00000      1a       1
```

Output Summary Comment

Edit Data - POSCAR_fcc.vasp

Phase: 1 Cell 1

Step (%): 10

Unit Cell Transformation

Transformation matrix

Rotation matrix P

1	0	0
0	1.5	0
0	0	1

Origin shift p

0.000000
0.000000
0.000000

View General Positions

Initialize current matrix

The new basis vectors a', b', c' are related to the basis vectors a, b, c by

$$(\boldsymbol{a}', \boldsymbol{b}', \boldsymbol{c}') = (\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c})\boldsymbol{P}$$

$$= (\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c}) \begin{pmatrix} P_{11} & P_{12} & P_{13} \\ P_{21} & P_{22} & P_{23} \\ P_{31} & P_{32} & P_{33} \end{pmatrix}$$

$$= (P_{11}\boldsymbol{a} + P_{21}\boldsymbol{b} + P_{31}\boldsymbol{c},$$
$$P_{12}\boldsymbol{a} + P_{22}\boldsymbol{b} + P_{32}\boldsymbol{c},$$
$$P_{13}\boldsymbol{a} + P_{23}\boldsymbol{b} + P_{33}\boldsymbol{c})$$

A shift of origin is defined by the shift vector

$$\boldsymbol{t} = (\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c})\boldsymbol{p}$$

$$= (\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c}) \begin{pmatrix} p_1 \\ p_2 \\ p_3 \end{pmatrix}$$

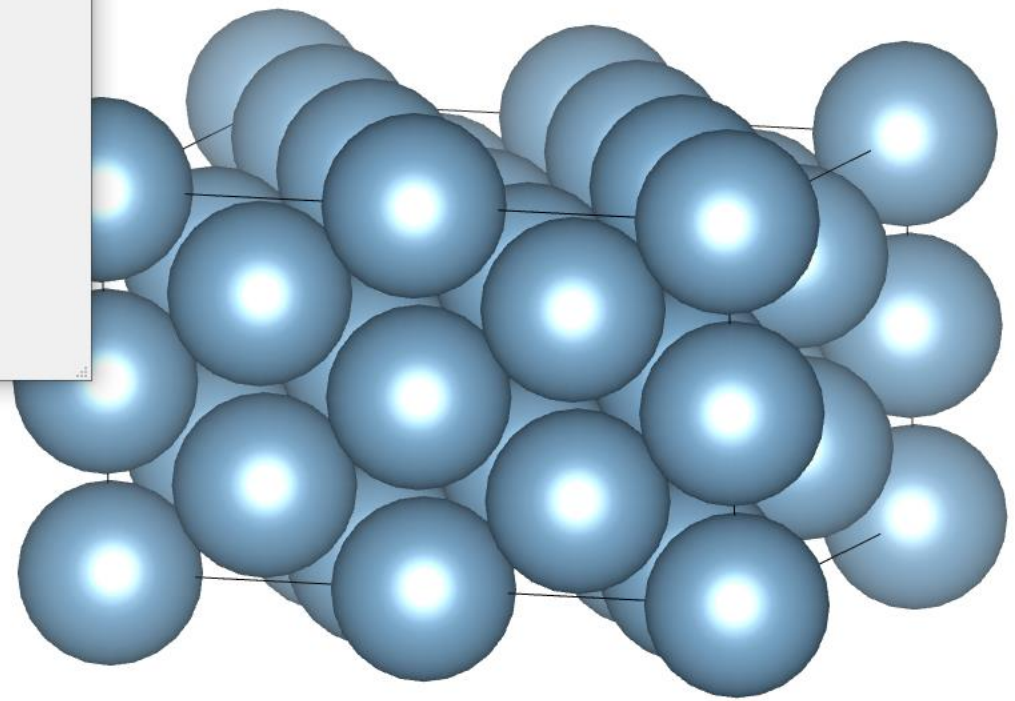
$$= p_1\boldsymbol{a} + p_2\boldsymbol{b} + p_3\boldsymbol{c}.$$

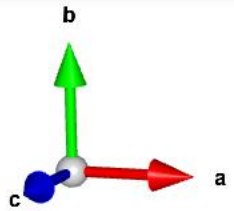
Normalize the range of fractional coordinates

OK Cancel

OK Cancel Apply

Adjust cell boundaries to change number of atoms in each layer (a,b) or number of layers in your slab model (c)





