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Determination of low strain interfaces via geometric matching

Determination of low strain interfaces via geometric matching

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This tutorial introduces the new **GeneralizedLatticeMatch** method for combining two bulk crystals into an interface.

On many occasions, one is interested in creating a realistic interface between two materials, even without having precise structural informations on the two surfaces that form the interface. The **GeneralizedLatticeMatch** method facilitates this process, by automatically finding all the possible interface supercells between the two crystals based only on their bulk crystalline structure. The method is an optimized version of the algorithm described in [JLS+17]. Compared to the lattice-matching method used in the **Interface Builder**, described in [The Interface Builder in QuantumATK](#), the present method is unbiased as it considers all the possible surfaces of the two crystals forming the interface.

A number of structural parameters are calculated for each interface, which allows one to easily analyze the matching pattern and choose the most appropriate interface to be used for further studies. The structure of the desired interface can then be easily created using the **Interface Builder** implemented in QuantumATK.



Method description

The following describes in the main steps of the algorithm used in the **GeneralizedLatticeMethod** method, which is very similar to that used in the **Interface Builder** (see [The Interface Builder in QuantumATK](#)).

1. Initially, the possible surface vectors

$[\mathbf{a}_1, \mathbf{a}_2]$ of the first of the two materials forming the interface are constructed, starting from a linear combination of the Bravais vectors of the primitive cell:

$$\mathbf{a}_1 = \sum_{i=1}^3 c_i \mathbf{u}_i \quad c_i \in \mathbb{Z},$$
$$\mathbf{a}_2 = \sum_{i=1}^3 c'_i \mathbf{u}_i \quad c'_i \in \mathbb{Z},$$

and by a subsequent projection of the resulting vectors from

\mathbb{R}^3 to

\mathbb{R}^2 . A similar procedure is applied to construct the surface vectors

$[\mathbf{b}_1, \mathbf{b}_2]$ of the second surface. As it will be shown in the Section [Input and output description](#), the number of generated surface cells can be limited by specifying:

- The maximum value of the Miller indexes $[h, k, l]$ that define each surface;
 - The maximum length of the lattice vectors $[\mathbf{a}_1, \mathbf{a}_2]$ and $[\mathbf{b}_1, \mathbf{b}_2]$.
2. Each couple of surface cells is matched by using the same lattice-match method as used in the **Interface Builder**, and described in the technical note [The Interface Builder in QuantumATK](#).
 3. The average strain is then calculated as:

$$\bar{\varepsilon} = \sqrt{\frac{\varepsilon_{11}^2 + \varepsilon_{22}^2 + \varepsilon_{11}\varepsilon_{22} + \varepsilon_{12}^2}{4}}$$

where

ε_{11} ,

ε_{22} and

ε_{12} are the components of the 2D strain tensor, as defined in the technical note [The Interface Builder in QuantumATK](#).

Note

Notice that this definition of the average strain differs from that used in the [The Interface Builder in QuantumATK](#). The present definition of strain is more appropriate for the present method as it is an invariant of the strain tensor.

Input and output description

In order to use the GeneralizedLatticeMatch method one can set up a simple script as follows:

```

1  # Read the BulkConfiguration of the primitive cell of the
2  # first material
3  configuration_1 = nload('InAs.py',BulkConfiguration)[-1]
4  # Read the BulkConfiguration of the primitive cell of the
5  # second material
6  configuration_2 = nload('Al.py',BulkConfiguration)[-1]
7
8  # Run the GeneralizedLatticeMatch method
9  generalized_lattice_match = GeneralizedLatticeMatch(
10     configuration_1,
11     configuration_2,
12     max_strain=0.02,
13     maximum_miller_index=3,
14     longest_surface_lattice_vector=50*Angstrom,
15     max_surface_area=200.0*Angstrom**2,
16     user_given_miller_index=None
17 )

```

The script reads two input files, each one containing a BulkConfiguration of the bulk primitive cell of one of the two materials that form the interface. Then, it applies the GeneralizedLatticeMatch method on these two structures. A number of **input parameters** can be set to control the precision and the extent of the search for possible interface supercells. The full list of input parameters is:

