



Article A Linear Strain-Free Matching Algorithm for Twisted Two-Dimensional Materials

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Abstract: As nano-electronic technology makes electronic devices gradually microscopic in size and diversified in function, obtaining new materials with superior performance is the main goal at this stage. Interfaces formed by adjacent layers of material in electronic devices affect their performance, as does the strain caused by lattice mismatch, which can be simulated and analyzed by theoretical calculations. The common period of the cell changes when the van der Waals (vdW) material is twisted. Therefore, it is a significant challenge to determine the common supercell of two crystals constituting the interface. Here, we present a novel cell matching algorithm for twisted bilayer vdW materials with orthogonal unit cells, where the resulting common supercell remains orthogonal and only angular strains exist without linear strains, facilitating accuracy control. We apply this method to 2-*Pmmn* twisted bilayer borophene. It can automatically find the resource-allowed common supercell at multiple rotation angles or fix the rotation angle to find the proper accuracy.

Keywords: lattice mismatch; twisted 2D material; algorithm; DFT calculations



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1. Introduction

Due to the rapid development of nano-electronics, electronic devices are gradually breaking through the barriers of their original size and dimensions, and this breakthrough has also led to a significant improvement in their performance [1,2]. In many cases, two layers of materials in an electronic device come into contact to form a new interface. The changes that occur at the interface affect the performance of the electronic device, unexpectedly not depending on the nature of the material itself [3,4]. In addition, the interface between two disproportionate materials generates unavoidable strains, which can strongly affect their mechanical and electronic properties. The interface structure can be characterized experimentally by transmission electron microscopy [5], X-ray diffraction [6], etc. However, complex internal atomic configurations are difficult to determine experimentally, and assessing the stability of the interface requires repeated tests that are time and material intensive. Therefore, the construction of accurate models is a necessary prerequisite to simulate and analyze the interface properties at the atomic scale and to provide some assistance for the design and development of electronic devices.

Van der Waals (vdW) interactions between two-dimensional (2D) materials have opened up new directions for selecting new materials for electronic and optoelectronic devices [7,8]. Such a material represents a so-called vdW material, which is composed of multiple monolayers connected by weak vdW forces and from which the layers can thus be stripped off relatively easily. They can also be stacked on other materials by vdW forces independently of chemical bonding, forming vdW heterostructures [9–13], which are potential materials for high-performance nano- and optoelectronic devices. Among them, the twisting effects in stacked 2D materials have sparked interest in multilayer structures composed of various monolayers. Further modulation of the electronic properties can be achieved by precise control of the interlayer rotation angle. Nevertheless, cell matching is a difficult issue for the theoretical calculations and analysis of twisted materials. After twisting two layers of fabric, though the structures of the upper and lower layers remain

the same, the common period of the two crystals has changed, while the periodic cell structure is the foundation for theoretical calculations. Therefore, to study the interface properties, it is first necessary to determine the common supercell of the two crystals forming the interface.

