

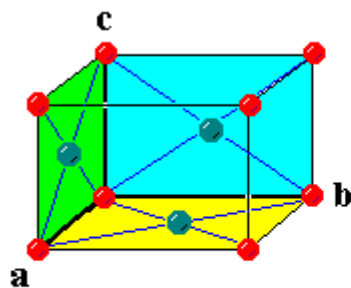
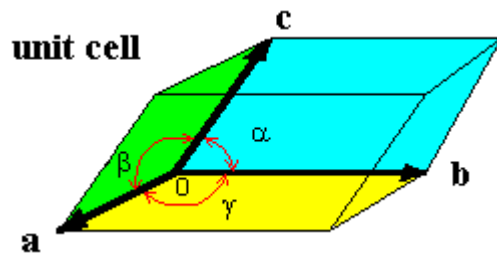
Multislice Assistance

This application software assists to make an input data file for the multislice program by Dr. Earl J. Kirkland.

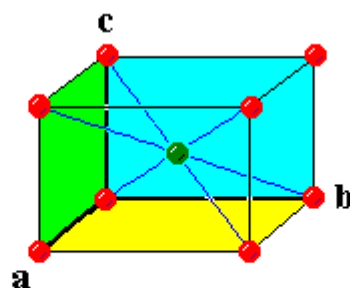
Regarding the unit cell, the meaning is as follows in this application;

- a) A minimum repeating structure which can make a crystal.
- b) Same type atoms at eight (8) corners of the structure.

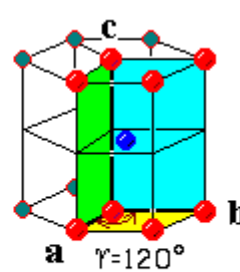
\$ 1. Unit cell



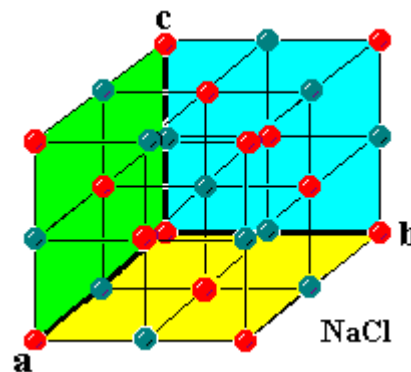
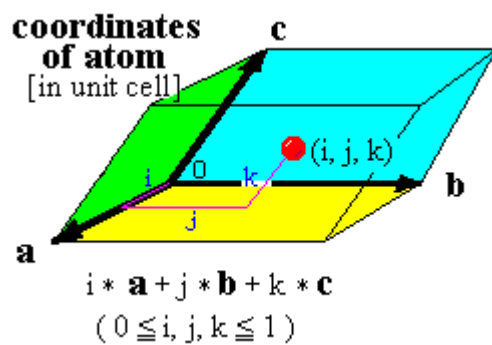
face centered



body centered



**hexagonal
close packed**



\$2. Input parameters

Set crystal parameters

Lattice constants

a axis (Ang.) b axis (Ang.) c axis (Ang.)

3.905 3.905 3.905

alpha (deg.) beta (deg.) gamma (deg.)

90 90 90

Coordinates and name of atom in a unit cell

a coordinate b coordinate c coordinate

0 0 0

Atom 0 Color pictured

Sr [Color] Next

Crystal direction perpendicular to sliced planes

u v w

1 0 0

Cancel OK

1. Crystal parameters;

- * a axis value of a unit cell in Angstrom
- * b axis value of a unit cell in Angstrom
- * c axis value of a unit cell in Angstrom
- * Angle (α) between b axis and c axis in degree
- * Angle (β) between c axis and a axis in degree
- * Angle (γ) between a axis and b axis in degree

2. Crystal direction $\langle u \ v \ w \rangle$ perpendicular to the planes to be sliced

3. Coordinates (i, j, k) of atom “i” with name;

1) Atom 0: The (0, 0, 0) atom making the unit cell.

