

Crystal Builder

Cleave plane

Fe (1 1 0) surface

V7.000

X-Ability Co,. Ltd.

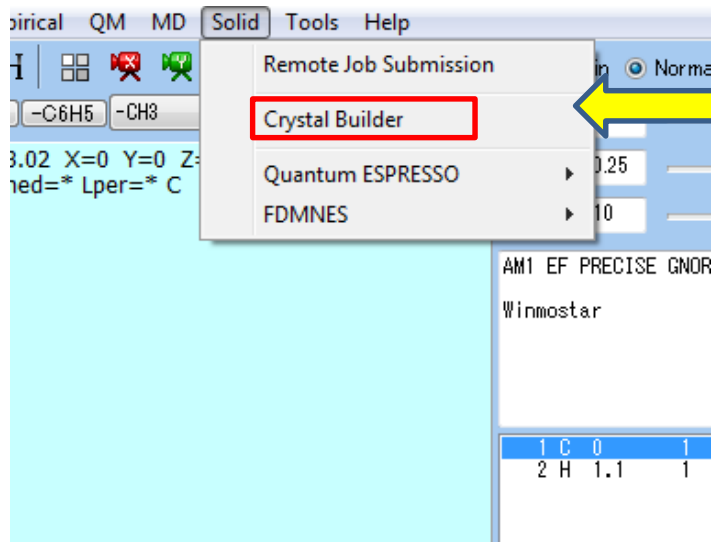
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2016/11/01

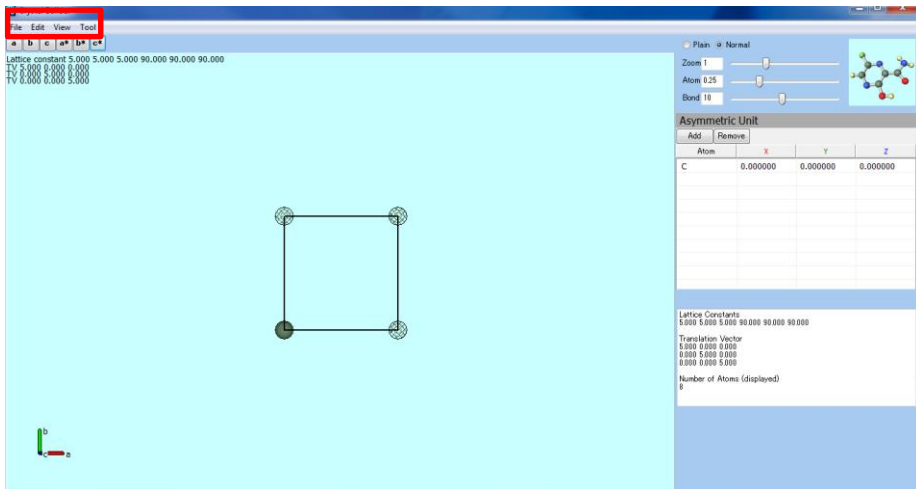
Contents

- I. Define a unit cell
- II. Cleave along (1 1 0) surface
- III. Convert to a tetragonal unit cell

