X-Ability
クロスアビリティ

Crystal Builder

Basics

Ni-Al alloy

V7.000

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Contents

I. Define a unit cell

About NiAl crystal

Crystal system：Cubic
Space group： Pm-3m (221)
Lattice constants：a=2.88 Å
Asymmetric Unit：Ni(0.0 0.0 0.0), Al (0.5 0.5 0.5)

II. Create a supercell

III. Save

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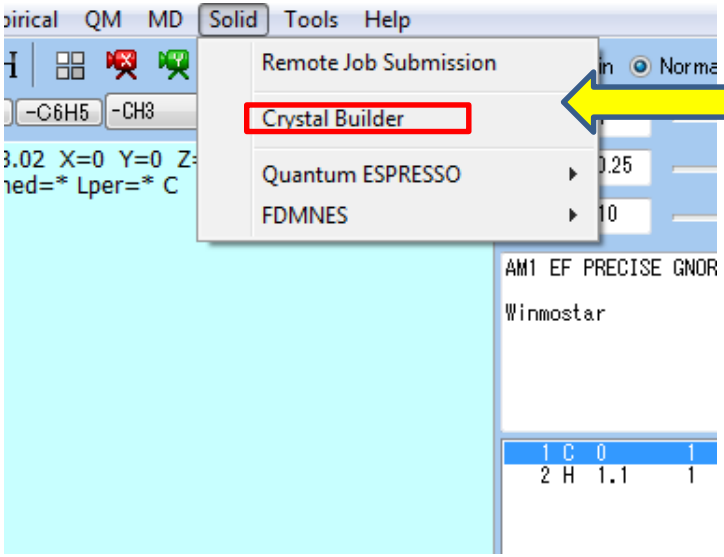
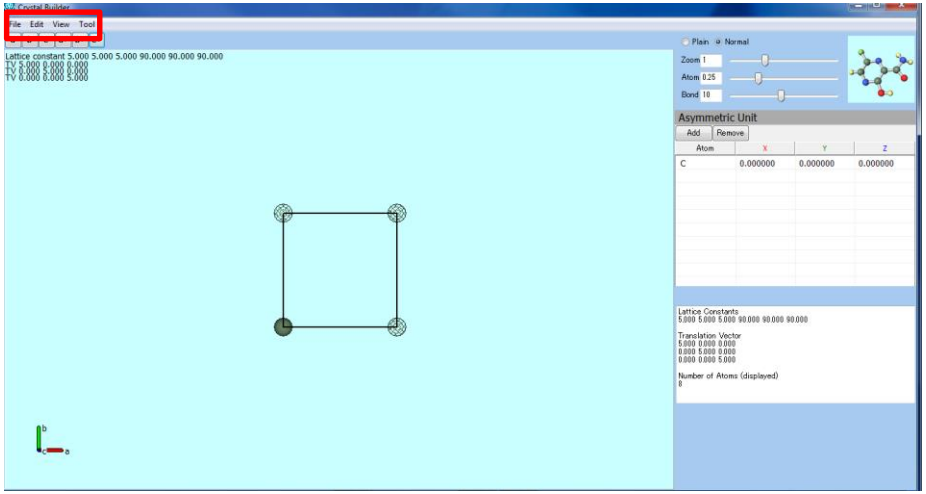
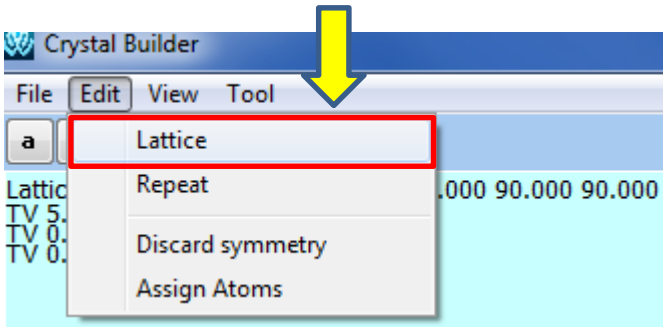
I. Define a unit cell