- `configuration_1`: BulkConfiguration of the bulk primitive cell of the first material.
- `configuration_2`: BulkConfiguration of the bulk primitive cell of the second material.
- `max_strain`: Maximum strain applied to each of the two surfaces.
- `maximum_miller_index`: Maximum value of the Miller indexes $[h, k, l]$ that define each of the two surfaces.
- `longest_surface_lattice_vector`: Maximum length of each surface lattice vector $[a_1, a_2]$ and $[b_1, b_2]$.
- `max_surface_area`: Maximum value of the surface area of the interface supercell.
- `user_given_miller_index`: Predefined Miller indexes of the surface of `configuration_1`.

Note

When the parameter `user_given_miller_index` is set to a value different than `None`, the search for the possible surfaces is restricted to the second material, whereas the surface of the first material is kept fixed. This option will be used in [Example 2: Lattice match between a bulk system with a predefined surface](#).

After the possible matches are calculated, the matching results are printed directly in the QuantumATK log file of the calculation. The matches will be listed in order of increasing strain, together with a number of output parameters that characterize each match.

```

+-----+
|  A          B          Strain  Atoms  Area  Aspect  Angle  Rotation  |
+-----+
| [ 1  0  0] >-< [ 1  0  0]  0.000110  29    72.9   1.0    90.0    0.0
| [ 2  2  1] >-< [ 1  0  0]  0.000110  23   163.9   2.2   153.4   26.6
| [ 3  3  2] >-< [ 1  1  1]  0.004030  28   170.9   1.2   162.6   60.3

```

The output parameters are:

- `A`: Miller indexes

$[h, k, l]$ of the first surface.


- **B** : Miller indexes

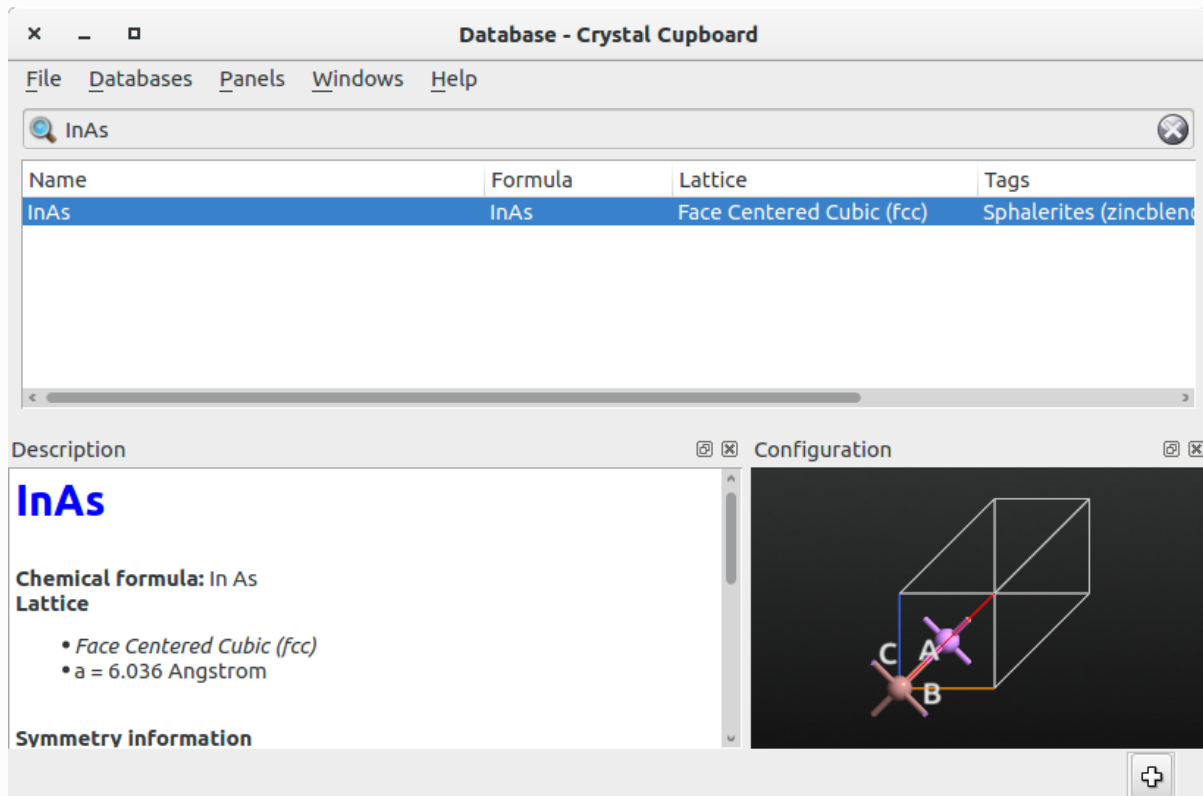
$[h, k, l]$ of the second surface.