Recently, researchers have come up with various approaches to this problem. Predrag Lazić et al. [14] used the method of enumerating lattice vectors to seek the common period of the interface between two materials with a given accuracy, where one of the materials would generate a particular strain to match the other. The method proposed in this work applies to searching for the minimum common period under the condition of a given lattice vector. However, the cell periods for different rotation angles cannot be searched automatically. In response to this issue, Daniele Stradi et al. [15] proposed a more specific matching scheme, which is divided into cell expansion, rotation, and strain, and can search for the smallest common period at different rotation angles. Line Jelver et al. [16] further proposed a matching algorithm for the 3D case. The lattice matching method in a program, ARTEMIS, developed by Ned Thaddeus Taylor et al. [17] is similar to it and is accomplished through three stages: cell generation, vector match, and angle match. Daniel S. Koda et al. [18] proposed a coincidence lattice method to find a solution that minimizes the area of the supercell. However, the global smallest common supercells found by these methods mentioned above tend to have low symmetry, which is not conducive to the subsequent simulation calculations. Bo Gao et al. [19] designed a lattice match toolkit that can automatically search for a superlattice with minimal lattice-mismatch strain between two materials by requiring only unit cells instead of the specific surface vectors. However, the two structure models it uses have some limitations. Félix Therrien et al. [20] tried a new approach that transforms crystal matching into an optimization problem by finding the best atom-to-atom map that minimizes the Euclidean distance between the atoms. Shiddartha Paul et al. [21] built a simulation cell by stretching the overlayer to match the supercell of the substrate and found the periodic variation in the mismatch strain versus the number of unit cells in a supercell. Dumitru Dumcenco et al. [22] constructed a simple model of adsorption accounting only for pairwise atom-atom interactions instead of introducing artificial strain. The model structures obtained by these methods are often not orthorhombic systems and have significant distortions. Moreover, these algorithms tend to introduce matching strains and rotation angles during cell matching, which is not suitable for cell matching where a fixed rotation angle is required.

We propose a cell matching method to address these problems, which is suitable for twisted bilayer vdW materials with orthogonal unit cells. The method can calculate the common period for maintaining the orthogonal cell with a given accuracy, that is, satisfying the three problems mentioned above. However, it should be noted that the common supercell obtained by this method is not necessarily the smallest supercell considering the maintenance of the orthorhombic structure. Nonetheless, the orthogonal system creates a significant start for further experimental or theoretical studies. Under the condition of a given rotation angle, this algorithm finds the nearest lattice point that meets the accuracy requirement by applying the successive approximation method to the angle bisector. Afterward, the method of lattice redefinition is used to make the cells of the upper and lower layers overlap, which keeps the rotation angle constant and the redefined lattice still orthogonal. In addition, unlike the other matching algorithms, which have both shear and normal strains, the algorithm proposed in this paper only has shear strains, which makes the precision control efficient and straightforward. It is worth mentioning that the presence of shear lattice deformation is also an effective way of regulating the key properties of heterostructures [23].

2. Materials and Methods

2.1. Algorithm Details

After setting a series of rotation angles, the program can automatically find common supercells under all rotations and sort the angles by the specific surface area, making it easy for the user to find the rotation angles allowed by computing resources. Further, the program can also investigate the relationship between the accuracy of the rotation angle and the supercell size by setting a fixed rotation angle with a series of unfixed precisions to find the appropriate accuracy at that rotation angle. The working of this cell matching algorithm is shown as a flowchart in Figure 1.



Figure 1. Flow chart of the cell matching algorithm.

By interpreting the model data in the POSCAR file, which is the mandatory VASP input file and contains the lattice geometry and the ionic positions of material, the matrix made up of all the atomic coordinates becomes the dot matrix. The program records the data about the lattice vectors and atomic coordinates of the material model. At the same time, the program establishes the lattice coordinate system and performs lattice redefinition. After setting the calculation accuracy and the rotation angle of the bilayer structure, the program constructs the angular bisector of the rotation angle and finds the lattice points on the angular bisector by a successive approximation method. Eventually, after finding the lattice points that meet the accuracy requirement, common supercells of the twisted bilayer material can be created, and the supercell sizes can be evaluated using the criterion of specific surface area. The program saves all the parameters and writes them to the new POSCAR file. In the following, we provide the details of the algorithm.