1. Click **Solid | Crystal builder**.



2. Click **Edit | Lattice**.



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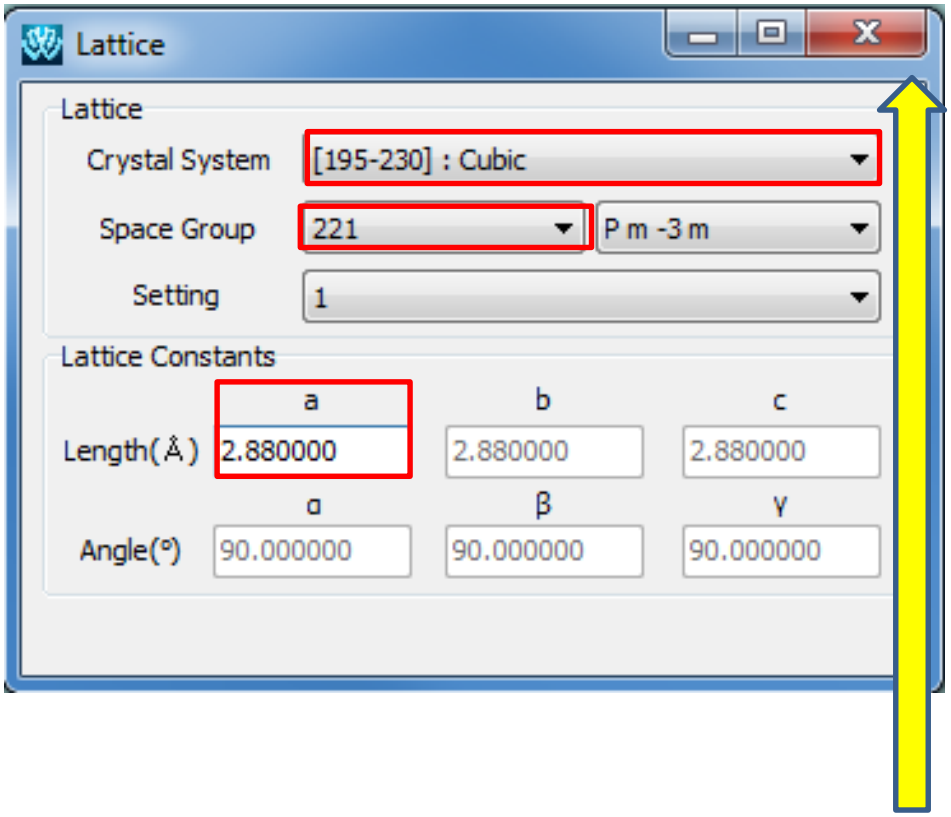
I. Define a unit cell

1. Set **Crystal System** to **Cubic**.
2. Set **Space Group** to **221**.

3. Set **a** to **2.88** and push the Enter key.



4. Click here to close.

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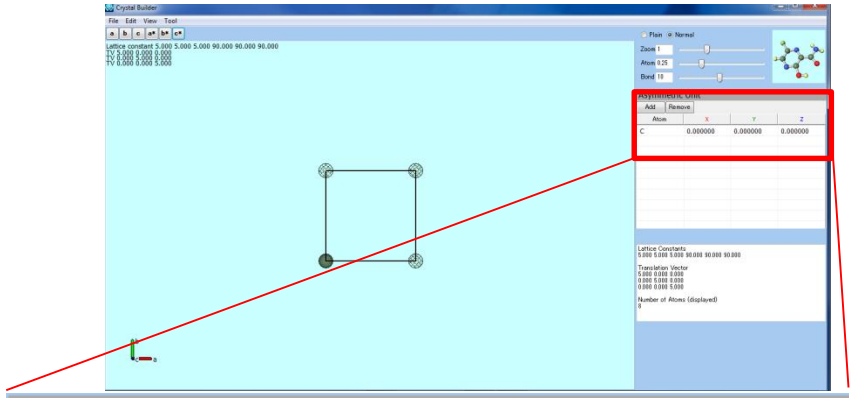
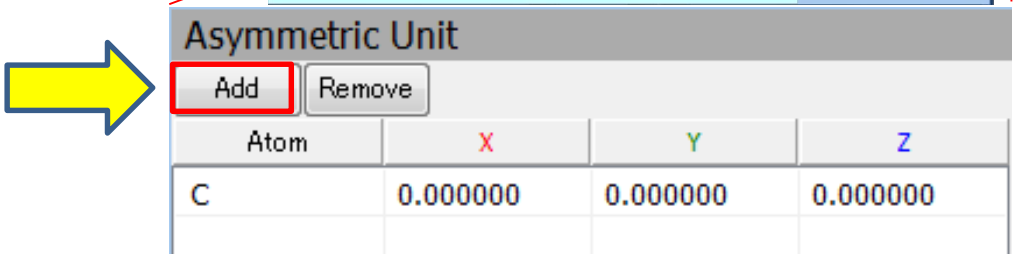
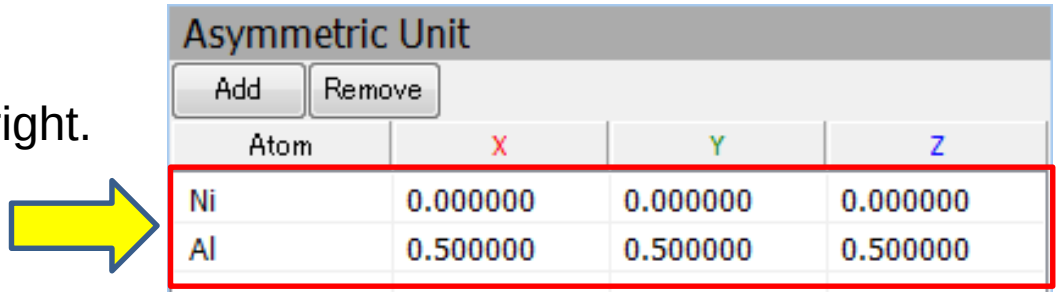
I. Define a unit cell



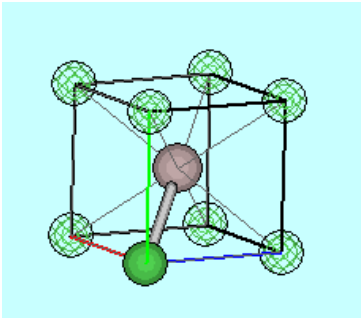
1. Click **Add**.