- **Strain** : Maximum strain of the two surfaces.
- **Atoms** : Total number of atoms in the interface supercell.
- **Area** : Surface area of the interface supercell.
- **Aspect** : Aspect ratio between two surface vectors of the interface supercell. The ratio is calculated by taking the largest vector at the numerator.
- **Angle** : Angle between the two vectors of the interface supercell.
- **Rotation** : Rotation between the two surfaces in the interface supercell.

Example 1: Lattice match between two bulk systems

In this first example, you will calculate the possible matches between indium arsenide and aluminum.

To obtain the structure file containing the BulkConfiguration of bulk InAs, open **QuantumATK**, go to the **Builder** and click on Add ▶ From Database.... In the **Database**, select the primitive cell of bulk InAs shown in the figure below, add it to the **Stash** by clicking on the  button.



The screenshot shows the 'Database - Crystal Cupboard' window. The search bar contains 'InAs'. The table below shows the search results:

Name	Formula	Lattice	Tags
InAs	InAs	Face Centered Cubic (fcc)	Sphalerites (zincblende)

The 'Description' panel for 'InAs' is visible, showing the following information:

- Chemical formula:** In As
- Lattice**
 - Face Centered Cubic (fcc)
 - a = 6.036 Angstrom
- Symmetry information**

The 'Configuration' panel shows a 3D model of the primitive cell of bulk InAs, which is a face-centered cubic (fcc) lattice. The atoms are represented by spheres, and the unit cell is outlined. The axes are labeled A, B, and C.

Repeat the same procedure to add to the **Stash** the structure of the primitive cell of bulk Al, which is shown in the figure below.

Database - Crystal Cupboard

File Databases Panels Windows Help

Aluminium/Aluminum (alpha)

Name	Formula	Lattice	Tags
Aluminium/Aluminum (alpha)	Al	Face Centered Cubic (fcc)	Elements Cubic Stand

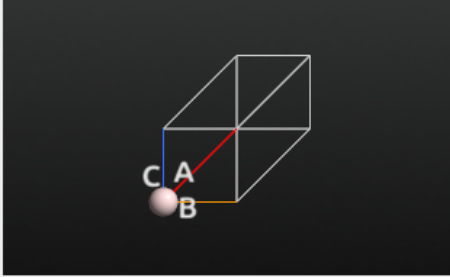
Description Configuration

Al (Aluminium/Aluminum (alpha))

Chemical formula: Al
Lattice

- Face Centered Cubic (fcc)
- a = 4.04958 Angstrom

Symmetry information



In the **Stash**, save the two configurations by right-clicking on each structure and selecting 'Save as'. Alternatively, you can download the two files from here: [InAs.py](#), [Al.py](#).

