

# Crystal Builder

Cleave plane

Fe (1 1 0) surface

V8.007

X-Ability Co., Ltd.

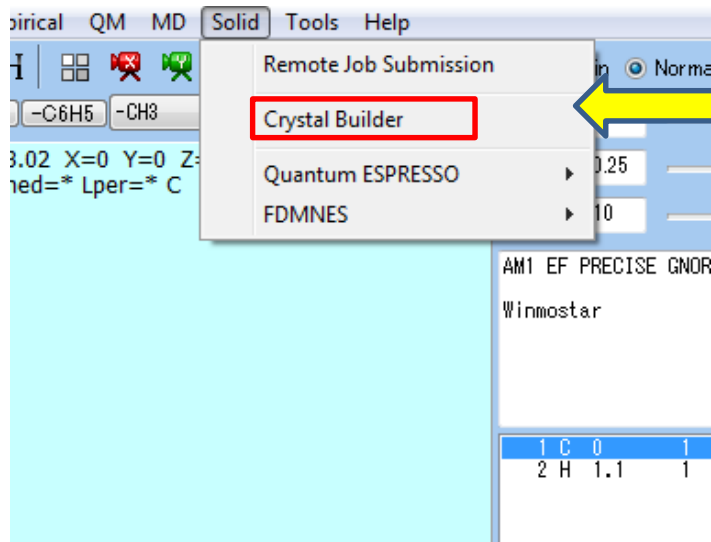
[question@winmostar.com](mailto:question@winmostar.com)

