

Crystal Builder

Basics

Ni-Al alloy

V8.007

X-Ability Co., Ltd.

question@winmostar.com

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Contents

I. Define a unit cell

About NiAl crystal

Crystal system: Cubic

Space group : Pm-3m (221)

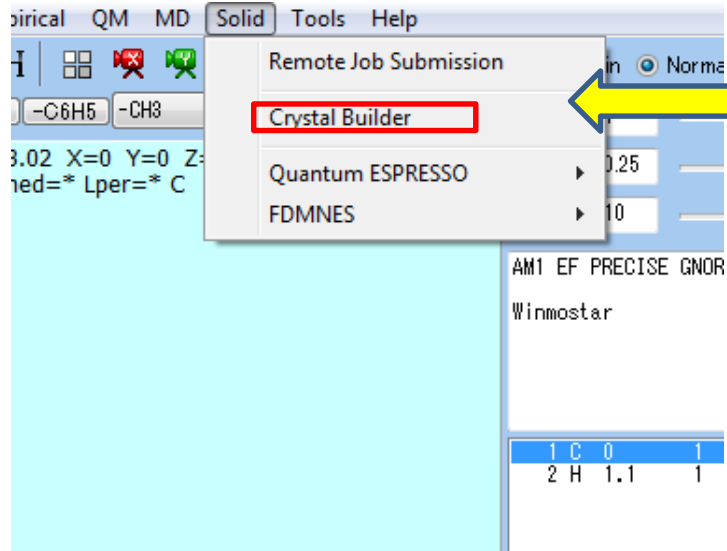
Lattice constants : $a=2.88 \text{ \AA}$

Asymmetric Unit: Ni(0.0 0.0 0.0), Al (0.5 0.5 0.5)

