A fast method for predicting the formation of crystal interfaces and heterocrystals

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Abstract

In order to address an important problem in Computational Materials Design, we have demonstrated the feasibility of an algorithm which rapidly scans through various surface configurations of two single crystals selected from a crystal structures database and identifies those pairs which are likely to form stable heterointerfaces. Any two crystals are cut along different planes and all possible heterocrystal interfaces are generated based on geometric criteria and predicted bond directions of atoms on both constituent surfaces. Each configuration is assigned two scores derived using deviations of interfacial bond lengths from ideal and electronegativity differences between atoms on each side of the interface. We present some results to illustrate our method for PtNi3 on Pt3Co, GaP on Si, and Si on SiO2. This technique can be used as a fast filter for further analysis by more detailed ab initio-based methods, and is meant to address the higher throughput methods needed in the Materials Genome Initiative for complex material structures.

1. Introduction

Heterocrystals consist of two or more regions of different composition. They are of fundamental importance in microelectronics and particularly the microchip industry since the junction between adjacent materials can have unique characteristics, and new materials can be engineered to have bulk properties not attainable in one material crystals. In order to address challenges raised by ever-shrinking transistor dimensions, materials with targeted properties, a combination of quantum methods and atomistic simulations is essential [1].

It is a challenge to search through numerous crystal structures in order to find the ideal heterocrystal configurations, since there are many different crystal facets and crystal structures. In principle, the best way to test if two surfaces are chemically compatible would be with density functional theory (DFT), which is an essentially parameter free quantum mechanical method. However, it is also a method that is computationally rather expensive. In order to reduce the amount of time doing DFT calculations, it is important to develop an initial screening step to test the compatibility of two surfaces rapidly. For two materials of interest, if we consider that each material has five crystal structures and taking into account only the low index planes, (100), (110), and (111), there would be a total of 15 planes of interest per material, totalling 225 possible heterocrystal combinations. It is an enormous task to test 225 heterocrystals with DFT, and a screening step will dramatically reduce the computational time by reserving DFT for only the most promising candidates. In a real application, there could be multiple atoms in a material and high index planes are also possible, leading to thousands of possibilities. In such systems, using our method will help in reducing the overall number of simulations that need to be done by an ab initio technique like DFT.

The formation of hetero-crystals depends fundamentally on the geometry of the crystal lattices and on the chemical interactions between the atoms on each surface at the interface. Several authors [2–6] have proposed methods to predict heteroepitaxial growth. These methods range from mathematical considerations [2,6] to complex and computationally intensive energy calculations [4,7].

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In this paper, we have developed a proof-of-concept algorithm to assist materials design and determine whether a hetero-crystal may be formed between two arbitrary inorganic crystal surfaces. Based on a mixture of geometric and chemical considerations, the algorithm scans through various combinations of materials rapidly and predicts surface combinations and relative orientations likely to result in hetero-crystal interfaces. The main algorithm models crystal structures using structural information from the Inorganic Crystal Structures Database (ICSD). It cuts crystals along various Miller index surfaces. The algorithm then determines whether the two surfaces satisfy a geometric matching criterion following previous ideas [2], and gives a set of possible candidate configurations that need to be ranked and compared in subsequent steps. Two such criteria that are based on the relative positions of the atoms on the two surfaces, and on their average electronegativity difference are used in this paper. The method itself is described below.

2. Methods and materials simulation

In order to decide whether two crystalline surfaces can form a hetero-crystal interface, we developed and tested an algorithm to evaluate whether the geometries of the planes are compatible based on the method suggested in [2]. Once the planes were found to have matching periodicities, we set an initial configuration by considering the expected bond directions of the atoms on the surfaces and matching periodicities, we set an initial configuration by considering the expected bond directions of the atoms on the surfaces and implemented methods to rank possible configurations, as well as combinations of different planes. We describe the different steps in the algorithm in sections below. In Sections 2.1 and 2.2, we describe the lattice and surface matching based on geometry; in Section 2.3, we describe a scoring metric based on chemistry. Our results as well as the DFT method used for validation are presented in Section 3.