2018/01/18

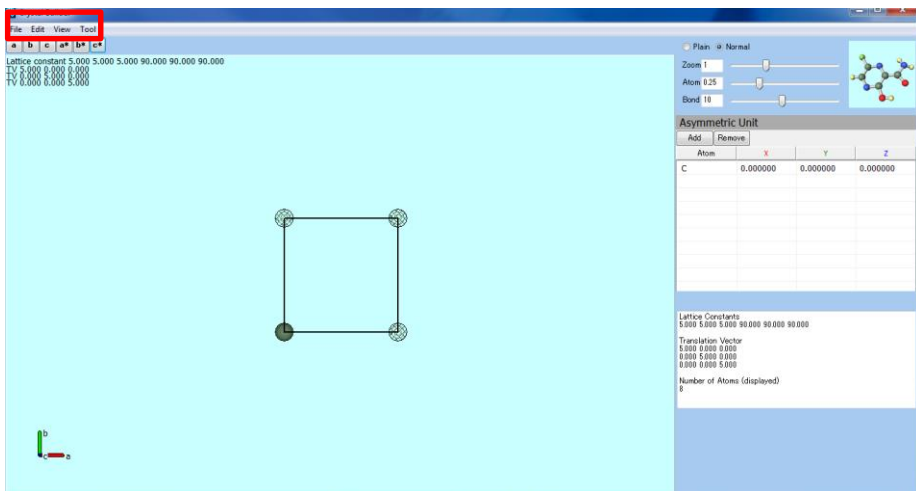
# Contents

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

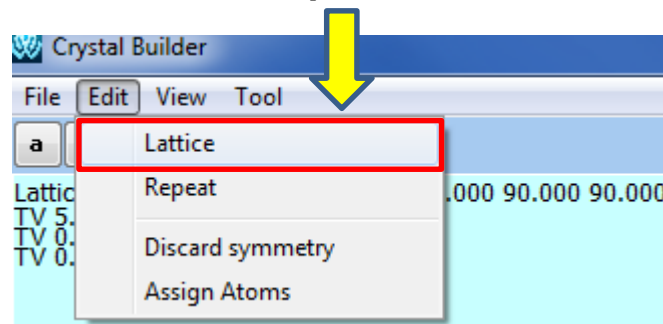
# I. Define a unit cell






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

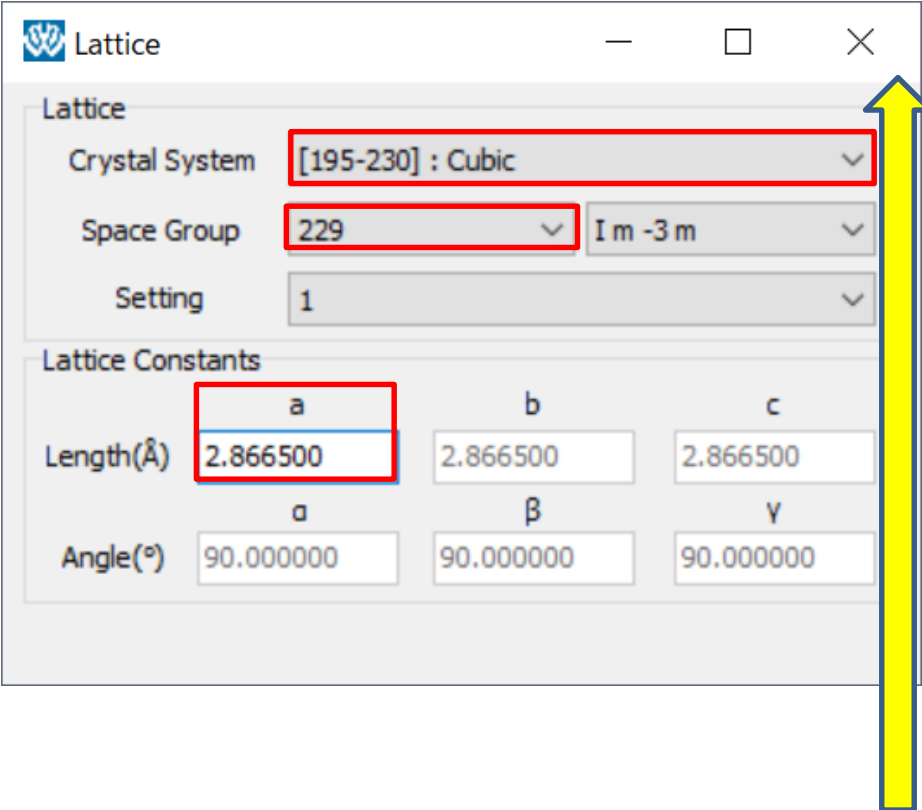


2. Click **Edit | Lattice**.



# I. Define a unit cell

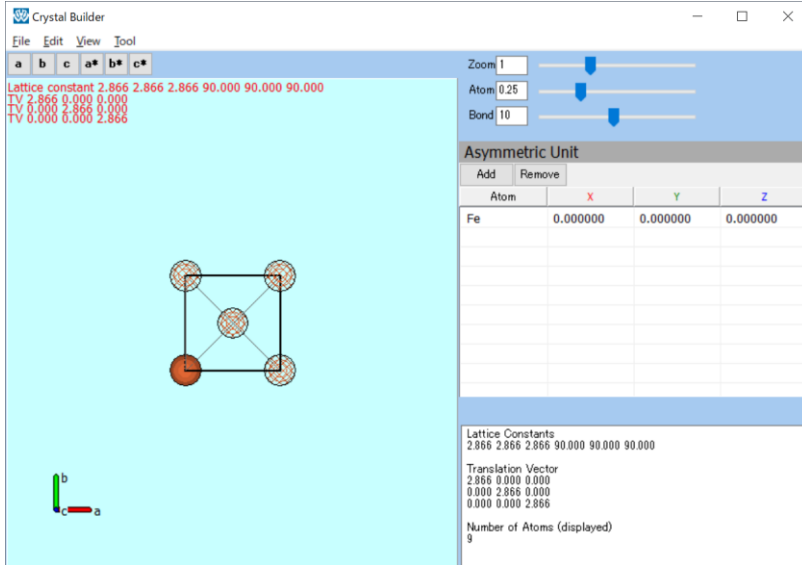
1. Set **Crystal System** to **Cubic**. 
2. Set **Space Group** to **229**. 
3. Set **a** to **2.8665** and push the Enter key. 



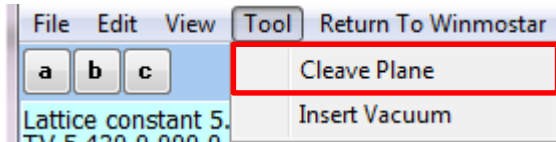
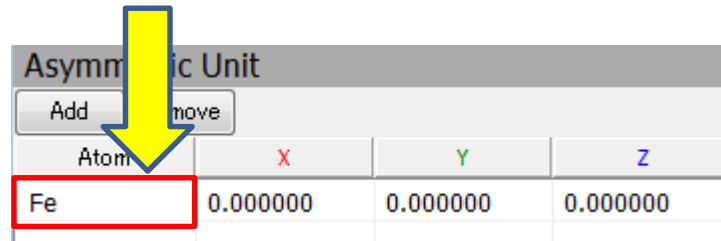
| Lattice           |                   |           |           |
|-------------------|-------------------|-----------|-----------|
| Crystal System    | [195-230] : Cubic |           |           |
| Space Group       | 229               | I m -3 m  |           |
| Setting           | 1                 |           |           |
| Lattice Constants |                   |           |           |
|                   | a                 | b         | c         |
| Length(Å)         | 2.866500          | 2.866500  | 2.866500  |
|                   | $\alpha$          | $\beta$   | $\gamma$  |
| Angle(°)          | 90.000000         | 90.000000 | 90.000000 |