2.1.1. Lattice Redefinition

In terms of the bilayer structure (Figure 2a), when the adjacent surfaces are deflected by a certain rotation angle, as shown in Figure 2b, the original unit cell does not correctly describe the periodicity shared by the upper and lower surfaces. Therefore, the unit cell of the twisted bilayer structure needs to be redefined. Solving this starts from a specific situation. When the upper and lower surfaces of the same orthorhombic lattices are rotated by exactly 90°, as in Figure 2c, the lattice constant after rotation is the least common multiple of the two lattice constants, and the lattice vectors remain orthogonal. Similarly, when the rotation angle of the upper and lower surfaces is not 90°, the primitive lattice vector of one surface can be redefined as a vector in the direction of the primitive lattice vector of the other surface. If the cell points in the primitive cell are arranged periodically, a lattice dot matrix can be obtained, and a lattice coordinate system can be established with the lattice dots. It can be concluded that the cell formed by any two non-collinear vectors of the lattice dot matrix is equivalent to any cell under the periodic boundary condition. Figure 2d shows that the blue, green, and red cells are equivalent to each other, so one can be redefined as the other cell. Starting from the unit cell of one surface with primitive vectors (\vec{a}, \vec{b}) , a new supercell consisting of vectors $(\vec{\mu}, \vec{\nu})$ can be constructed from the lattice redefinition. The expression is described as:

$$\vec{\mu} = n_{11}\vec{a} + n_{12}\vec{b} \tag{1}$$

$$\vec{\nu} = n_{21}\vec{a} + n_{22}\vec{b}$$
(2)

in which n_{ij} are the components of the redefined lattice vectors on the primitive ones, taken as a positive integer. n_{ij} can form a 2 × 2 square matrix *N*. *N* takes the form [24]:

$$N = \begin{pmatrix} n_{11} & n_{12} \\ n_{21} & n_{22} \end{pmatrix}$$
(3)



Figure 2. (a) Atomic configuration and primitive cell of borophene; (b) sketch diagram of twisted bilayer borophene; (c) 90° -twisted bilayer borophene; (d) sketch diagram of lattice redefinition. The black dotted line indicates the crystal cell. Blue lines indicate non-twisted structures, orange lines indicate twisted structures, and red dashed lines are angle bisectors.

2.1.2. Supercell Matching

A primitive lattice dot matrix is a dot matrix formed by multiple, periodically arranged primitive crystalline cell sites. Let \vec{a}^t be the lattice vector of one surface, where *t* represents rotation. If $\vec{\mu}$ is to be made collinear with \vec{a}^t , i.e., $\vec{\mu} = k \vec{a}^t$, it can be deduced that there

is at least one lattice point of the primitive lattice dot matrix falling in the $\vec{\mu}$ direction. Furthermore, the lattice constant of the common supercell of the twisted bilayer structure is the least common multiple of the length of the redefined lattice vector $|\vec{\mu}|$ and the length of the primitive lattice vector after rotation $|\vec{a}^t|$. This is a simple way to obtain the common period of a twisted bilayer structure.

However, it should be noted that, on the one hand, lattice constants in theoretical calculations are often floating-point numbers, so accuracy errors need to be introduced in solving the least common multiple of two lattice vectors. Meanwhile, the potential demand for the smallest possible supercell size also requires introducing accuracy errors. On the other hand, it is sometimes difficult to find the lattice points of the original lattice dot matrix that fall in the \vec{a}^{t} direction when redefining the lattice vector. Two cases need to be discarded. Firstly, the distance between the lattice point and the origin is large, making the common supercell size larger and the number of atoms higher, making the subsequent theoretical calculation difficult or even impossible. Secondly, there is no lattice point in the \vec{a}^{t} direction when the problem has no solution. It is worth noting that, in reality, an utterly ideal state of the material in the process of mutual bonding via vdW forces can hardly exist, and it is more or less subject to strain. Consequently, under certain circumstances, it is reasonable to treat specific accuracy errors in the calculation as the strain generated

in practice. The strain tensor ε in a deformed surface is a symmetric matrix defined as [15]:

$$\varepsilon = \begin{pmatrix} \varepsilon_{xx} & \varepsilon_{xy} \\ \varepsilon_{yx} & \varepsilon_{yy} \end{pmatrix} \tag{4}$$