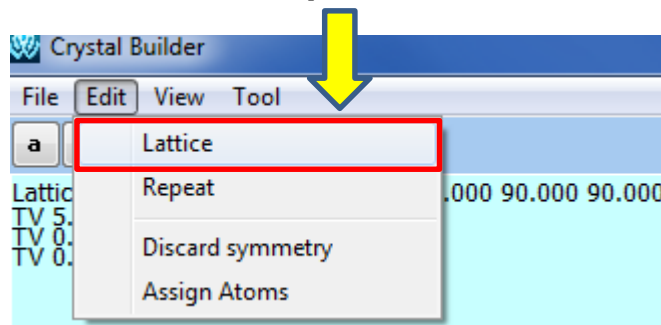
I. Define a unit cell



1. Click **Solid | Crystal Builder**.

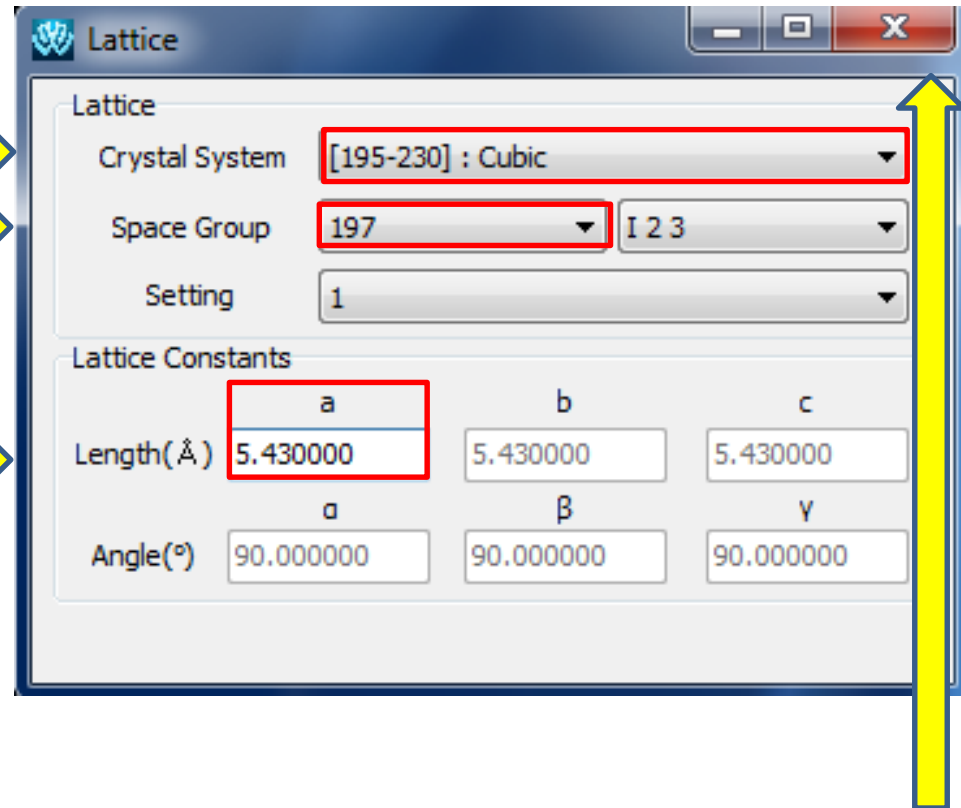


2. Click **Edit | Lattice**.



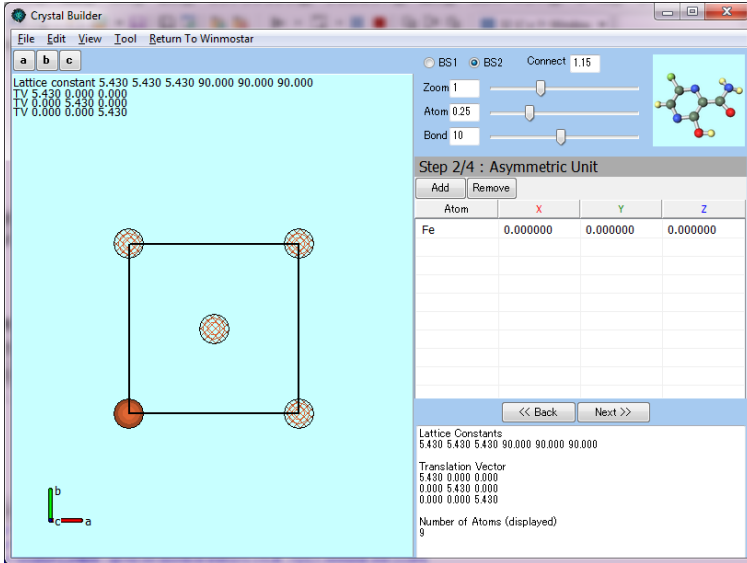
I. Define a unit cell

1. Set **Crystal System** to **Cubic**.
2. Set **Space Group** to **197**.
3. Set **a** to **5.43** and push the Enter key.