Note: It is not necessary to input the coordinates (0, 0, 0).

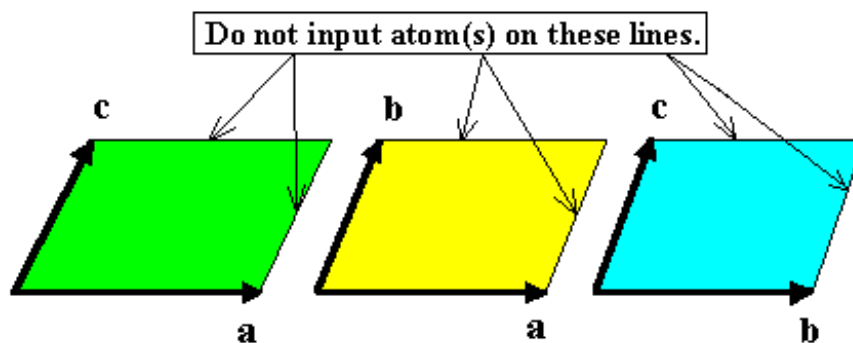
2) Atom “x” (x = 1, 2, 3, ...) : Atoms on the face planes of the unit cell, and in the unit cell.

Coordinates of the atom “x” must be reduced coordinates in the unit cell.

***** IMPORTANT *****

In the case of atoms on the face planes of the unit cell, ONLY atoms on the a-b face plane, b-c face plane, and c-a face plane must be inputted.

Refer to the following picture.



Atoms on the face plane of unit cell

After inputting “coordinates (i, j, k) of the atom x, its name, and its color displayed,” press <Next> button.

Repeat the procedure sequentially, until inputting the “last” atom data.

When all necessary parameters are inputted, press <OK> button instead of <Next> button.

NOTE :

If you want to use the previous inputted data for the different <u v w> value, just press <OK> button after inputting the different <u v w> value. In this case, do not press <Next> button, and do not change parameters other than the <u v w> value.

\$3. An example of input parameters

Specimen is strontium titanate (SrTiO₃).

Sliced planes are perpendicular planes to the <100> axis.

* Input 3.905 (Angstroms) as “a axis” value.

* Input 3.905 (Angstroms) as “b axis” value.

* Input 3.905 (Angstroms) as “c axis” value.

* Input 90 (degrees) as “ α ” value.

* Input 90 (degrees) as “ β ” value.

* Input 90 (degrees) as “ γ ” value.

* Input 1 as “u” value.

* Input 0 as “v” value.

* Input 0 as “w” value.

* Select Sr, and black color.

Press <Next> button, then

* Select O, and input coordinates (0.5, 0.5, 0), and select blue color.

Press <Next> button, then

* Select O, and input coordinates (0.5, 0, 0.5), and select blue color.

Press <Next> button, then

* Select O, and input coordinates (0, 0.5, 0.5), and select blue color.

Press <Next> button, then

* Select Ti, and input coordinates (0.5, 0.5, 0.5), and select red color.

Then, press <OK> button instead of <Next> button.

\$4. Display of atoms on sliced layers

When pressing <OK> button, the atoms on each sliced plane appear on the screen.

First sliced plane: left top picture

Second sliced plane: left bottom picture

Third sliced plane: right top picture

Fourth sliced plane: right bottom picture

If existing more than 4 sliced planes, press <Next> button. In this case, you can get 5th sliced plane (left top), 6th sliced plane (left bottom), and so on.

\$5. Saving the data

1) Displayed pictures on the screen can be saved as a bitmap.

2) Furthermore, the reduced coordinates of atoms (in the unit cell) on all sliced layers and the inputted crystal data can be saved as a text file.

