A Lattice Matching Algorithm for Layered Heterostructures

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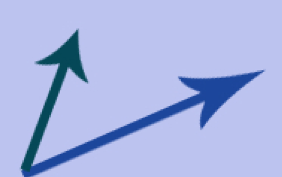
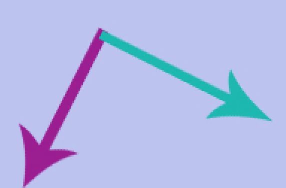
Introduction

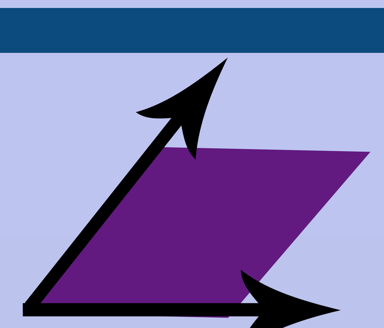
Epitaxy is the process of growing a crystal subtance on another crystal substance. This process is called *heteroepitaxy* when the crystals are different. Predicting if the epitaxial growth of different materials will work is tricky since the lattice parameters do not necessarily match. I have designed and implemented an algorithm based on one discussed by Zur and McGill[1] that compares the geometry of the materials and characterizes the lattice mismatch.



Overview



This algorithm does not exactly determine whether heteroepitaxial growth of two materials is possible since the chemistry at the interface is the main determining factor, however the geometry of the two materials is also important. This algorithm compares in plane 2-D symmetry of the materials described by the *lattice vectors* of the materials.



Step 1

The algorithm takes in two pairs of vectors that describe each material in the x-y plane. It then proceeds to calculate the area of the parallelogram spanned by each pair of vectors.

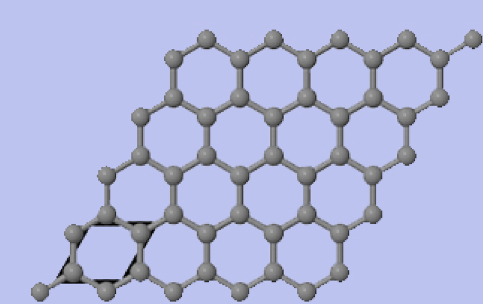
Step 2

Then the algorithhm takes the ratio of areas and calculates a rational approximation to within a specified tolerance.

For example, if the ratio of the areas is 3.14 and a 1% tolerance is specified it returns the rational approximation $\frac{19}{6}$

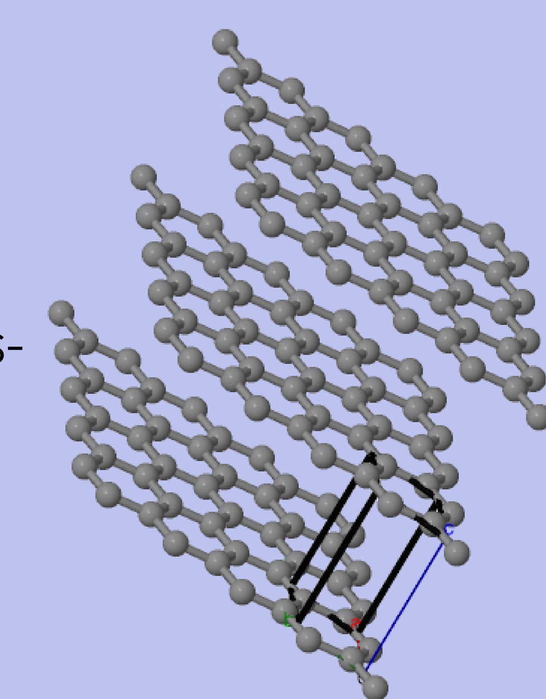
Example Outputs

Graphene has lattice vectors: $2.46\begin{pmatrix}\frac{\sqrt{3}}{2}\\ -\frac{1}{2}\end{pmatrix}, 2.46\begin{pmatrix}\frac{\sqrt{3}}{2}\\ \frac{1}{2}\end{pmatrix}$



Single layer of graphene.

3 layers of graphene. My algorithm use the identity matrix to transform the vectors, as expected.



To test the algorithm for heterostructures, I attempted to reproduce the results in [2], matching the lattice of In_2Te_2 and graphene.