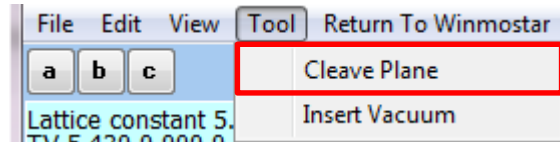
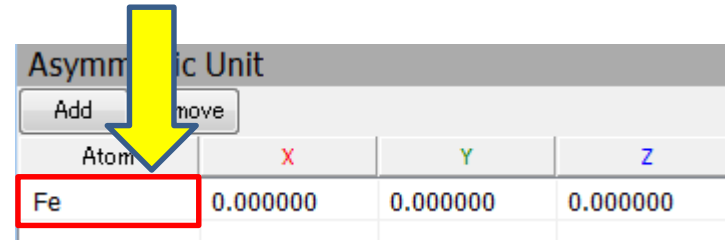


4. Click here to close.

I. Define a unit cell

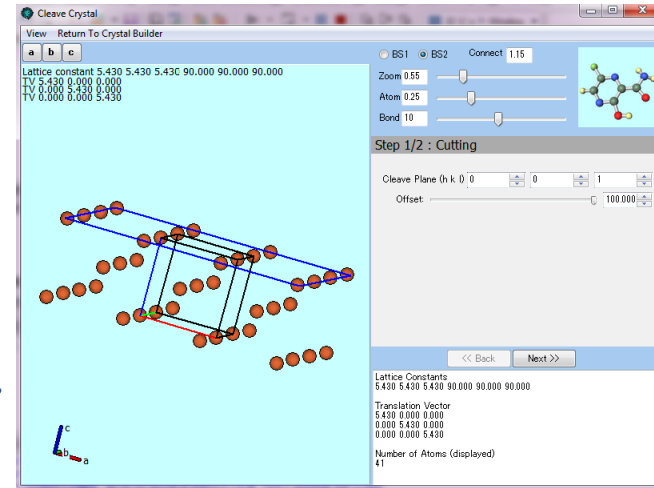


1. Input Fe.

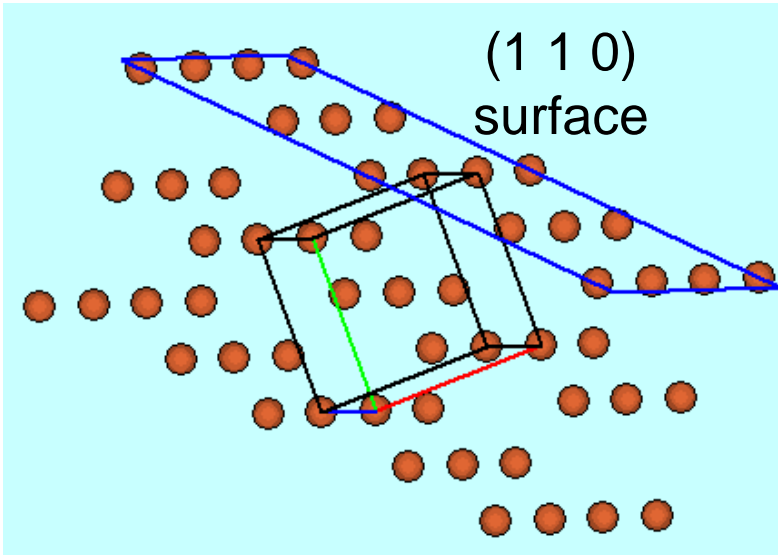
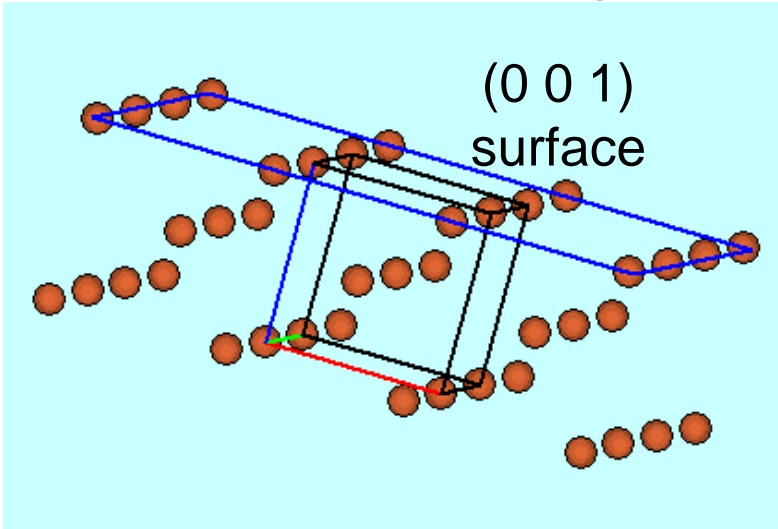


2. Click.

Cleave Plane mode will start.