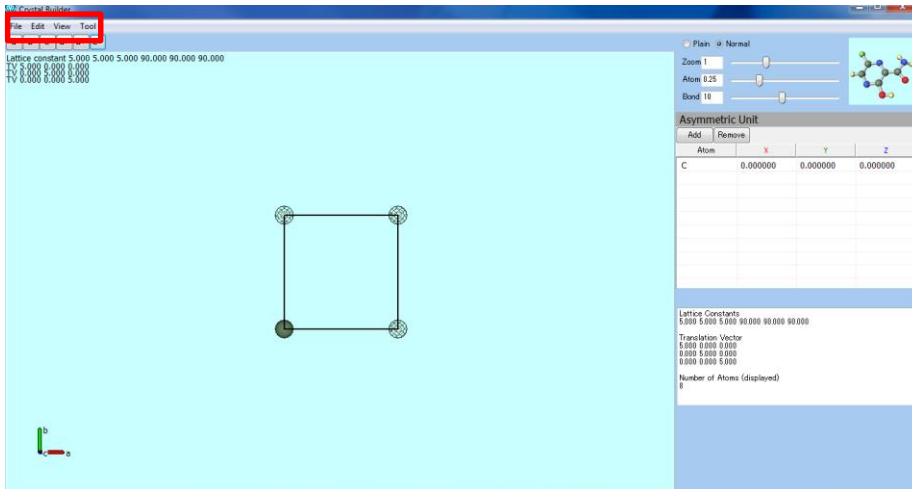
II. Create a supercell

III. Save

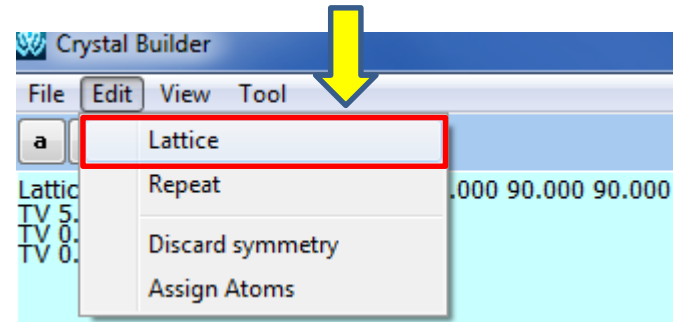
I. Define a unit cell



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



2. Click **Edit | Lattice**.

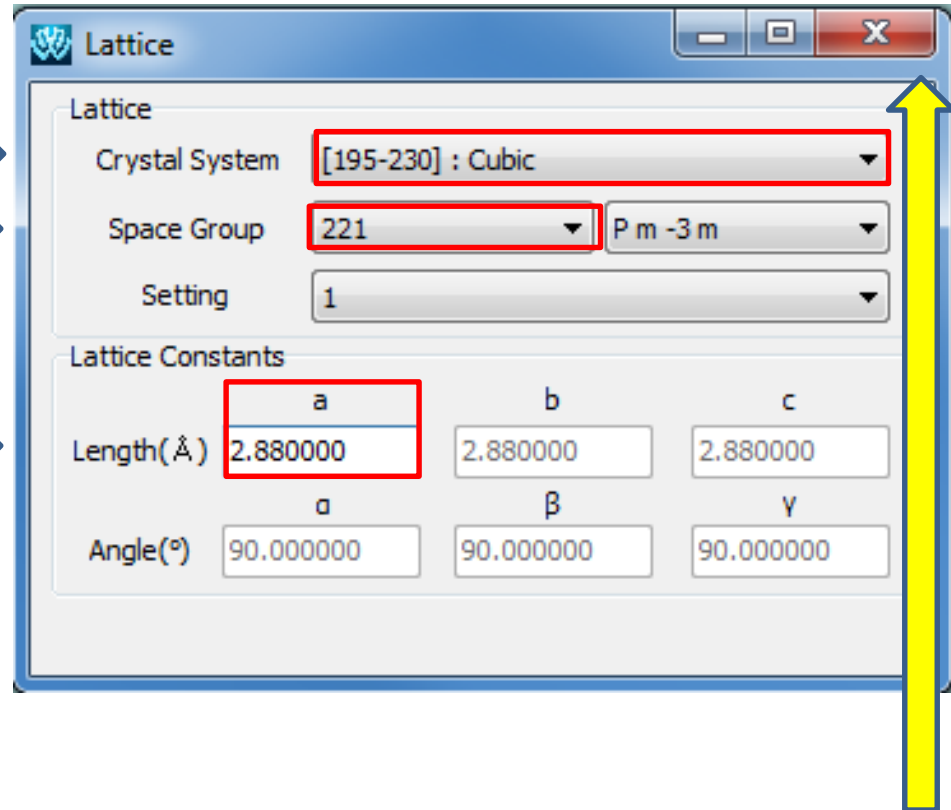


I. Define a unit cell

1. Set **Crystal System** to **Cubic**.

2. Set **Space Group** to **221**.

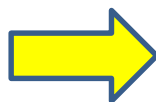
3. Set **a** to **2.88** and push the Enter key.



4. Click here to close.

I. Define a unit cell

1. Click **Add**.



The screenshot shows the Crystal Builder software interface. The main window displays a unit cell with four atoms at the corners. A red box highlights the 'Asymmetric Unit' table in the bottom right corner. The table has columns for Atom, X, Y, and Z. The 'Add' button is highlighted with a red box.

Atom	X	Y	Z
C	0.000000	0.000000	0.000000

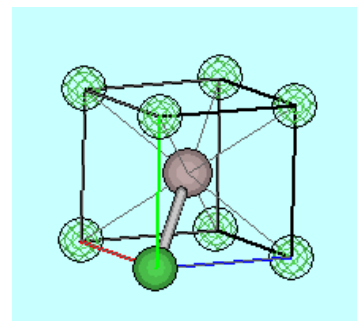
2. Change **Atom**, **X**, **Y** and **Z** (fractional coordinates) as the right.



