

# Crystal Builder

Basics

Ni-Al alloy

V7.000

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2016/11/01

# Contents

## I. Define a unit cell

About NiAl crystal

Crystal system: Cubic

Space group : Pm-3m (221)

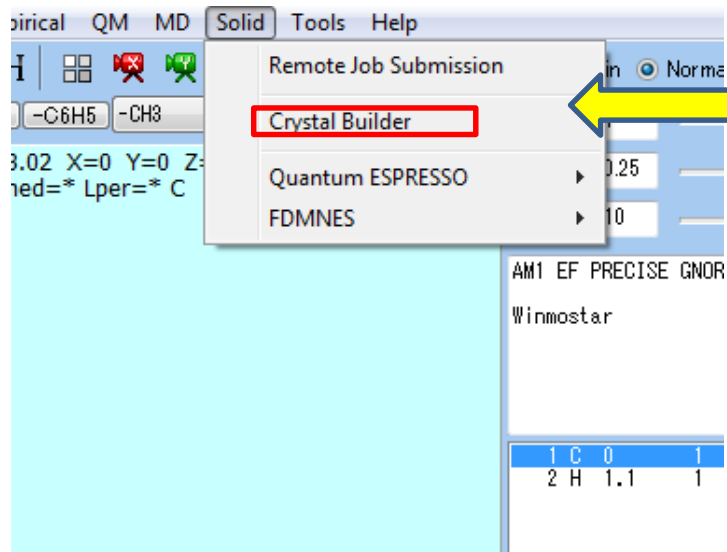
Lattice constants :  $a=2.88 \text{ \AA}$

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

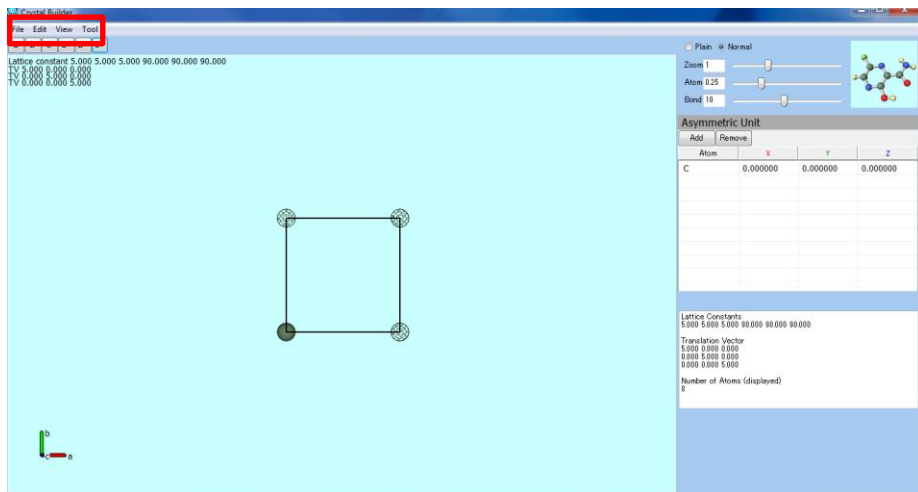
## II. Create a supercell

## III. Save

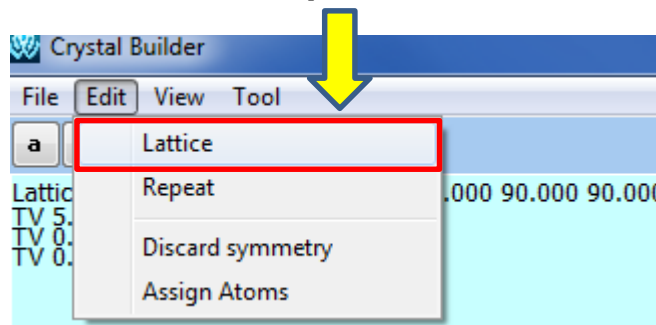
# I. Define a unit cell



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.

Lattice

Crystal System [195-230] : Cubic

Space Group 221 P m -3 m

Setting 1

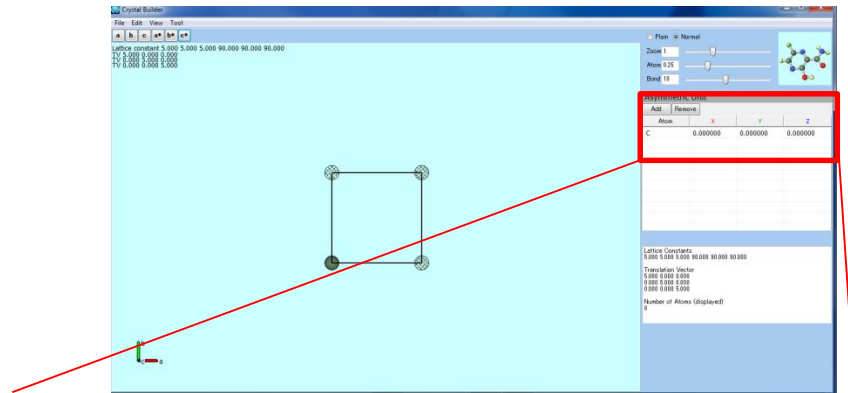
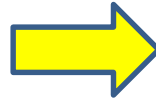
Lattice Constants

	a	b	c
Length(Å)	2.880000	2.880000	2.880000
Angle(°)	90.000000	90.000000	90.000000