Set up the script for the GeneralizedLatticeMatch method as shown below:

```

1  # Read the BulkConfiguration of the primitive cell of the
2  # first material
3  configuration_1 = nread('InAs.py',BulkConfiguration)[-1]
4  # Read the BulkConfiguration of the primitive cell of the
5  # second material
6  configuration_2 = nread('Al.py',BulkConfiguration)[-1]
7
8  # Run the GeneralizedLatticeMatch method
9  generalized_lattice_match = GeneralizedLatticeMatch(
10     configuration_1,
11     configuration_2,
12     max_strain=0.02,
13     maximum_miller_index=3,
14     longest_surface_lattice_vector=50*Angstrom,
15     max_surface_area=200.0*Angstrom**2,
16     user_given_miller_index=None
17 )

```

Alternatively, you can download the script from here: [match_InAs_Al.py](#)

In this example, the scan will be performed by considering surfaces with a maximum strain of 0.02, with Miller indexes $h, k, l \leq 3$, with a maximum length of the lattice vectors of 50 Å, and with an upper threshold for the surface area of 200 Å².

Run the script in the terminal as `atkpython match_InAs_Al.py > match_InAs_Al.log`. The output will look as shown below. There are several possible matches, so for brevity only the first 20 matches are shown.

```

+-----+
|
| Atomistix ToolKit 2017.1 [Build ce08f12]
|
+-----+

Miller planes for A : |-----|
                    : =====
                    |-----|

Miller planes for B : |-----|
                    : =====
                    |-----|

Matching Miller planes : =====
+-----+
| A          B          Strain   Atoms   Area   Aspect   Angle   Rotation |
+-----+
[ 1 0 0] >-< [ 1 0 0] 0.000110 29    72.9    1.0    90.0    0.0
[ 2 2 1] >-< [ 1 0 0] 0.000110 23   163.9    2.2   153.4   26.6
[ 3 3 2] >-< [ 1 1 1] 0.004030 28   170.9    1.2   162.6   60.3
[ 3 1 1] >-< [ 2 1 1] 0.004030 10   120.8    1.7    90.0    0.0
[ 3 1 1] >-< [ 3 1 1] 0.004250 16   120.8    1.7   106.8   33.6
[ 3 3 1] >-< [ 3 3 1] 0.004250 16   158.8    2.2   102.9    0.0
[ 3 3 1] >-< [ 3 3 1] 0.005470 13   158.8    2.2   102.9    0.0
[ 3 1 1] >-< [ 3 1 1] 0.005470 13   120.8    1.7   106.8   33.6
[ 2 1 1] >-< [ 2 1 1] 0.005470 17   178.5    2.4    90.0    0.0
[ 2 1 0] >-< [ 2 1 0] 0.005470 13   162.9    1.2   114.1    0.0
[ 1 1 1] >-< [ 1 1 1] 0.005470 13    63.1    1.0   120.0   60.0
[ 1 1 0] >-< [ 1 1 0] 0.005470 17   103.0    1.4    90.0    0.0
[ 1 0 0] >-< [ 1 0 0] 0.005470 13    72.9    1.0    90.0    0.0
[ 1 0 0] >-< [ 2 2 1] 0.005470 7    72.9    1.0    90.0    0.0
[ 3 2 2] >-< [ 1 1 1] 0.005940 23   150.2    1.2   157.6   60.5
[ 1 0 0] >-< [ 2 1 1] 0.006130 19   182.2    3.9    39.8    0.6
[ 3 1 1] >-< [ 1 1 0] 0.007160 18   151.0    1.7    73.2   22.6
[ 3 1 1] >-< [ 1 0 0] 0.007730 19   120.8    1.7    90.0    0.0
[ 3 2 2] >-< [ 3 1 1] 0.008250 13   150.2    2.3   115.9   35.2
[ 1 0 0] >-< [ 1 1 0] 0.008420 28   200.4    2.2    79.7   38.2

```

Notice how the match with the least strain is that between the $\langle 100 \rangle$ surface of InAs and the $\langle 100 \rangle$ surface of Al.

Example 2: Lattice match between a bulk system with a predefined surface

In some cases, one could be interested in finding the possible matches of a bulk material to a given surface. In this second example, you will investigate how to find the possible matches of bulk aluminium to the InAs(111) surface. InAs nanowires with $\langle 111 \rangle$ -oriented facets have been synthesized in Ref. [KZC+15], and it has been demonstrated experimentally that $\langle 111 \rangle$ -oriented Al layers can be grown on this surface.