 ε_{xx} and ε_{yy} are uniaxial tensile strains along the x and y directions, respectively, which are called linear strains in the following. ε_{xy} and ε_{yx} are shear strains, which are called angular strains in the following. Then, a unified coordinate system is introduced to rotate the vectors of the supercells $(\vec{\mu}, \vec{\nu})$ and (\vec{a}^t, \vec{b}^t) , so that $\vec{\mu}$ and \vec{a}^t are aligned along the *x*-axis to facilitate the calculation of the strain tensor ε . At this point, $\mu_y = a^t_y = 0$. A 2 × 2 matrix *e* is applied on one of the supercells to match the other [19]:

$$\varepsilon = \frac{1}{2}(e + e^T) - I \tag{5}$$

$$(p\overrightarrow{\mu}, m\overrightarrow{\nu}) = e \cdot (q\overrightarrow{a}^t, n\overrightarrow{b}^t)$$
(6)

The errors introduced by cell redefinition and the solution of the least common multiple of the lattice vectors are both present in the literature and can often be converted into linear and angular strains generated by the configuration. The specific calculation can be derived from Equations (4)–(6), so that:

$$\varepsilon_{xx} = \left| \frac{p\mu_x}{qa^t_x} \right| - 1 \tag{7}$$

$$\varepsilon_{yy} = \left| \frac{m v_y}{n b^t_y} \right| - 1 \tag{8}$$

$$\varepsilon_{xy} = \frac{1}{2} \frac{m v_x - \frac{p \mu_x}{q a^t_x} n b^t_x}{n b^t_y} \tag{9}$$

in which $p\vec{\mu} = q\vec{a}^t$, $m\vec{\nu} = n\vec{b}^t$. The strain can be borne by one surface or shared by both surfaces. If taking the latter approach, the strain in each surface is half of that borne by one.

2.1.3. Angular Bisector Matching Method

Figure 3a shows a sketch diagram of the lattice vector matching method. If the original monolayer cell is orthogonal, it is possible to find the orthogonal cell of the bilayer structure with a given accuracy using this method. Further, based on this work, we propose constructing angular bisectors to realize lattice matching and eliminate the linear strain in the matching process, while only the angular strain exists, and effectively control the balance between strain and size.



Figure 3. (a) The lattice vector matching method; (b) the angular bisector matching method; (c) lattice redefinition for the original layer of the bilayer structure; (d) lattice redefinition for the twisted layer of the bilayer structure.

Figure 3b shows that instead of finding the lattice point on the straight line where the lattice vector is located after twisting, the lattice point is found by constructing the angle bisector of the deflection angle and finding the lattice point on the angle bisector. Assuming that in the lattice coordinate system of the non-twisted monolayer structure, the coordinates of the lattice points on the two angular bisectors are (-p,q) and (m,n), respectively. Then, the lattice vectors of the non-twisted monolayer structure can be redefined as the vectors $\vec{\mu}(-p,q)$ and $\vec{\nu}(m,n)$, as shown in Figure 3c. Furthermore, if the cell is orthogonal (Figure 3d), it can be concluded that the above $\vec{\mu}$ and $\vec{\nu}$ are lattice vectors of the twisted monolayer structure, and the coordinates in its lattice coordinate system are (p,q) and (m, -n), respectively. As a simple proof, if the unit cell is orthogonal, the following conclusions can be drawn that its structure is mirror-symmetric about any lattice vector. When there is a rotation angle between the two layers, it is easy to obtain that the bilayer structure is mirror-symmetric about the angle bisector. Therefore, if the lattice point of one surface falls on the angle bisector, the other surface must have the same lattice point falling on the angle bisector. Conversely, if it is required that the lattice points in the bilayer structure falling on the angle bisector are the same, the vectors \vec{v} and \vec{v}^t corresponding to the lattice point must be equal, namely, $|m\vec{a} + n\vec{b}| = |m\vec{a} - n\vec{b}|$, then $\vec{a} \cdot \vec{b} = 0$, that is to say, the unit cell is orthogonal. Therefore, the algorithm requires the unit cells to be orthogonal. For non-orthogonal unit cells, it is often feasible to convert them to orthogonal unit cells, so the algorithm still has an extensive range of applicability.

