



Interface construction of Al(111)|graphene

Introduction

The present tutorial describes how to build an Al (111)| graphene interface.

1. Outline of procedure

- Construct the Al (111) surface
- Construct the Al(111) | graphene interface

2. Geometric aspects of modeling interfaces

A number of geometrical aspects have to be considered when studying and modeling interfaces:

In most cases there are special requirements on how to match the two contacting materials: e.g. the use of periodic boundary conditions requires the lattice constants of the two materials to be commensurate.

When modeling coherent structures using *ab initio* methods with periodic boundary conditions it is desirable to find geometries which minimize the elastic strain (misfit) at the interface. The reason is that with decreasing misfit, the coherent regions between misfit dislocations at an interface become larger. Consequently, for decreasing misfit, the interface model employed in the periodic approach becomes an increasingly realistic representation of the real systems.

In a composite material the two phases can differ in their elastic properties. You may want to account for this by adapting the lattice parameter of the softer material to the one of the harder material when building an interface.

Because periodic boundary conditions (slab model) are applied to model the interface, the resulting supercell contains two interfaces. In order to get a clear value of the interface energy you need to make sure both interfaces present in the cell are identical. Otherwise, an interface energy calculation gives an average value over the two interfaces.

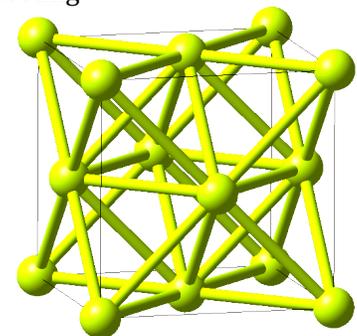
1. Construct the Al surface

Required: *Al.sci*..... **Face-centered cubic Al (Fm-3m)**

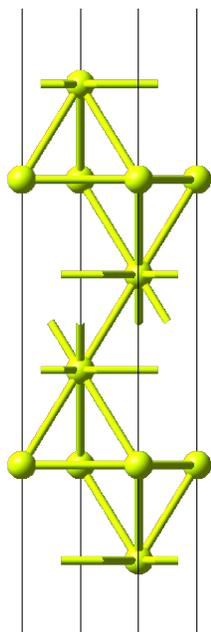
Result: *Al_111.sci*..... **Al (111) surface**

Open the Al bulk structure by >>**File**>>**Open**>>**File from disk** and selecting MD/Structures/Elements/Al.sci. This will retrieve the Al face-centered cubic (Fm-3m) structure from the disk.

Alternatively, you can also build the structure from scratch by opening an empty bulk system with >>**File**>>**New bulk System**. **Right-click** on the empty structure in the viewer and select **Edit symmetry**.... Set the symmetry to **Fm-3m**. Open the **Add Atom** panel (**right-click** and select **Add Atom**...) and add Al to the a-Wyckoff position ($a -- 0.000, 0.000, 0.000$). Set the lattice constant A to 4.0494 Å (**right-click** >>**Edit Cell**...). You now have created the bulk Al structure from scratch.



To construct the Al (111) surface open the surface builder with >>**Builders**>>**Build surfaces**... . Set the Miller indices h: **1** k: **1** l: **1** and click on **Search**. Leave the variables Repeats: **2** and Gap(Ang): **10** unchanged and click on **Create**. Select the option **Symmetric** and confirm with **OK**. This will create an Al (111) surface slab containing 6 Al atoms.



Al 1 1 1 surface_2, symmetry = P-3m1

slab thickness = 14.0275
total thickness = 24.0275

Plane 1 altitude

Plane 0 altitude

Create as P1 Symmetric Centered P1

New Symmetry : P-3m1 Formula : (Al)6

2. Build an interface between Al (111) and graphene

Required: *C-graphite.sci*..... *Carbon in the graphite structure*

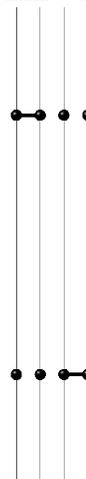
Result: *Al_111_graphene_interface.sci*..... *Al (111) graphene interface*

1. Build graphene

Retrieve the graphite structure by opening MD/Structures/Elements/C-graphite.sci (>>**File**>>**Open**>>**File from disk**).

You can also build graphite from scratch by setting the symmetry to P6₃/mmc, the lattice constants to A=2.447 Å and C=6.66 Å, and adding carbon to the 2c and 2b Wyckoff positions.

Create out of the graphite structure two layers of graphene by changing the C lattice constant from 6.66 to 26.66 Å (**right-click** on the structure >>**Edit Cell...**). This will separate the two graphene layers so that they do not interact with each other effectively creating two isolated graphene layers. Rename the structure to **C 2 layer graphene** with >>**Edit**>**Rename....**



2. Build the Al(111) graphene interface

Select the **Interfaces** tool from the MEDEA® **Tools** menu.

Activate one of the previously constructed surface structure windows (let it be the Al (111) surface model), and choose **Define and run** from the **Interfaces** menu, select the two layer graphene structure as **Second System**.

Set all tolerance values and **# Cells to search** equal to 3. Put all **Weight of first system lattice parameter** to be on Al by adjusting the corresponding slider. In our case, the Al surface is the first system, so the weight should be 1.00. Press **Run Job** to submit a search for interface geometries.

The search algorithm uses Bravais lattice vectors in both surface planes to construct matching surfaces. From the many possibilities to match the surfaces, it lists those systems which fulfill the specified tolerance criteria. On a laptop with two cores, this search takes about 10 seconds.



You can check the status of the Job through MEDEA®'s **Job Control** menu.

Once finished, click on **Retrieve** in the **Interfaces** menu and load the relevant job through the file selection dialogue.

MEDEA® displays a spreadsheet containing results of the interface search. Given the above search criteria you should see the result:

ID	Identical Interfaces	nAtoms	Spacegroup	Area (Ang2)	dArea	A (Ang)	dA	B (Ang)	dB	Theta (degree)	dTheta	BedAngle (degree)
1.1	Yes	34	P-3	21.30	2.7	4.959	1.3	4.959	1.3	120.0	0.0	30.0

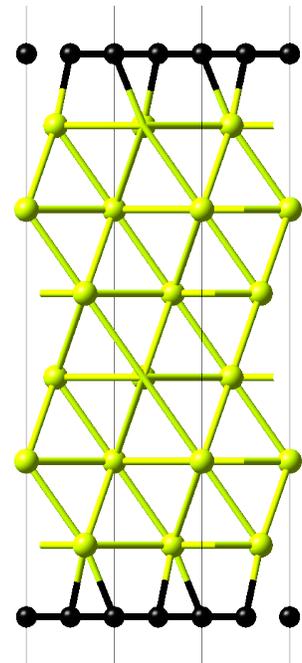
Highlight the entry and open it by **right-clicking** and select the **Create Interface** option.

In the builder window, the distance between the Al (111) surface and the graphene planes can be adjusted by setting the **Gap in Angstroms**. You can set the **Total Gap** to 4 Å or both **Upper Gap** and **Lower Gap** to 2 Å each, which is a reasonable starting value to optimize the interface structure. Confirm the gap setting with **Apply**.

Furthermore, the relative positions can be adjusted by specifying x-, and y-fractional shifts. For now, keep the default settings.

Create the interface by clicking the **OK** button.

This procedure should result in a supercell containing two equivalent Al (111) graphene interfaces. There are in total 34 atoms in the structure; 18 Al, and 16 C atoms, respectively. Study the structure with **Geometric analysis** in MEDEA®'s **Analysis** menu.



Modules Required:

- **Interfaces**