Use the same structure files as in [Example 1: Lattice match between two bulk systems](#), and setup the script for the GeneralizedLatticeMatch calculation as follows:

```

1 # Read the BulkConfiguration of the primitive cell of the
2 # first material
3 configuration_1 = nload('InAs.py',BulkConfiguration)[-1]
4 # Read the BulkConfiguration of the primitive cell of the
5 # second material
6 configuration_2 = nload('Al.py',BulkConfiguration)[-1]
7
8 # Run the GeneralizedLatticeMatch method
9 generalized_lattice_match = GeneralizedLatticeMatch(
10     configuration_1,
11     configuration_2,
12     max_strain=0.02,
13     maximum_miller_index=3,
14     longest_surface_lattice_vector=50*Angstrom,
15     max_surface_area=200.0*Angstrom**2,
16     user_given_miller_index=(1,1,1)
17 )

```

Notice how the `user_given_miller_index` option, highlighted in yellow, has now been set to `user_given_miller_index=(1,1,1)`. Therefore, in this case only the matches of bulk Al to the InAs(111) surface will be considered. You can also download the script from here: [match_InAs111_Al.py](#)

Run the script in the terminal as `atkpython match_InAs111_Al.py > match_InAs111_Al.log`. The output will look as shown below. Notice how there are fewer possible matches than those in the output of [Example 1: Lattice match between two bulk systems](#). This is because only one surface is now considered for the material denoted `A`.

```

+-----+
|
| Atomistix ToolKit 2017.1 [Build ce08f12]
|
+-----+

Miller planes for B : =====

Matching Miller planes : =====
+-----+
| A          B          Strain   Atoms   Area   Aspect   Angle   Rotation |
+-----+
| [ 1 1 1] >-< [ 1 1 1]  0.005470   13     63.1    1.0     120.0    60.0
| [ 1 1 1] >-< [ 3 3 1]  0.010100   17    142.0    1.2     46.1     18.4
| [ 1 1 1] >-< [ 2 1 0]  0.010710   15    110.4    4.0     30.0     5.9
| [ 1 1 1] >-< [ 3 1 1]  0.011070   26    110.4    2.6     19.1    77.9
| [ 1 1 1] >-< [ 3 1 1]  0.012770   15    110.4    2.6     19.1    77.9
| [ 1 1 1] >-< [ 1 1 0]  0.013260   24    126.2    2.6     40.9    12.1
| [ 1 1 1] >-< [ 1 0 0]  0.014880   23    126.2    1.7      8.2     1.1
| [ 1 1 1] >-< [ 2 2 1]  0.014880   13    126.2    2.3     10.9    31.1
| [ 1 1 1] >-< [ 3 2 1]  0.016000   18    189.3    2.6     26.3    75.4
| [ 1 1 1] >-< [ 3 1 2]  0.016000   18    189.3    3.5     19.1    44.6
| [ 1 1 1] >-< [ 2 1 0]  0.016150   13    110.4    4.0     30.0     5.9
| [ 1 1 1] >-< [ 2 1 1]  0.016420    9     78.9    2.9     30.0    20.8
| [ 1 1 1] >-< [ 1 1 0]  0.016510   19    126.2    2.6     40.9    12.1
+-----+

```

In this case, the match to the InAs(111) surface with the lowest strain is that with the Al(111) surface, which is in agreement with the experimentally measured structure reported in Ref. [\[KZC+15\]](#).

References

[JLS+17] Line Jelver, Peter Mahler Larsen, Daniele Stradi, Kurt Stokbro, and Karsten Wedel Jacobsen. Determination of low-strain interfaces via geometric matching. *Phys. Rev. B*, 96:085306, Aug 2017. doi:10.1103/PhysRevB.96.085306.

[KZC+15] (1,2) P. Krogstrup, N. L. B. Ziino, W. Chang, S. M. Albrecht, M. H. Madsen, E. Johnson, J. Nygård, C. M. Marcus, and T. S. Jespersen. Epitaxy of semiconductor–superconductor nanowires. *Nature Materials*, 14:400–406, 2015. doi:10.1038/nmat4176.



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