The coordinates of the lattice points near the angle bisector can be solved directly within a given precision limitation. First, assuming that the rotation angle is θ , the slope of the angle bisector is $k = \tan(\theta/2)$. In the case of known lattice constants, we can obtain $b \times n/a \times m = k$, i.e., n/m = ck. Arbitrarily, take ck = 1.1425, if the given accuracy is 0.1,

then n/m = 11/10 after the reduction. Thus, the coordinate of the lattice point (11, 10) can be taken. However, the lattice point obtained by the simple reduction method may not be the nearest one satisfying the precision requirement. In the above example, if the lattice point is (8, 7), the accuracy error is about 0.00036, which is smaller than that of (11, 10) while the size is also smaller.

2.1.4. Successive Approximation Method

To avoid the lattice points that are not the nearest neighbors when directly approximated at a given accuracy, the successive approximation method is used to obtain the point that meets the accuracy requirement. A sketch diagram of the successive approximation method to find the nearest lattice point is shown in Figure 4. The red dotted line indicates the direction of the angle bisector of the twisted bilayer structure. Due to the symmetry, only one direction needs to be considered. The specific steps of the successive approximation method are as follows. First, take the lattice point **A**, calculate the corresponding slope of the point. If the slope of the lattice point is smaller than the slope of the angle bisector, take one lattice point upward, i.e., point **B**. If the situation is just the opposite, take one lattice point to the right, i.e., point C. Repeat the calculation steps until the lattice point meets the accuracy requirement. From the approximate method above, when the coordinates of the lattice points are large enough, the lattice point with the required accuracy can always be obtained. In addition, it should be noted that for a certain numerical accuracy, the slope is not uniform over different angles. Therefore, the angular accuracy rather than the slope accuracy is needed. In summary, the successive approximation method can be summarized in the following equation:

$$\left(\operatorname{arctan}\left(\frac{bn}{am}\right) < \frac{\theta}{2} \to n = n+1$$

$$\operatorname{arctan}\left(\frac{bn}{am}\right) > \frac{\theta}{2} \to m = m+1$$

$$(10)$$

where θ is the rotation angle.



Figure 4. Successive approximation method. Red dashed line is angle bisector.

Although the computational effort of the successive approximation method is greater than that of the direct reduction method, the computational effort increases geometrically for each additional atom in the theoretical calculation. Therefore, as long as the cell size can be reduced as reasonably as possible, the successive approximation method is still worthwhile for the total simulation time spent.

2.1.5. Supercell Sizes Evaluation

After constructing angular bisectors and using the successive approximation method, the information of the common supercell of the bilayer structure can be obtained. As mentioned before, the supercell size has a significant influence on the entire calculation.

An excessive size can even make the calculation impossible. Therefore, after obtaining the common supercell, a thorough evaluation of the size is required. Assuming that the lattice point coordinates of the two lattice vectors of the common supercell are (-p,q) and (m,n), the lengths of the two lattice vectors are $L1 = \sqrt{(a \times m)^2 + (b \times n)^2}$ and $L2 = \sqrt{(a \times p)^2 + (b \times q)^2}$, respectively. In this paper, the specific surface area is taken as the evaluation quantity of the supercell size, which is defined as $S = L1 \times L2/a \times b$. If the number of atoms in the primitive unit cell of the monolayer structure is N, the number of atoms in the common supercell of the twisted bilayer structure can be obtained as $2 \times S \times N$. Supposing that the number of atoms in the primitive unit cell of the twisted bilayer borophene is 2, the number of atoms in the common cell of the twisted bilayer borophene is $4 \times S$.