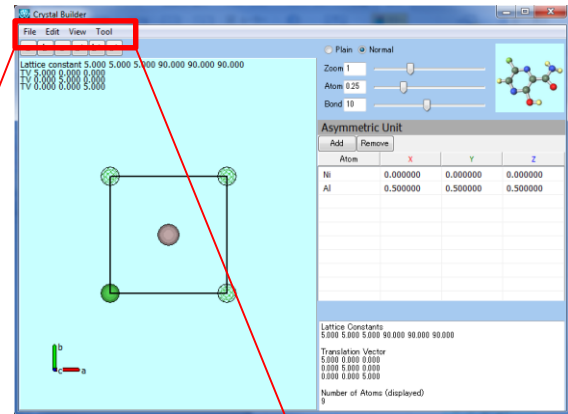
The screenshot shows the updated 'Asymmetric Unit' table. The 'Add' and 'Remove' buttons are visible. The table has columns for Atom, X, Y, and Z. The 'Atom' column is highlighted with a red box. The 'X', 'Y', and 'Z' columns are also highlighted with a red box.

Atom	X	Y	Z
Ni	0.000000	0.000000	0.000000
Al	0.500000	0.500000	0.500000

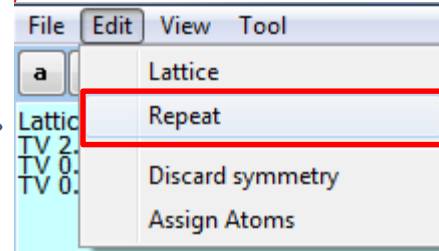
3. The resulting structure will appear.



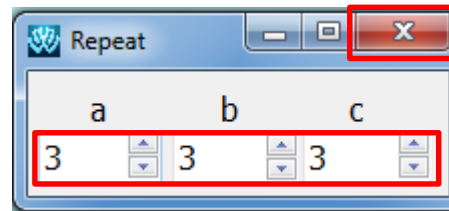
II. Create a supercell



1. Click **Edit | Repeat**.

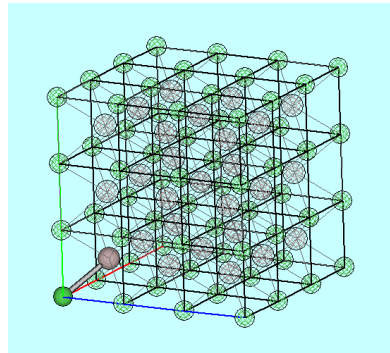


2. Input like this.

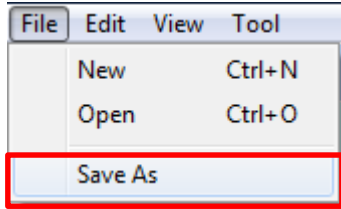


3. Click here to close.

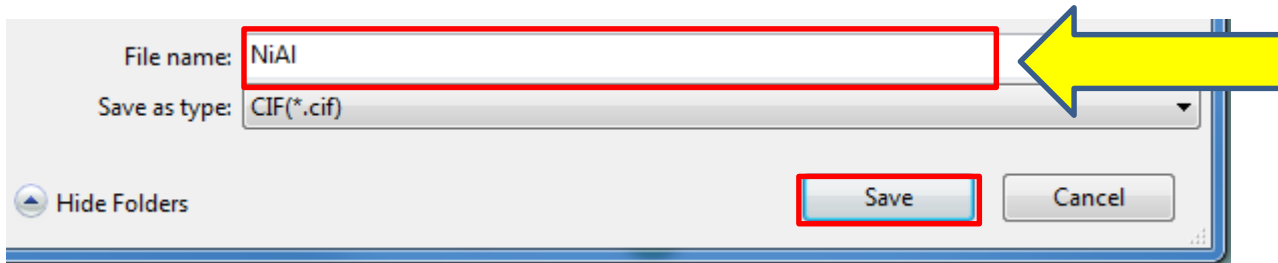
4. 3x3x3 super cell will appear.



III. Save



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



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