In_2Te_2 has lattice vectors

$$4.23\begin{pmatrix}\frac{\sqrt{3}}{2}\\ -\frac{1}{2}\end{pmatrix}, 4.23\begin{pmatrix}\frac{\sqrt{3}}{2}\\ \frac{1}{2}\end{pmatrix}$$

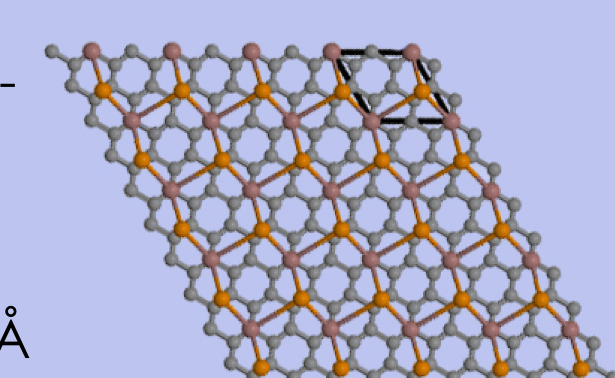
To best preserve angles and match vector magnitudes and spanned area, the algorithm determined to transfrom the graphene vectors by $\begin{pmatrix}1 & 0\\ 0 & 3\end{pmatrix}$

and In_2Te_2 by $\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}$

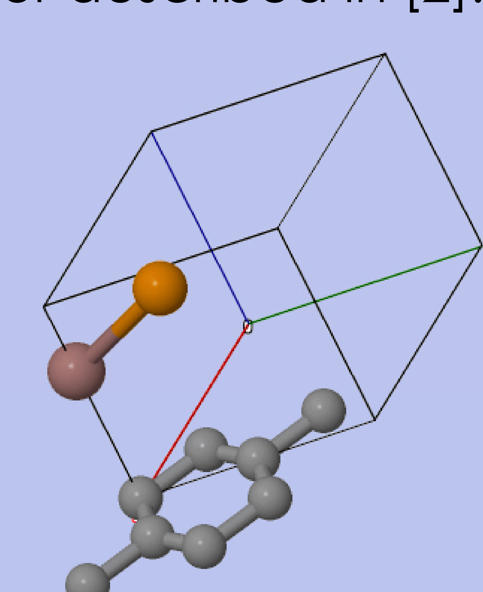
the combined supercell is described by

$$\begin{pmatrix}2.13\\ -3.69\end{pmatrix}, \begin{pmatrix}2.13\\ 3.69\end{pmatrix}$$

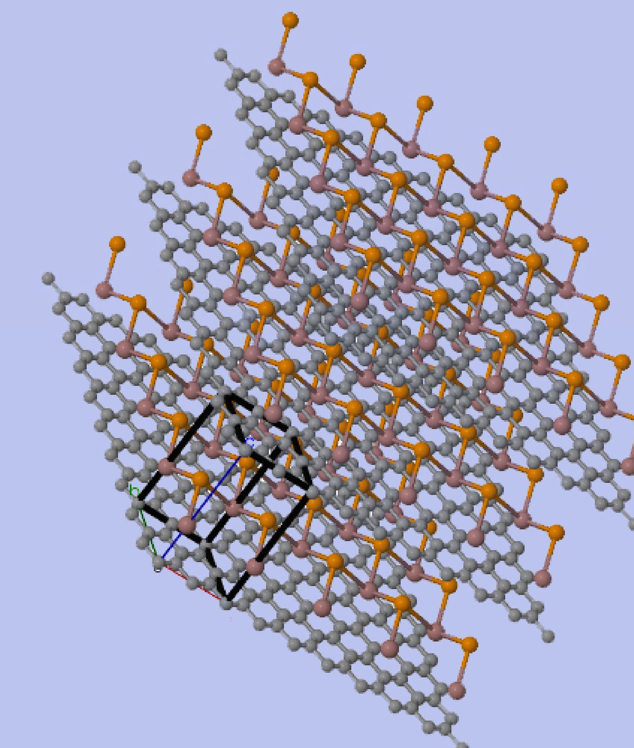
with lattice constant of 4.261Å which is within the 1% margin of error described in [2].



Top view of heterostructure



Unit cell of of the output



Step 3

The next step is to determine a supercell that has an area that is *n* times greater than the input unit cells, where *n* is an integer. Extending the previous example, it woul be 19 times one cell and 6 times the other. It does this by transforming the vectors using this matrix:

$$\begin{pmatrix}i & j\\ 0 & m\end{pmatrix}$$
$$i, j, m \in \mathbb{Z}$$
$$i \cdot m = n$$
$$i, m > 0$$
$$0 \le j \le m-1$$

Final Steps

Lastly, the algorithm goes through the Gaussian reduction algorithm, similar in form to Euclid's greatest common divisor algorithm, and compares the magnitudes of the vectors, angles between them, and the spanned areas and selects the set that are within a specified tolerance of each other.

References

[1] Lattice match: An application to heteroepitaxy Zur, A. and McGill, T. C., Journal of Applied Physics, 55, 378-386 (1984)

[2] Kekulé textures, pseudospin-one Dirac cones, and quadratic band crossings in a graphne-hexagonal indium chalcogenide bilayer Giovannetti, et al., Phys. Rev. B, 91, 12, 12-17 (2015)

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