2.2. Elastic Contribution to the Interface Energy

Additional elastic contributions are introduced into the interface energy due to the presence of strains in the structures on both sides of the interface, and the magnitude of the contribution is strongly related to the strength of the interaction between the upper and lower surfaces. For the upper and lower surfaces with orthorhombic symmetry, we can write the total energy per unit area as [15]:

$$E = E^{int} + E^{surf} + (\frac{1}{2}\varepsilon_{xx}^{2}C_{11} + \frac{1}{2}\varepsilon_{yy}^{2}C_{22} + \varepsilon_{xx}\varepsilon_{yy}C_{12} + 2\varepsilon_{xy}^{2}C_{44})t$$
(11)

in which E^{int} is the interface energy between the upper and lower layers, E^{surf} is the energy of the free surface of the upper layer, ε_{xx} , ε_{yy} , and ε_{xy} have already been defined in Equations (7)–(9), C_{11} , C_{12} , and C_{44} are the elastic constants of the upper layer material, and t is its thickness. Since the algorithm eliminates the linear strain by the angular bisector matching method and only the angular strain exists, the equation can be further simplified as:

$$E = E^{int} + E^{surf} + 2\varepsilon_{xy}^2 C_{44}t \tag{12}$$

Neglecting the interaction between the interface and the upper free surface and the effect of strain, E^{surf} will not depend on the interface geometry. For weak interfaces, the interface energy E^{int} is expected to be independent of geometry. Thus, the contribution of elastic energy plays the vast majority of the role and will influence the stability trends for different geometries.

2.3. Accuracy

After giving the details related to the cell matching algorithm, we analyzed the relationship between accuracy and structural strain. As shown in Figure 5, the blue lattice point obtained by the cell matching algorithm tends not to fall on the angle bisector, so some angular error exists. Assuming the given accuracy is *E*, the angular error in the lattice point of the non-twisted monolayer structure is $-\Delta 1$, then $|-\Delta 1| < E$. Furthermore, due to the symmetry, the angular error in the lattice point of the twisted monolayer structure is $\Delta 1$. Similarly, for the other lattice vector, there is $|\Delta 2| < E$. When the two layers overlap through strain, the angular strain can be obtained as $\varepsilon_{\theta} = 2 \times (\Delta 2 - (-\Delta 1))$, i.e., $\varepsilon_{\theta} < 4E$. When the strain is equally distributed to each layer of the structure, the strain in each layer is 2*E*.

2.4. Cartesian Coordinate System Conversions

The data conversion method of the calculation file in VASP to this cell matching algorithm should be supplemented. In the structure file named POSCAR in VASP, the lattice vector is often defined in the Cartesian coordinate system. If the original lattice vector is:

$$\vec{a} = a_x \vec{x} + a_y \vec{y}$$
(13)

$$\overrightarrow{b} = b_x \overrightarrow{x} + b_y \overrightarrow{y} \tag{14}$$

Combining with Equations (1) and (2), the lattice vector of the common supercell is obtained in VASP as:

$$\vec{\mu} = (n_{11}a_x + n_{12}b_x)\vec{x} + (n_{11}a_y + n_{12}b_y)\vec{y}$$
(15)

$$\vec{\nu} = (n_{21}a_x + n_{22}b_x)\vec{x} + (n_{21}a_y + n_{22}b_y)\vec{y}$$
(16)

For the atomic coordinate of a point (x, y) in the common period, from Equations (1) and (2) it can be deduced that:

$$x \quad y \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} x & y \end{bmatrix} N^{-1} \begin{bmatrix} u \\ v \end{bmatrix}$$
 (17)

i.e., $\begin{bmatrix} x & y \end{bmatrix} N^{-1}$ is the coordinate value for this atom in the coordinate system defined by the lattice vector of the common supercell. Furthermore, lattice redefinition and the establishment of bilayer structures can be achieved using the existing modeling tools.



Figure 5. Accuracy analysis of cell matching algorithm. Blue lines indicate non-twisted structures, orange lines indicate twisted structures and red dashed lines are angle bisectors.