\$6. Reading the crystal data

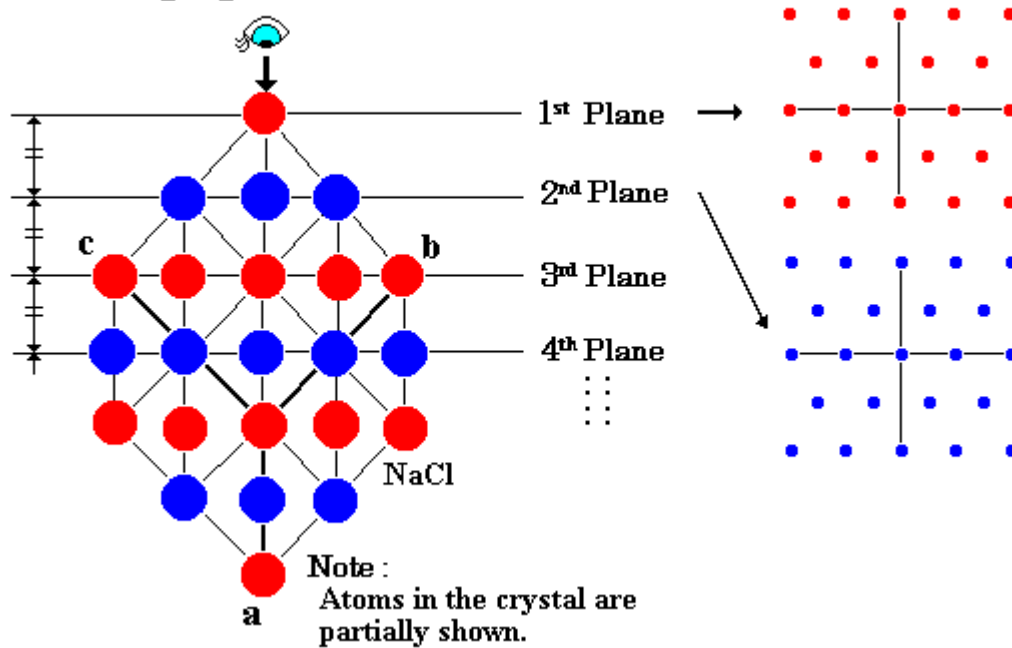
1) The saved crystal data file can be read and applied to the sliced planes displayed.

2) The attached file, SrTiO₃.TXT, is an example file of SrTiO₃ crystal which can be read by this application, and you can get pictures of sliced planes of the crystal on the screen if you read the file.

\$7. Example

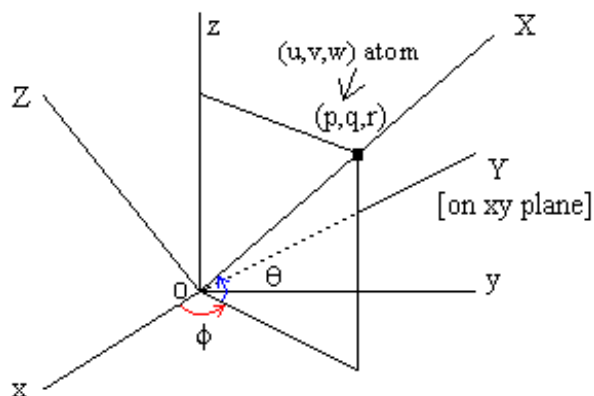
An example of sliced planes by “Multislice Assistance” is as follows;

Planes perpendicular to $\langle 1\ 1\ 1 \rangle$



\$8. Supplements

8.1) Coordinates Rotation



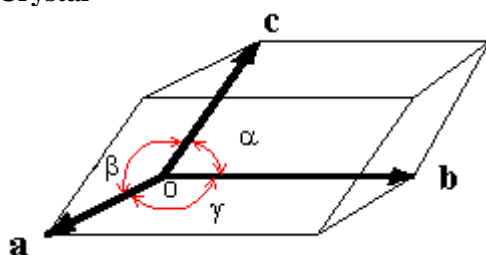
NOTE: $-90 \text{ deg} \leq \phi \leq +90 \text{ deg}$
 $-90 \text{ deg} \leq \theta \leq +90 \text{ deg}$
 $0 \leq p$

$$X = +\cos(\theta) \cdot \cos(\phi) \cdot x + \cos(\theta) \cdot \sin(\phi) \cdot y + \sin(\theta) \cdot z$$

$$Y = -\sin(\phi) \cdot x + \cos(\phi) \cdot y$$

$$Z = -\sin(\theta) \cdot \cos(\phi) \cdot x - \sin(\theta) \cdot \sin(\phi) \cdot y + \cos(\theta) \cdot z$$