4. Click here to close.

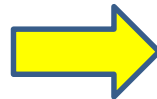
# I. Define a unit cell

1. Click **Add**.



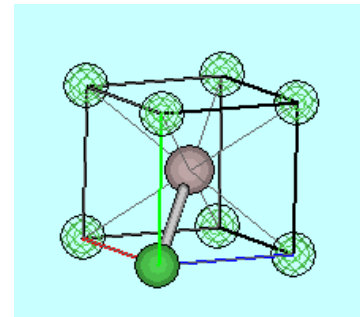
Asymmetric Unit			
Add Remove			
Atom	X	Y	Z
C	0.000000	0.000000	0.000000

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

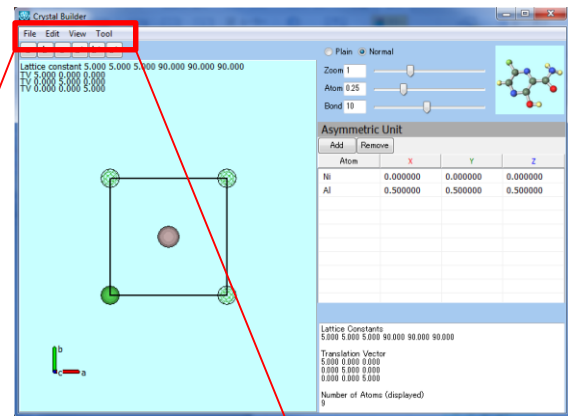


Asymmetric Unit			
Add Remove			
Atom	X	Y	Z
Ni	0.000000	0.000000	0.000000
Al	0.500000	0.500000	0.500000

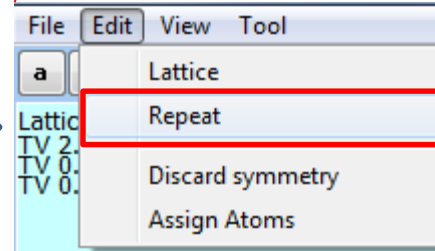
3. The resulting structure will appear.



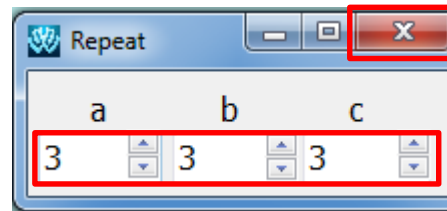
# II. Create a supercell



1. Click **Edit | Repeat**.



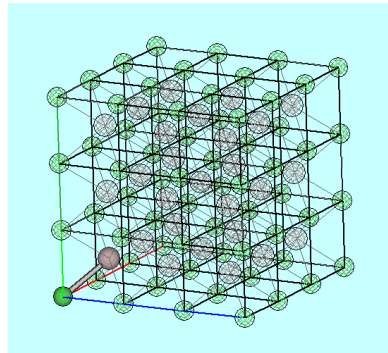
2. Input like this.



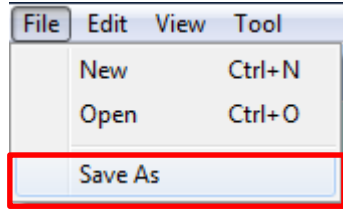
3. Click here to close.



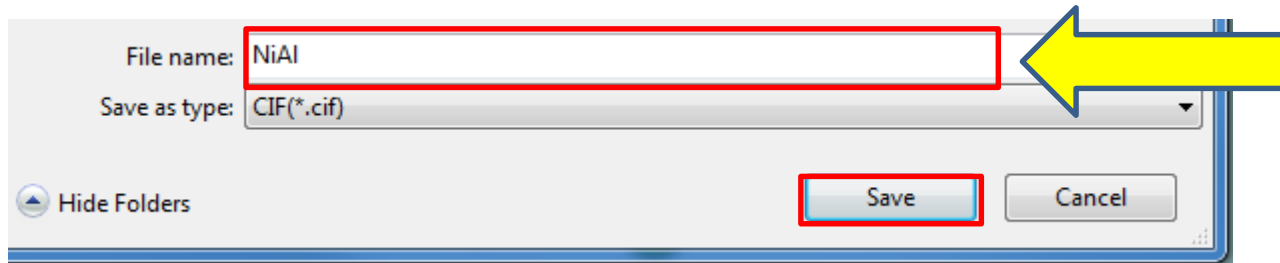
4. 3x3x3 super cell will appear.



## III. Save



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



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