2.1. Lattice matching

Previous research has shown that hetero-epitaxial growth requires interfacial translational symmetry, which must be compatible with the lattice symmetry of the bulk on both sides of the interface [2]. Several examples in the literature discuss geometric lattice matching. Some of the methods outlined include the consideration of crystallographic space groups [6], finding linear transformations between the substrate and the over-layer lattices [7] and generation of possible superlattices followed by pairwise comparison of the constituent unit cells [2]. The latter method was chosen since it appeared to apply to some of the most general cases and proved to be faster than methods based on computation of pair potentials.

Fig. 1 shows there is not a unique choice of basis vectors for a two-dimensional lattice. In order to compare two two-dimensional lattices, it is necessary to describe them in unique ways. A pair of basis vectors \( \mathbf{u} \) and \( \mathbf{v} \) of a 2D lattice was found using the Miller indices of the corresponding plane [8]. These vectors were reduced to a primitive basis, following an algorithm outlined in [2]. \( \{ \mathbf{a}, \mathbf{b} \} \) is defined to be a primitive basis for a two-dimensional lattice if the angle between \( \mathbf{a} \) and \( \mathbf{b} \) is less than 90° and if \( \mathbf{a} \) and \( \mathbf{b} \) are the shortest possible lattice basis vectors. It is further conventionally required that \( |\mathbf{a}| \leq |\mathbf{b}| \). For the example shown in Fig. 1, the algorithm would convert the blue\(^1\) basis (in the right panel) to the red one (in the left panel).

Once the reduced primitive basis vectors were determined, geometric lattice matching is assumed to be possible if two superlattices, describing a substrate and overlayer, consist of unit cells of similar dimensions. Superlattice unit cells (supercells) contain integer numbers of reduced unit cells and can be described in terms of two superlattice basis vectors. If a supercell consists of \( n \) reduced unit cells, a basis \( \{ \mathbf{u}, \mathbf{v} \} \) for the superlattice may be generated using:

\[
\mathbf{u} = i \mathbf{a} + j \mathbf{b} \quad \text{and} \quad \mathbf{v} = m \mathbf{b}
\]

where \( \{ \mathbf{a}, \mathbf{b} \} \) is the primitive basis, \( 1 \leq i, j, m \leq n - 1 \) and \( \{ \mathbf{u}, \mathbf{v} \} \) are coprime. In all, the number of possible superlattices which supercells consisting of \( n \) primitive unit cells is less or equal to the sum of the divisors of \( n \) [9]. Figs. 2 and 3 illustrate the superlattices formed for \( n = 4, m = 2 \) and \( i = 2 \).

Lattice matching requires supercells of nearly equal area. Let \( A_1 \) and \( A_2 \) be the primitive unit cell of the two surfaces. The smallest positive integers \( p, q \) such that \( pA_1 \approx qA_2 \) were found using the convergents of the continued fraction representation [10] of \( \frac{A_1}{A_2} \), such that

\[
\left| \frac{p}{q} - \frac{A_2}{A_1} \right| \leq \varepsilon
\]

where \( \varepsilon > 0 \) is some small tolerance.

All possible superlattice basis vectors \( \{ \mathbf{u}_1, \mathbf{v}_1 \} \) and \( \{ \mathbf{u}_2, \mathbf{v}_2 \} \) in the two planes were generated using Eq. (1). To conclude whether matching was possible, the algorithm compared supercell side lengths corresponding to the two superlattices, \( \frac{|\mathbf{u}_1|}{|\mathbf{v}_1|} \) and \( \frac{|\mathbf{u}_2|}{|\mathbf{v}_2|} \), as well as \( \frac{|\mathbf{u}_1|}{|\mathbf{v}_2|} \) and \( \frac{|\mathbf{u}_2|}{|\mathbf{v}_1|} \) were evaluated. If any of these pairs of ratios were within \( \varepsilon \) of 1, where \( \varepsilon > 0 \) is a user-specified tolerance on the allowed strain, we concluded the superlattices are of roughly equal dimensions and the two surface lattices match.