8.2) Crystal



NOTE: $0 \text{ deg} < \alpha \leq 90 \text{ deg}$
 $0 \text{ deg} < \beta \leq 90 \text{ deg}$
 $0 \text{ deg} < \gamma < 180 \text{ deg}$

An atom position (p, q, r), including atoms in the cell and atoms on the faces

$$p = u \cdot a$$

$$q = v \cdot b$$

$$r = w \cdot c$$

where

u, v, and w are real numerical value, and $0 \leq u$.

Set the point O to the origin of the xyz coordinates, and set **a** axis to the x axis, and set **b** axis on the xy plane.

Then point (p, q, r) is described as follows at xyz coordinates;

$$p = u \cdot |a| + v \cdot |b| \cdot \cos(\gamma) + w \cdot |c| \cdot \cos(\beta)$$

$$q = v \cdot |b| \cdot \sin(\gamma) + w \cdot |c| \cdot \frac{\cos(\alpha) - \cos(\beta) \cdot \cos(\gamma)}{\sin(\gamma)}$$

$$r = w \cdot |c| \cdot \frac{\sqrt{1 - \cos(\alpha) \cdot \cos(\alpha) - \cos(\beta) \cdot \cos(\beta) - \cos(\gamma) \cdot \cos(\gamma) + 2 \cdot \cos(\alpha) \cdot \cos(\beta) \cdot \cos(\gamma)}}{\sin(\gamma)}$$

8.3) ϕ and θ

$$\cos(\phi) = p / \sqrt{p^2 + q^2} \quad ; \text{ except } p=q=0$$

$$\sin(\phi) = q / \sqrt{p^2 + q^2} \quad ; \text{ except } p=q=0$$

$$\cos(\theta) = \sqrt{p^2 + q^2} / \sqrt{p^2 + q^2 + r^2} \quad ; \text{ except } p=q=r=0$$

$$\sin(\theta) = r / \sqrt{p^2 + q^2 + r^2} \quad ; \text{ except } p=q=r=0$$

where

$$p = u \cdot |a| + v \cdot |b| \cdot \cos(\gamma) + w \cdot |c| \cdot \cos(\beta)$$

$$q = v \cdot |b| \cdot \sin(\gamma) + w \cdot |c| \cdot \frac{\cos(\alpha) - \cos(\beta) \cdot \cos(\gamma)}{\sin(\gamma)}$$

$$r = w \cdot |c| \cdot \frac{\sqrt{1 - \cos(\alpha) \cdot \cos(\alpha) - \cos(\beta) \cdot \cos(\beta) - \cos(\gamma) \cdot \cos(\gamma) + 2 \cdot \cos(\alpha) \cdot \cos(\beta) \cdot \cos(\gamma)}}{\sin(\gamma)}$$

8.4) Input parameters

(1) Unit cell parameters

* $|a|, |b|, |c|$ --- Angstrom unit

* α, β, γ ----- degree unit

* "AtomName[0]" denotes an atom name making the unit cell

(2) Atom positions in the unit cell / on the unit cell faces, and their names

* Atom position (E[i], F[i], G[i]) ----- reduced coordinates of the unit cell

* Atom name "AtomName[i]" at (E[i], F[i], G[i]) position

NOTE: $0 \leq E, F, G \leq 1$

E[0] = F[0] = G[0] = 0 denotes an atom making the unit cell.