4. Click here to close.

# I. Define a unit cell

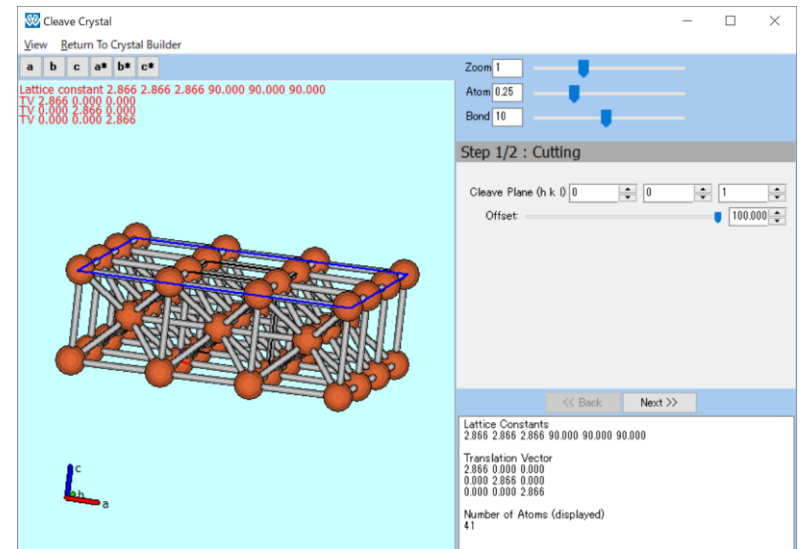


1. Input Fe.

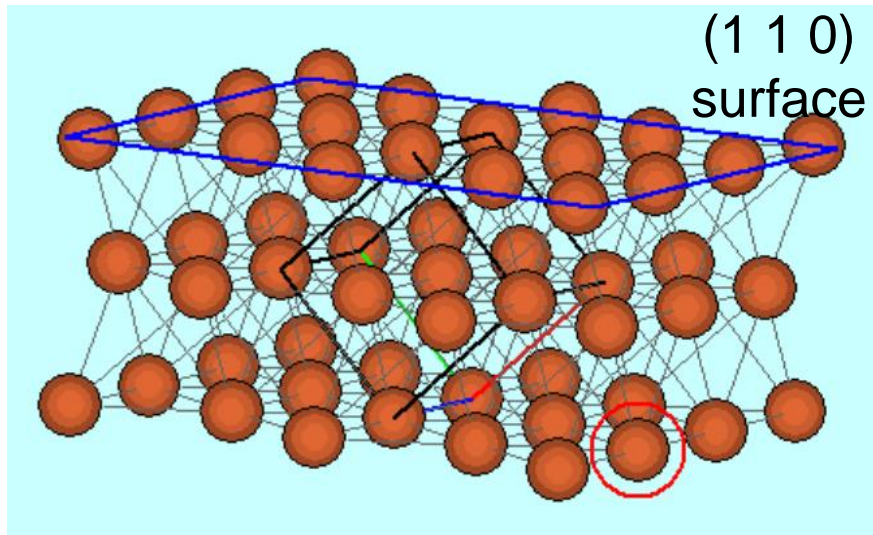
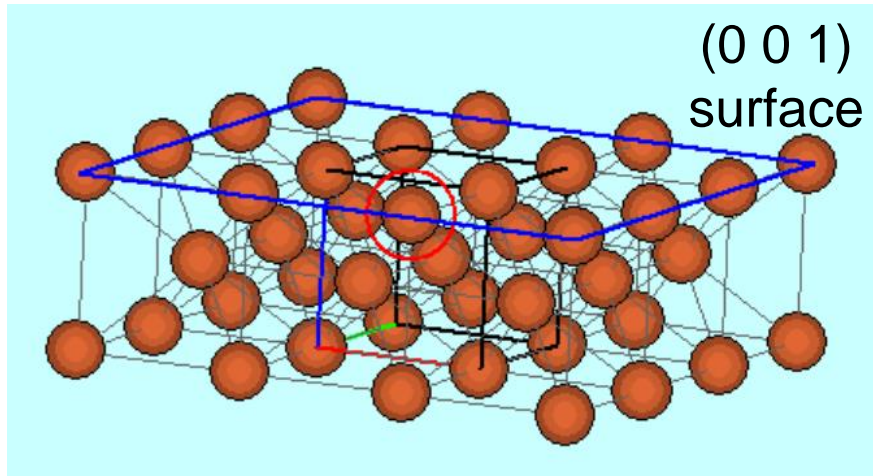