Custom color

Wireframe

Properties...

Boundary... Orientation...

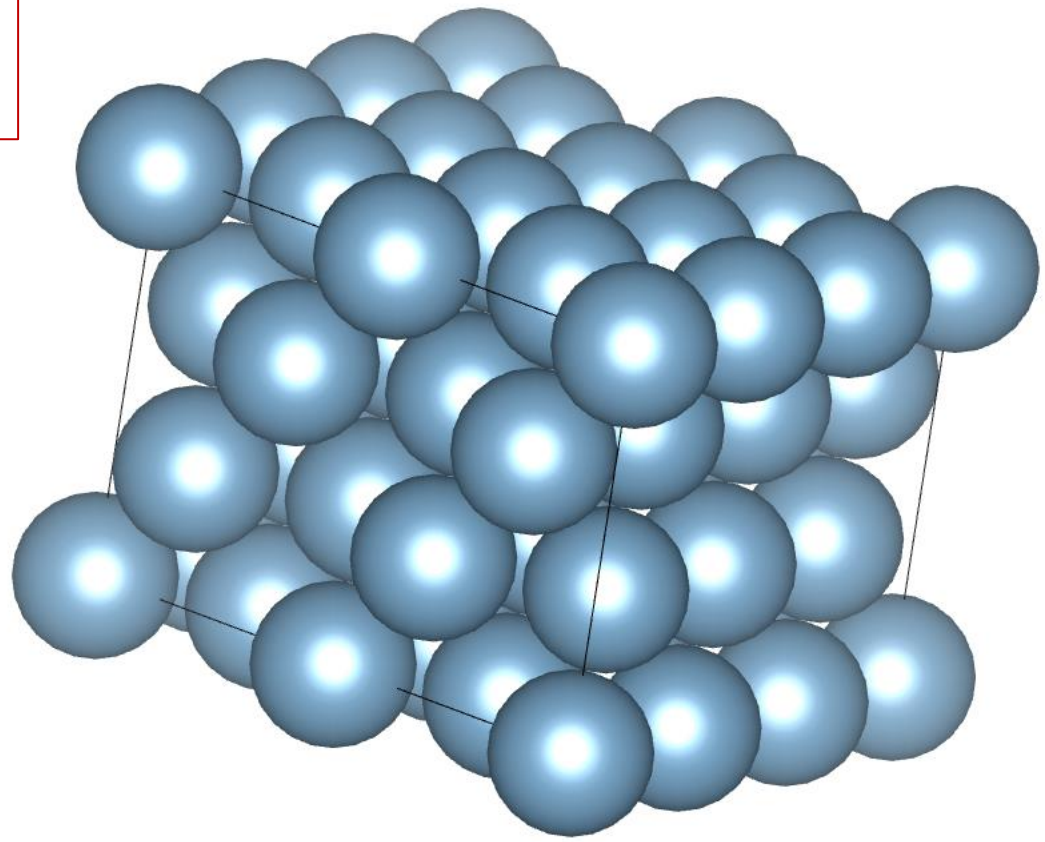
```
 23 Al  Al23        0.58333    0.25000    0.66667    1.000    0.000    1a         1
 24 Al  Al24        0.25000    0.25000    0.00000    1.000    0.000    1a         1
================================================================================

Number of polygons and unique vertices on isosurface = 0 (0)
46 atoms, 0 bonds, 0 polyhedra; CPU time = 0 ms
```

Output Summary Comment

POSCAR_fcc.vasp - VESTA

File Edit View Objects Utilities Help

Here is a FCC slab model with 18 atoms/layer and 4 layers




```
  23 Al  Al23        0.58333    0.16667    0.66667    1.000    0.000    0  (  0 )
  24 Al  Al24        0.25000    0.16667    0.00000    1.000    0.000    0  (  0 )
================================================================================

Number of polygons and unique vertices on isosurface = 0 (0)
64 atoms, 0 bonds, 0 polyhedra; CPU time = 1 ms
```

add_vacuum.py — [redacted]

File Edit View Selection Find Packages Help

write_poscars.py | add_vacuum.py

```python
import ase
import ase.io.vasp
import numpy as np

def add_vacuum(vac):
    slab = ase.io.vasp.read_vasp("POSCAR")
    slab.center(vacuum=vac, axis=2)
    ase.io.vasp.write_vasp('POSCAR',slab,direct=True,sort=True)


add_vacuum(10)

```

Easily add vacuum to surface slab using ASE

add_vacuum.py 11:15 CRLF UTF-8 Python GitHub Git (0)