Once two matching superlattices were found, they were deformed to an intermediate lattice via a linear transformation and both planes were rotated to lie parallel to each other in the xy plane of the Cartesian coordinate system. The lengths of the intermediate superlattice basis vectors \( \mathbf{u} \) and \( \mathbf{v} \) and the angle \( \theta \) between them were computed using:

\[
|\mathbf{u}| = f|\mathbf{u}_1| + (1 - f)|\mathbf{u}_2|
\]

\[
|\mathbf{v}| = f|\mathbf{v}_1| + (1 - f)|\mathbf{v}_2|
\]

\[
\theta = f\theta_1 + (1 - f)\theta_2
\]

where \( f \) is a user specified weight. For example, setting \( f = 0 \) is equivalent to deforming the first superlattice only to match the second exactly and \( f = 0.5 \) results in deforming both superlattice vectors to averages of the initial ones.

The linear transformation matrices \( L_1 \) and \( L_2 \) were found by solving the following equations:
and comparing them to the expected bond distances. The expected bond distance between two atoms was assumed to be equal to the sum of their atomic radii. We assumed two atoms were bonded if the distance between them in the bulk was less or equal than $1.1 \times$ (sum of their covalent radii) [11].

The broken bonds of each atom on the two surfaces were identified by taking the scalar products of the bond vectors in the bulk with the unit normal to the planes. Fig. 5 shows the initial and the broken bonds of the atom at the center of the unit cell. Positive scalar products were associated with the broken bonds or ‘anticipatory bond vectors’. Under the assumption that a particular atom on one of the surfaces is likely to form new bonds at the interface pointing in the directions of the broken bonds, the scalar products of all pairs of anticipatory bond vectors, one from each plane, were considered. For scalar products equal to $-1$, the anticipatory bond vectors point in exactly opposite directions. In this case a bond should form in the direction of the vectors, ideally with atoms separated by a distance equal to the sum of their corresponding covalent radii. In practice, we assume that a bond is likely to form if the anticipatory bond vectors point in approximately the same direction, or if their scalar product is close to $-1$ within a chosen tolerance.

When evaluating the scalar products between anticipatory bond vectors corresponding to atoms on the two surfaces, only the atoms in the superlattice unit cells were considered. The atoms inside a unit supercell were found by converting the position vectors of the atoms on the surface (with respect to an origin on the plane) from Cartesian coordinates to the superlattice basis.

For every scalar product found to be less than the set tolerance, the surfaces were translated such that the corresponding pair of atoms lies at the origin and shifted in the directions of an intermediate bond vector. This was determined by taking the difference between the two matching anticipatory bond vectors. Its length was set to be equal to the ideal distance between the atoms. The crystallographically distinct elements were identified using ICSD labels and only these were considered when finding an initial configuration as described above. We did this under the assumption that elements labeled identically are equivalent, so their bonds point in the same directions.

Every initial configuration was set up with a supercell of one material placed above an extended surface region consisting of $3 \times 3$ supercells of the other material. This configuration ensured that all interactions between the atoms in the two planes were accounted for when evaluating the corresponding scores.

2.3. Scoring metrics

For two materials, combinations of planes and different configurations were assigned scores and ranked using two criteria. The two different scoring processes rely on nearest neighbor distances and electronegativity differences between atoms on two surfaces. The first checks that the atoms at the surface are not bonded to the other surface at distances too close or too far from their ideal
bond distance. The second checks that the electronegativity difference of the atoms at the surface interface are maximized. Since there are many different initial configurations determined from the surface matching algorithm, these two scoring metrics will rank these configurations based on their chemical compatibility. The most promising configurations can then be compared with more accurate (and computationally more expensive) methods. Density functional theory (DFT) is the rigorous method for this purpose. In this paper, we will give an example that DFT can indeed be used to further quantify and rank different configurations. Our intent here is to use the ranking (of the cheap methods) as a downselection method for further analysis by DFT. A detailed study for this (or any other) material system that uses DFT as a final step is elaborate and is beyond the scope of this paper. We emphasise for this (or any other) material system that uses DFT as a final step that atoms inside the supercells on two distinct surfaces can have different nearest neighbors. A final score for a given configuration was divided by the maximum electronegativity difference between atoms on the two surfaces, best scores are the ones closest to 1. For single element crystals scores of 1 are generated as long as all atoms on the two surfaces have at least one nearest neighbor.