II. Cleave along (1 1 0) surface



1. Enter **1 1 0**.

Step 1/2 : Cutting

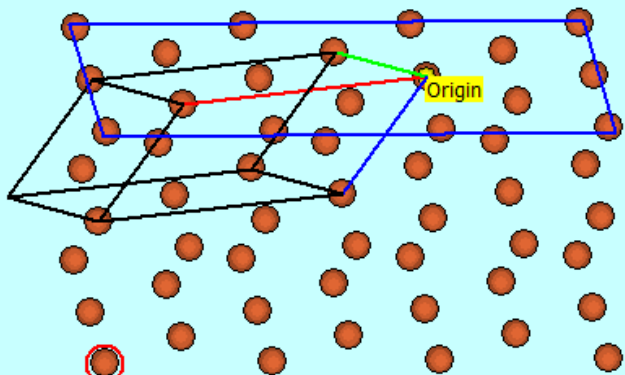
Cleave Plane (h k l)

Offset:

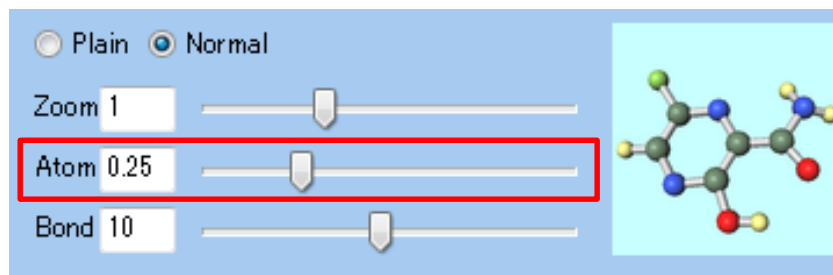
2. Click [Next >>].

<< Back

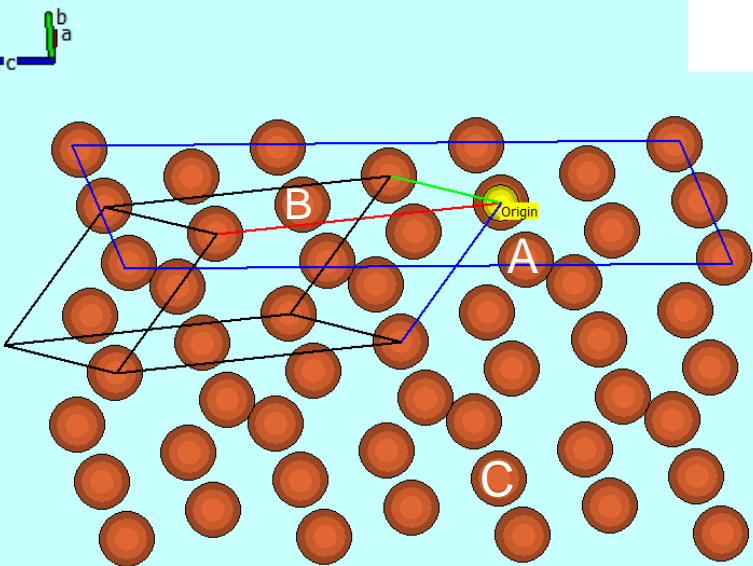
III. Convert to a tetragonal unit cell



1. Adjust the camera angle like the left.



2. The size of atoms can be changed. (if you need)



Step 2/2 : Transform Unit Cell

Origin	5.430000 5.430000 0.000000	Set
LatticeVector A	8.145000 2.715000 8.145000	Set
LatticeVector B	2.715000 8.145000 2.715000	Set
LatticeVector C	2.715000 2.715000 2.715000	Set

Execute

3. Click atom A, and click **Set**.
4. Click atom B, and click **Set**.
5. Click atom C, and click **Set**.

* The white alphabets "A, B, C" is just for explanation here (These will not appear in the graphics.)