3. Results

3.1. Computational Details

In this section, the cell matching algorithm proposed above is applied to the structure of twisted bilayer borophene as an example. All simulation results were obtained using density functional theory (DFT) implemented in the Vienna Ab Initio Simulation Package (VASP). The electron–ion interactions were described by the projector-augmented wave (PAW) potentials [25]. The exchange and correlation (XC) were described using the Perdew–Burke–Ernzerhof (PBE) approximation under the generalized gradient approximation (GGA) [26]. For the bilayer structure, the optPBE-vdW model is adopted, considering the interlayer vdW forces. Our algorithm required the lattice constants of the smallest unit cell of the monolayer borophene as raw data, where a = 1.614 Å and b = 2.865 Å, in good agreement with previous results [27]. The visualization of the model structure was achieved using Material Studio. Full relaxation of the model is required before it can be used for DFT calculations to avoid very few adjacent layer atoms being too close together.

3.2. Twisted Bilayer Borophene

Currently, bilayer borophene has been reported to be generated on Ag(111) and Cu(111) substrates, and they are more stable than monolayers due to bonding coupling between the layers [28,29]. Further, the injection of rotation angles allows the bilayer structure to exhibit

more interesting properties, such as superconductivity in twisted bilayer graphene [30,31]. This shows that the accurate construction of different twisted bilayer structures is an important basis for predicting the specific properties of the material. As shown in Figure 2a, the 2-*Pmmn* borophene shows a longitudinal armchair shape and a transverse zigzag shape, where the black dashed line marks one of the primitive cells with periodicity in the monolayer borophene.

As shown in Figure 6, aiming at bilayer borophene, we calculated the specific surface area of the common supercell and the unit cell at rotation angles from 10° to 90° using the cell matching algorithm. Figure 6a,b correspond to accuracies of 0.5 degrees and 0.05 degrees, respectively. Obviously, the comparison of different accuracies shows that the higher the accuracy, the larger the supercell size. In addition, there are larger supercell sizes at about 60° and 83° rotation angles. Furthermore, the variation in specific surface area with angle is not monotonic but constantly fluctuates, which may be related to the crystal orientation of the common supercell fixed by this cell algorithm.



Figure 6. The specific areas of the common supercells of bilayer borophene corresponding to different angles obtained by the cell matching algorithm under the accuracies of (**a**) 0.5 degrees and (**b**) 0.05 degrees are calculated.

The band structures of bilayer borophene with torsion angles of 32.2°, 58.0°, and 83.6° under the accuracies of 0.5 degrees and 0.05 degrees are tested [32]. Unlike single-layer borophene and multilayer boronene without torsion angles [33], the torsion angle of twisted bilayer boronene can split the bands and transform the bands into straight lines, similar to the Dirac cone band structure, suggesting that this type of double-layered torsional boronene may have a superconducting property similar to that of graphene, and at the same time, the torsion angle can effectively regulate the electrical properties of the double-layer torsion boronene and produce peculiar and rich properties.

4. Conclusions

This paper presents a cell matching algorithm for twisted bilayer orthogonal structures. As for hexagonal or trigonal grids, the principle of our algorithm is still valid after adjusting the parameters of the algorithm. Compared with the previous work, the algorithm has the advantages of (1) less computational effort; (2) only angular strain is generated and the algorithm can effectively control the supercell size by changing the accuracy; and (3) for the orthogonal cell in a monolayer structure, the common supercell of its twisted bilayer structure is still orthogonal. From the perspective of algorithm design, the starting point of previous work is often to find the smallest common supercell of different materials, while the starting point of this work is to find the supercell that remains orthogonal for a given rotation angle of a bilayer vdW material. Thus, this work allows a reasonable model to be found with small mismatch strains in the bilayer vdW materials with specified

torsion angles under conditions of customized accuracy. The strategy of this algorithm can also provide ideas for lattice matching of multilayer materials. However, compared with other algorithms, the algorithm has the disadvantages of (1) the common supercell is not necessarily the global minimum; and (2) the limitations of the applications.

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