2.3.1. Nearest neighbor distance criterion

This method is based on evaluating the nearest neighbor distances between atoms in a supercell and atoms on the opposite surface once an initial configuration is set. For each atom inside surface 1 as defined in Fig. 4, the nearest neighbor on surface 2 was determined and the associated nearest neighbor distance was computed. We defined the deviation of this distance from ideal as:

$$r_{\text{NN}} - r_{\text{ideal}}$$

where $r_{\text{NN}}$ is the nearest neighbor distance and $r_{\text{ideal}}$ is the expected distance between two atoms assumed to be equal to $f \times (\text{sum of the covalent radii})$. $f = 1$ was used in generating the scores reported in Section 3. The covalent radii of the elements used to compute the distances were measured.

The squared deviations over all atoms inside the supercell on surface 1 were averaged and used to enhance effects of large deviations and reduce effects of small ones. The calculations were repeated with surfaces 1 and 2 interchanged to account for the fact that atoms inside the supercells on two distinct surfaces can have different nearest neighbors. A final score for a given configuration and combination of planes was generated by averaging the two scores. In this case, scores as close to 0 as possible are preferable, since a good configuration is characterized by most atoms being separated by distances as close as possible to the expected bond length.

2.3.2. Electronegativity difference criterion

For each atom inside a supercell on surface 1 all neighbors on surface 2 were identified. The electronegativity differences between the atoms on surface 1 and their nearest neighbors on surface 2 were computed. To compute electronegativity differences between atoms we used the Pauling scale values of the electronegativities of the elements, $\epsilon_P$, from [11].

Average electronegativity differences for the atoms inside a supercell on surface 1 were generated and averaged over all atoms. Similarly to the approach described previously, the calculations were repeated with surfaces 1 and 2 interchanged. The final score was divided by the maximum electronegativity difference between two atoms on surfaces 1 and 2 respectively. Assuming ‘good’ configurations maximize the average electronegativity difference between atoms on the two surfaces, best scores are the ones closest to 1. For single element crystals scores of 1 are generated as long as all atoms on the two surfaces have at least one nearest neighbor.

3. Results

We have demonstrated our methodology on heterocrystals of several combinations of materials. GaAs on CdTe was chosen to validate the lattice matching algorithm. PtNi$_3$ on Pt$_3$Co was chosen as an important application to catalysis. Si on GaP was chosen because it allowed a comparison with DFT data that was published by [12]. SiO$_2$ on Si was chosen due to their importance in semiconductor technology.

3.1. GaAs on CdTe

The lattice matching algorithm was tested by considering combinations of GaAs and CdTe surfaces and comparing the results with the ones reported in scientific literature. These two materials are treated in detail in [2]. We were able to reproduce the main result of this work, finding matching superlattices with $p$ and $q$ as defined in Section 2.1 equal to 4 and 3 respectively for the GaAs and CdTe surfaces.

3.2. PtNi$_3$ on Pt$_3$Co

Here, we examine heterocrystal combinations of PtNi$_3$ [13] and Pt$_3$Co [14] given these alloys are used as cathode catalysts in fuel cells. Both alloys have face-centered-cubic structures and have similar lattice parameters. For each material, we considered cuts along the (100), (110), and (111) planes. For this system, $p$ and $q$ are equal. Table 1 shows the nearest neighbor (NN) and electronegativity (EN) scores of the best matches. We see that the best EN score is between either two (110) or two (100) surfaces. This is because there are cuts along these directions that are 100% Pt for Pt$_3$Co and 100% Ni for PtNi$_3$, which when formed into a heterocrystal, maximize the EN difference. For the (111) surface, it is impossible to avoid Pt–Pt or Co–Ni bonds, making the electronegativity difference non-ideal and lowering the EN score.