2. Click.

**Cleave Plane** mode will start.



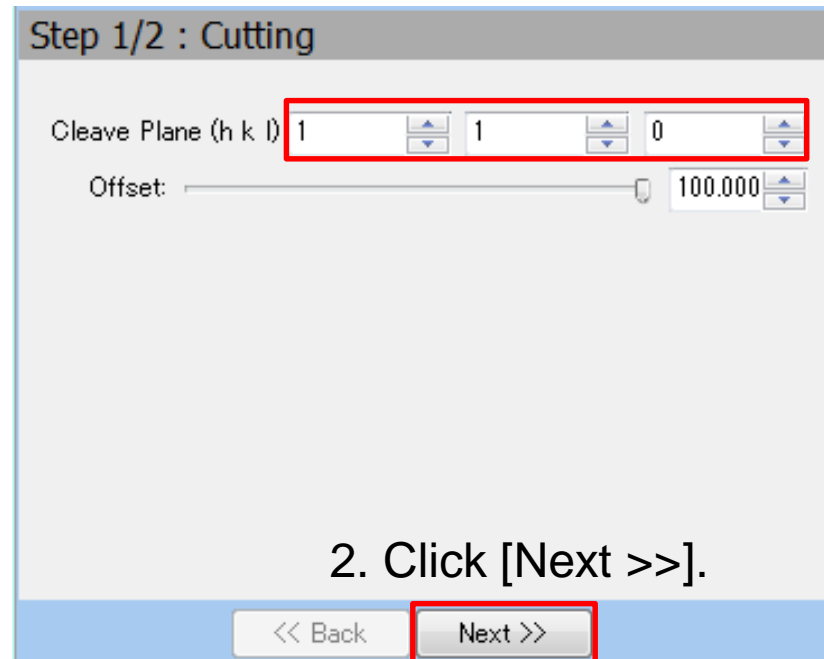
## II. Cleave along (1 1 0) surface



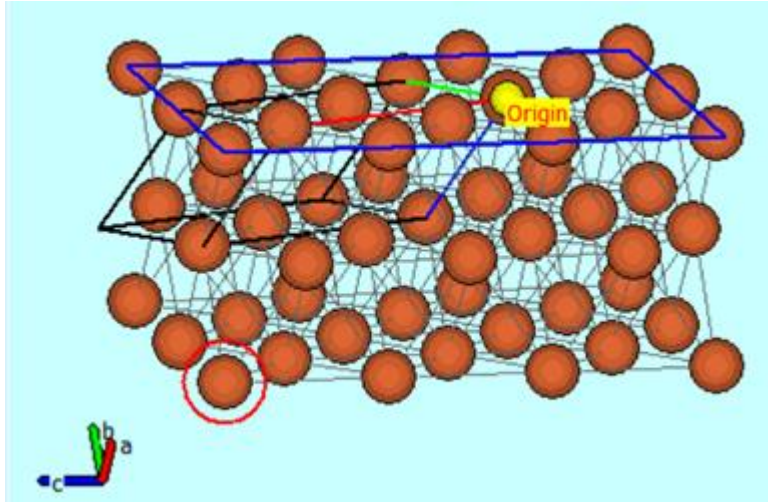
1. In order to change thickness of bonds, Adjust slider as below.



2. Enter **1 1 0**.



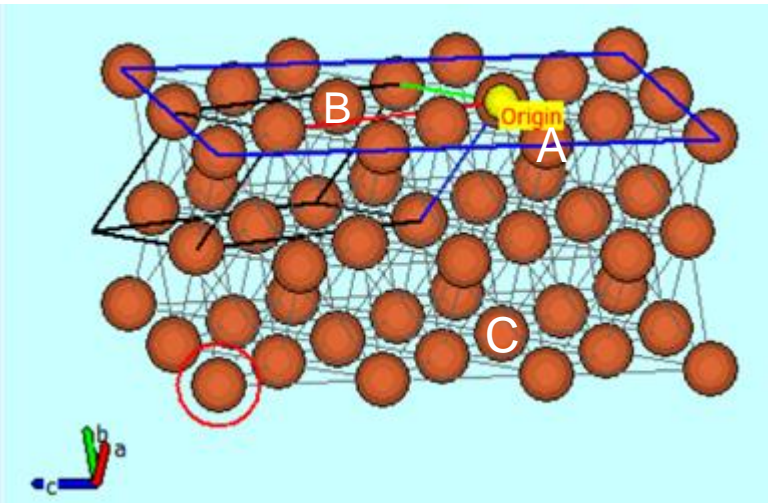
# III. Convert to a tetragonal unit cell