(3) Crystal direction $\langle u, v, w \rangle$ which is perpendicular to the planes to be sliced

* u, v, w ----- integers

NOTE: $\text{abs}(u) + \text{abs}(v) + \text{abs}(w) = 0$ is not allowed.

8.5) Calculation

(1) Conversion of "u"

If $u < 0$, then convert u, v, w as follows;

"new" u = -u

"new" v = -v

"new" w = -w

(2) $\cos(\phi)$, $\sin(\phi)$, $\cos(\theta)$, and $\sin(\theta)$

$$\begin{aligned}\cos(\phi) &= p / \sqrt{p^2 + q^2} && ; \text{ except } p=q=0 \\ \sin(\phi) &= q / \sqrt{p^2 + q^2} && ; \text{ except } p=q=0 \\ \cos(\theta) &= \sqrt{p^2 + q^2} / \sqrt{p^2 + q^2 + r^2} && ; \text{ except } p=q=r=0 \\ \sin(\theta) &= r / \sqrt{p^2 + q^2 + r^2} && ; \text{ except } p=q=r=0\end{aligned}$$

where

$$p = u|a| + v|b|\cos(\gamma) + w|c|\cos(\beta)$$

$$q = v|b|\sin(\gamma) + w|c|\text{abs}\{\cos(\alpha) - \cos(\beta)\cos(\gamma)\}/\sin(\gamma)$$

$$r = w|c|\sqrt{\text{abs}\{1 - \cos(\alpha)\cos(\alpha) - \cos(\beta)\cos(\beta) - \cos(\gamma)\cos(\gamma) + 2\cos(\alpha)\cos(\beta)\cos(\gamma)\}}/\sin(\gamma)$$

NOTE: Use “new” u, v, and w.

(3) Atom positions

Actual “m-th” atom position (e[m], f[m], g[m]) and its name AtomName[m]:

$$e[m] = (E[m]+i)|a| + (F[m]+j)|b|\cos(\gamma) + (G[m]+k)|c|\cos(\beta)$$

$$f[m] = (F[m]+j)|b|\sin(\gamma) + (G[m]+k)|c|\text{abs}\{\cos(\alpha) - \cos(\beta)\cos(\gamma)\}/\sin(\gamma)$$

$$g[m] = (G[m]+k)|c|\sqrt{\text{abs}\{1 - \cos(\alpha)\cos(\alpha) - \cos(\beta)\cos(\beta) - \cos(\gamma)\cos(\gamma) + 2\cos(\alpha)\cos(\beta)\cos(\gamma)\}}/\sin(\gamma)$$

where E[m], F[m], G[m] denote “m-th” atom position (E[m], F[m], G[m]), which has been inputted in the section 8.4) - (2), at xyz coordinates.

i, j, k denote all integers ($-\infty \sim +\infty$).

m = 0, 1, 2, (m = 0 denotes an atom making the unit cell.)

(4) “m-th” atom position at the rotated (X, Y, Z) coordinates

$$X[m] = +\cos(\theta)\cos(\phi)e[m] + \cos(\theta)\sin(\phi)f[m] + \sin(\theta)g[m]$$

$$Y[m] = -\sin(\phi)e[m] + \cos(\phi)f[m]$$

$$Z[m] = -\sin(\theta)\cos(\phi)e[m] - \sin(\theta)\sin(\phi)f[m] + \cos(\theta)g[m]$$

by assigning the above e[m], f[m], g[m], $\cos(\phi)$, $\sin(\phi)$, $\cos(\theta)$, and $\sin(\theta)$ --- i.e. (3) and (2).

(5) Display of atom positions

Show each atom position (Y[i], Z[i]), under the condition of “X[...] = constant,” on the PC screen.

NOTE:

* Colored position circle should correspond to the kind of atom assigned.

* If $0 < u$, show atoms from $-X$ to $+X$ direction.

Else, show atoms from $+X$ to $-X$ direction.

* A rectangle for the “super cell” should be displayed in the “atom pattern” on the PC screen.