We evaluate the (111) surface further because it is the most atomically dense and the surface cut of lowest energy. We performed further DFT calculations to verify the scoring algorithm. We compared the DFT mixing energy between two slabs of the (111) configuration that have different scores in Table 2. These two configurations correspond to different alignments.

Config. 1 has a better EN score of 0.76 and we see that it has better mixing energy of $-241$ meV/$\AA^2$. The reason Config. 1 has a higher EN score is because it results in stronger bonds between the Pt and Co. For Config. 2 with the lower EN score of 0.43, the Co at the interface is always bonded to Ni on the PtNi$_3$. The smaller electronegativity difference between Co and Ni compared to Co and Pt results in a lower EN score for Config. 2 than for Config. 1 which favors Co–Pt bonds. Config. 2 also has a nonzero NN score,
which confirms that a heterocrystal interface is less likely to form than in the case of Config 1. The positive NN score indicates that there is a deviation of the distance between Co and Ni from $t_{\text{ideal}}$ in the latter configuration.

### 3.3. Si on GaP

The interface of Si on GaP has been studied by [12] with DFT. They found that the interface energies for (111)/(111), (311)/(311), and (110)/(110) are 33.1 meV/Å², 32.4 meV/Å², and 14.2 meV/Å² respectively (note that the interface energy as defined in [12] is different from $E_{\text{int}}$ defined by us below; it does not include the contribution of the top and bottom surface, and therefore is a positive number). Our algorithm assigns high scores to these three interfaces (cf. Table 3), which confirms that the algorithm does indeed distinguish in general good from bad interfaces. The exact order of these 3 interfaces is not properly reproduced, which is not surprising, and which is the reason that DFT is needed in a subsequent step.

### 3.4. Si on SiO$_2$

The ICSID lists 38 different SiO$_2$ structures and 11 different Si structures. We considered 4 different SiO$_2$ structures and 2 different Si structures. Table 4 lists the tested structures.

For each material, we considered cuts along the (100), (110), (111), and (210) planes. In all, we found and scored 128 configurations. Table 5 lists some of the resulting interfaces and the associated scores.

The SiO$_2$ surface for the first interface in Table 5 contains only O atoms, while those of the second and third entries contain only Si atoms. This explains why the associated EN scores are relatively high: there are only Si–O or Si–Si bonds across each interface, both corresponding to maximum EN assignments of 1 between pairs of nearest neighbor atoms. EN scores which are not exactly 1 indicate that some atoms at the interface have no nearest neighbors. For the last two interfaces in Table 5, the SiO$_2$ surface contains both Si and O, with the reference element for the EN score being O. A low electronegativity difference score associated with a low nearest neighbor score for the (110) Si (Zn Blende)-(110) SiO$_2$ (Quartz, $\beta$) interface suggests that Si–Si bonds dominate. The highest nearest neighbor score for the (110) Si (Wurtzite)-(111) SiO$_2$ (Tridymite) interface suggests that some atoms are under-coordinated. The (110) Si (Zn Blende)-(110) SiO$_2$ (Quartz, $\beta$) interface should be preferred due to apparent high bond density at the interface.

As discussed earlier, the next step in a thorough prediction of interfaces is to rank the most likely candidate configurations with DFT. Here, we will use DFT to show that for the two most promising interfaces this is indeed a feasible approach, and that our algorithm does indeed give useful results in the quest of reducing the pool of candidate configurations. We have calculated the interface energy $E_{\text{int}}$ for two possible configurations of (111) Si (Zn Blende)-(100) SiO$_2$ (Cristobalite $\beta$). We define the interface energy as the difference between the energy of the entire system (with the substrate and deposit joined) and the energy of the system given deposit and substrate separated (with the surfaces that otherwise form the interface completely exposed). Thus, a negative value for $E_{\text{int}}$ means that the two sub-systems want to join each other (and form an interface), while a positive value for $E_{\text{int}}$ means that the substrate and deposit prefer to be separated.