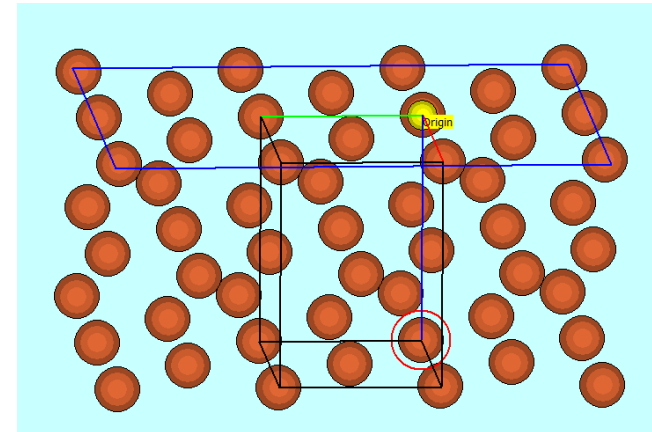
III. Convert to a tetragonal unit cell

1. If your system is the same as the right, click **Execute**.

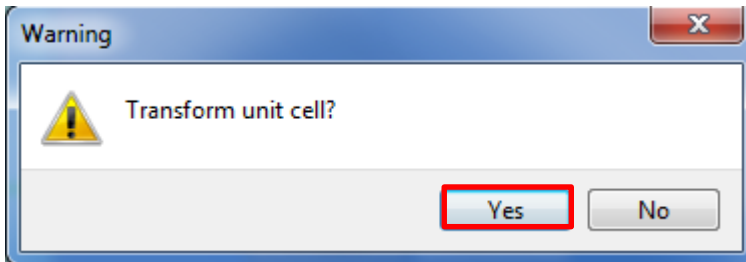
Step 2/2 : Transform Unit Cell

Origin	5.430000 5.430000 0.000000	Set
LatticeVector A	10.860000 0.000000 0.000000	Set
LatticeVector B	5.430000 5.430000 5.430000	Set
LatticeVector C	0.000000 0.000000 0.000000	Set

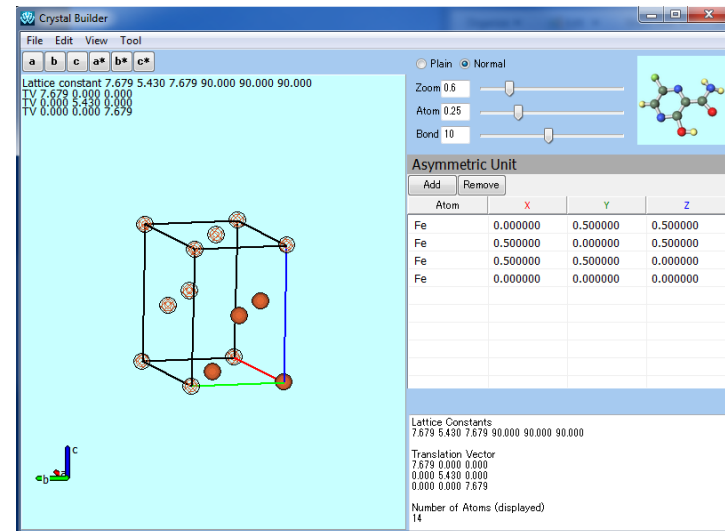
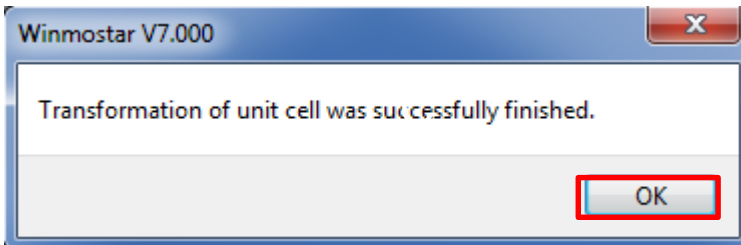
Execute



2. Click **Yes**.



3. Click **OK**.



After converting, Cleave Plane mode will end.