1. Adjust camera as left picture.

Note:

In the next step, The default selected cell will be converted to the tetragonal cell. For convenience of description, this series of processes will be explained using a picture from a single direction. In practical usage, users need to rotate camera and choose lattice points carefully.



Step 2/2 : Transform Unit Cell

|                 |                            |     |
|-----------------|----------------------------|-----|
| Origin          | 2.866500 2.866500 0.000000 | Set |
| LatticeVector A | 4.299750 1.433250 4.299750 | Set |
| LatticeVector B | 1.433250 4.299750 1.433250 | Set |
| LatticeVector C | 1.433250 1.433250 1.433250 | Set |

Execute

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

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



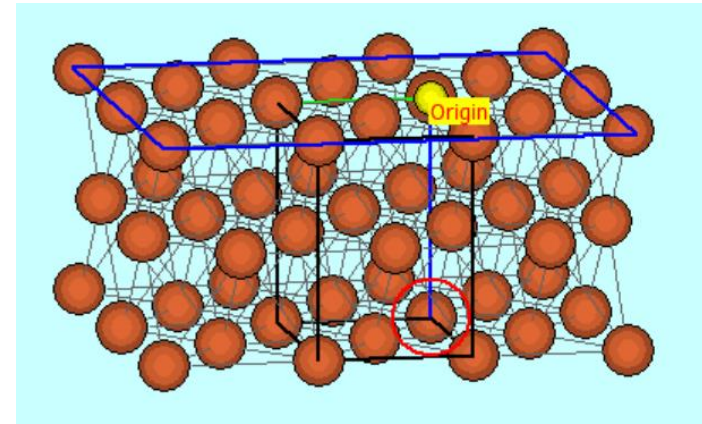
# III. Convert to a tetragonal unit cell

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

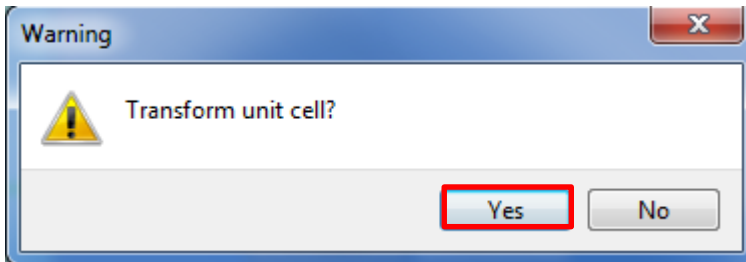
Step 2/2 : Transform Unit Cell

|                 |                             |     |
|-----------------|-----------------------------|-----|
| 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 |

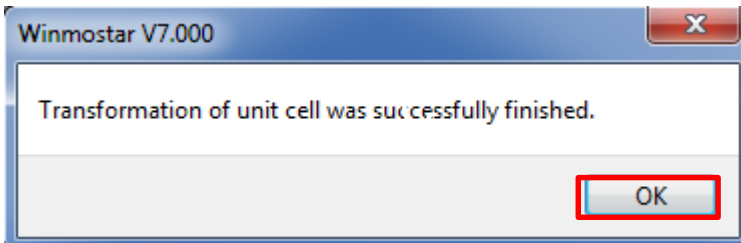
**Execute**



2. Click **Yes**.



3. Click **OK**.



| Atom | X        | Y        | Z        |
|------|----------|----------|----------|
| Fe   | 0.000000 | 0.500000 | 0.500000 |
| Fe   | 0.500000 | 0.000000 | 0.500000 |
| Fe   | 0.500000 | 0.500000 | 0.000000 |
| Fe   | 0.000000 | 0.000000 | 0.000000 |

Lattice Constants  
4.054 2.866 4.054 90.000 90.000 90.000

Translation Vector  
4.054 0.000 0.000  
0.000 2.866 0.000  
0.000 0.000 4.054

Number of Atoms (displayed)  
14

After converting, Cleave Plane mode will end.