The FHI-AIMS [15] code was used for all DFT calculations presented here. It is an all electron code that uses atom centered basis sets and DFT exchange-correlation functional (PBE [16]). The CPU time it took to do 128 configurations with our algorithm was 880 s and we note that our algorithm was not yet optimized for computational speed. On
the other hand, the CPU time for DFT calculations to determine the interface energy of one configuration is approximately two weeks. This is the reason for not presenting detailed DFT results in this paper.

The most stable heterocrystal from the DFT calculations was found to be Config. 2 in Table 6 with an energy of ~58.1 meV/Å. This shows that the algorithm is able to find probable heterocrystal configurations that are energetically favorable to form between Si and SiO2. The reason Config. 2 has a lower DFT energy than Config. 1 is that the atoms along the interface rearrange quite a bit during the relaxation step. In contrast, the EN and NN scores are based on the bulk atomic configuration. Therefore, the predicted scores work best and give the correct order when the atoms do not move much from their bulk positions after the heterocrystal forms, as in the case of PtNi3 on Pt3Co. On the other hand, the Si and SiO2 DFT results show that the configuration with a worse score actually formed a better heterocrystal, due to the atoms relaxing and moving away from their bulk position after the heterocrystal forms.

### 4. Conclusions

We have developed an algorithm to generate any two crystal structures from the ICSD, cut them along different planes and rapidly screen all possible combinations in order to determine the ones likely to form hetero-crystals. Since the method we developed was based entirely on a combination of geometry and local chemistry, more detailed methods may be necessary to cover the range of different materials. For example, we started from the assumption that epitaxial growth is only possible if the lattices of the two crystalline surfaces match. This assumption has been confirmed experimentally in many cases [2,7,17], but does not apply to non-periodic surfaces and may not hold for very complex interfaces. Our algorithm generates the smallest possible “parallelograms” or supercells of nearly equal areas to within a set precision, with corners at lattice points. The effect of the area tolerance as described in Sections 2.1 and 3.1 needs to be investigated in more detail. Relaxing the area tolerance leads to smaller values of p and q as defined in Section 2.1 (which may be more realistic), but it will increase the difference in areas of the resulting supercells. It is reasonable to believe that larger supercells are an indication of the fact that the interfaces have very different symmetries, thus it would be less probable for a hetero-crystal to form in practice. However, the smaller the supercells, the smaller the number of possible superlattices, so the less likely it is to find a good match. More tests need to be done to find a balance between these two factors. We believe the limit on the supercell sizes which still allow for hetero-crystal formation is strongly dependent on the test materials and can only be determined experimentally.

The purpose of our method is to rapidly find and rank possibly good configurations and combinations of planes and generate an output which can be used for further modeling. Further use of quantum mechanical calculations to estimate interfacial energies is still crucial as the next step in predicting heterocrystal formation accurately. In our approach we assumed that the ideal bond length between two atoms is roughly equal to the sum of their covalent radii. This is not always the case and our algorithm could potentially place the two surfaces too close together or too far apart. This in turn influences the scores associated with the configurations and therefore their ranking. For example, the bond distance between Pt and Co atoms in the bulk was found to be close to 1.04(r_{\text{Pt}} + r_{\text{Co}}), whereas in the case of other materials this might reach 0.9(r_{\text{atom}} + r_{\text{mole}}). These approximations might be improved by generating a list of expected bond lengths for pairs of elements, rather than storing covalent radii of single elements.

The current scoring methods can be improved and other ways of evaluating the surfaces can be developed. Our algorithm is set up in such a way that it allows for other scoring methods to be incorporated. For example, one suggestion would involve counting the electrons in the outer shells of nearest neighbor atoms on the two surfaces. However, this method might be difficult to implement for transition metals since in this case the outer shells can have several valid electronic configurations. Another approach that we are currently working on is to include a hierarchy of empirical potentials of increasing accuracy (and increasing computational cost) to reduce the number of configurations obtained with geometric methods, before using DFT.

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