2. Change **Atom**, **X**, **Y** and **Z** (fractional coordinates) as the right.



3. The resulting structure will appear.



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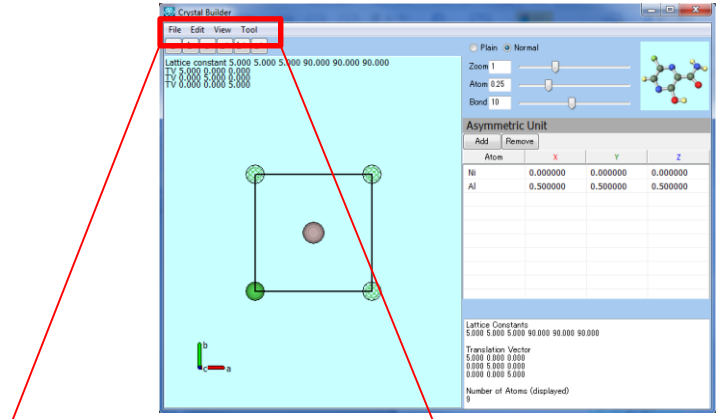
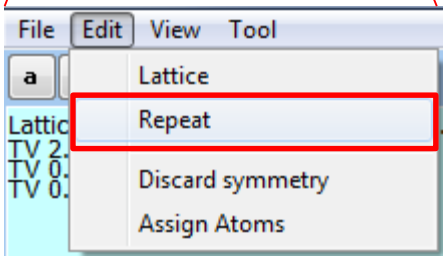
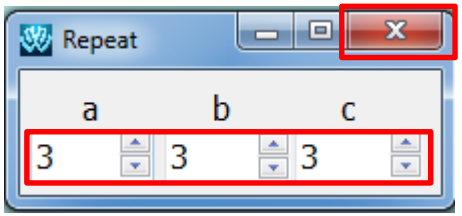
II. Create a supercell



1. Click **Edit | Repeat**.

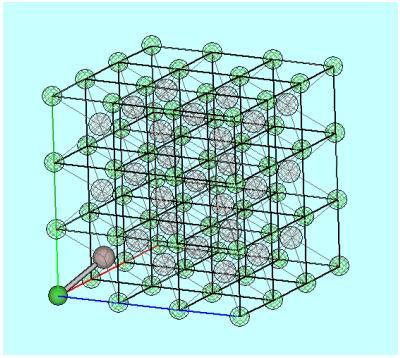


2. Input like this.



3. Click here to close.

4. 3x3x3 super cell will appear.



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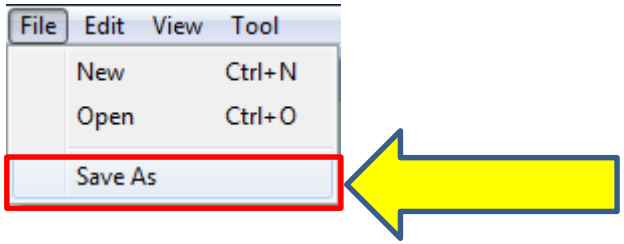
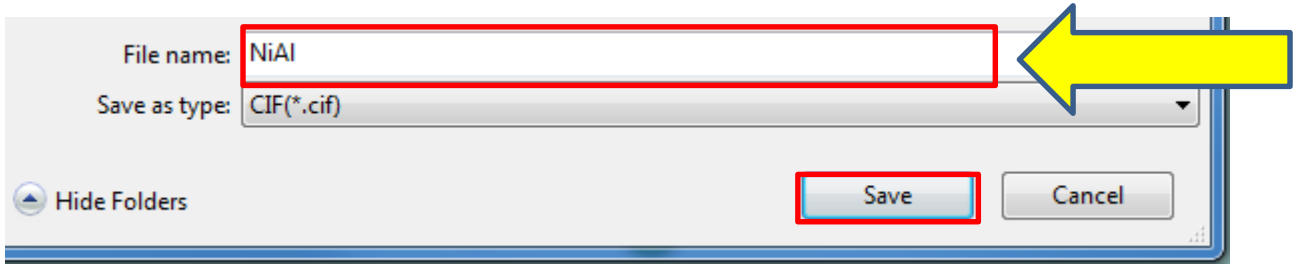
III. Save



1. Click **File | Save As**.



2. Enter a file name and click **Save**.