|  |  |
| --- | --- |
| 姓名： | 王建伟 |
| 电子邮箱： | Jianwei\_wang@uestc.edu.cn |
| 代码所用编程语言： | Fortran |
| 代码已实现功能：   1. 可构造异质结的体系：x-y平面内基矢为六角晶格（比如60°，120°）或者直角晶格（90°），z方向为异质结生长方向； 2. 通过旋转矩阵以及平移操作实现不同堆叠顺序的设置； 3. 可设置真空层的厚度； 4. 可设置异质结界面处的层间距； 5. 可以完成5种基本的异质结搭建； | |
| 操作说明（请附上操作截图）：  共有3个程序，需要3个步骤：  （1）读入输入的两个结构，获得晶格参数，运行lattice\_match\_hex.f(六角) 或者lattice\_match\_rect.f(直角)，搜索寻找晶格匹配的可能结构，输出相应的旋转矩阵TRAN\_A1, TRAN\_B1,TRAN\_A2, TRAN\_B2, 等等；  （2）利用上一步得到的旋转矩阵，运行vaspkit得到变换后的超元胞结构，分别为SUPERCELL\_A.vasp 和SUPERCELL\_B.vasp;  (3) 以第（2）步得到的两个超元胞结构为输入，将两个超元胞结构组合起来，可设置真空层高度，界面处的层间距，平移矢量等。  **2D/2D异质结简单版本**：  AA  编译lattice\_match\_hex.f，即ifort -o lattice\_match\_hex.x lattice\_match\_hex.f, 并运行lattice\_match\_hex.x,得到多个旋转矩阵，选取第一组如下  TRAN\_A1=  TRAN\_B1=  运行heterojunction\_building.x,将在屏幕上显示如下提示内容，按要求输入参数设置：  input the height of vallcum:  15  input the distance between nearby layers  3  MoS2  3.19031572340000  3.19031572343695  Found 2 atom type(s)  Number of atom for each type:  Type No.  1 1  2 2  Total No. atom: 3  A off\_centre = (x,y,z) as new origine  0 0 0  9  WSe2  3.32706928250000  3.32706928252858  Found 2 atom type(s)  Number of atom for each type:  Type No.  1 1  2 2  Total No. atom: 3  B off\_centre = (x,y,z) as new origine  0 0 0  lattice mismatch is: -4.110330969640696E-002  combination of A and B:MoS2 \_WSe2  delta A distance is : 3.01219692109860  delta B distance is : 3.34618175320219  得到构造好的异质结结构画图如下：    AA’  运行lattice\_match\_hex.x,得到多个旋转矩阵，选取如下旋转矩阵  TRAN\_A1=  TRAN\_B1=  对01\_WSe2\_POSCAR进行旋转操作:  cp 01\_WSe2\_POSCAR POSCAR  cp TRAN\_B1 TRANSMAT.in  运行vaspkit,输入400，得到POSCAR  由于此时得到的POSCAR基矢不是标准形式，进一步运行vaspkit并输入923，得到标准化的POSCAR.  cp POSCAR SUPERCELL\_B.vasp  运行heterojunction\_building.x,将在屏幕上显示如下提示内容，按要求输入参数设置：  input the height of vallcum:  15  input the distance between nearby layers  3  MoS2  3.19031572340000  3.19031572343695  Found 2 atom type(s)  Number of atom for each type:  Type No.  1 1  2 2  Total No. atom: 3  A off\_centre = (x,y,z) as new origine  0 0 0  9  SUPERCEL  3.32706928250000  3.32706928252858  Found 2 atom type(s)  Number of atom for each type:  Type No.  1 1  2 2  Total No. atom: 3  B off\_centre = (x,y,z) as new origine  0 0 0  lattice mismatch is: -4.110330969640696E-002  combination of A and B:MoS2 \_SUPERCEL  delta A distance is : 3.01219692109860  delta B distance is : 3.34618175320219  计算得到的结构如下图所示：    AB’  运行lattice\_match\_hex.x,得到多个旋转矩阵，选取如下旋转矩阵  TRAN\_A1=  TRAN\_B1=  运行heterojunction\_building.x,将在屏幕上显示如下提示内容，按要求输入参数设置：  input the height of vallcum:  15  input the distance between nearby layers  3  MoS2  3.19031572340000  3.19031572343695  Found 2 atom type(s)  Number of atom for each type:  Type No.  1 1  2 2  Total No. atom: 3  A off\_centre = (x,y,z) as new origin point  0.333333 0.666666 0  9  WSe2  3.32706928250000  3.32706928252858  Found 2 atom type(s)  Number of atom for each type:  Type No.  1 1  2 2  Total No. atom: 3  B off\_centre = (x,y,z) as new origin point  0.666666 0.333333 0  lattice mismatch is: -4.110330969640696E-002  combination of A and B:MoS2 \_WSe2  delta A distance is : 3.01219692109860  delta B distance is : 3.34618175320219  得到结果如图所示：    A’B  得到旋转矩阵  TRAN\_A1=  TRAN\_B1=  运行heterojunction\_building.x,将在屏幕上显示如下提示内容，按要求输入参数设置：  input the height of vallcum:  15  input the distance between nearby layers  3  MoS2  3.19031572340000  3.19031572343695  Found 2 atom type(s)  Number of atom for each type:  Type No.  1 1  2 2  Total No. atom: 3  A off\_centre = (x,y,z) as new origine  0.666666 0.33333330 0  9  WSe2  3.32706928250000  3.32706928252858  Found 2 atom type(s)  Number of atom for each type:  Type No.  1 1  2 2  Total No. atom: 3  B off\_centre = (x,y,z) as new origine  0.333333 0.666666 0  lattice mismatch is: -4.110330969640696E-002  combination of A and B:MoS2 \_WSe2  delta A distance is : 3.01219692109860  delta B distance is : 3.34618175320219    AB  得到旋转矩阵  TRAN\_A1=  TRAN\_B1=  对01\_WSe2\_POSCAR进行旋转操作:  cp 01\_WSe2\_POSCAR POSCAR  cp TRAN\_B1 TRANSMAT.in  运行vaspkit,输入400，得到POSCAR  由于此时得到的POSCAR基矢不是标准形式，进一步运行vaspkit并输入923，得到标准化的POSCAR.  cp POSCAR SUPERCELL\_B.vasp  运行heterojunction\_building.x,将在屏幕上显示如下提示内容，按要求输入参数设置：  input the height of vallcum:  15  input the distance between nearby layers  3  MoS2  3.19031572340000  3.19031572343695  Found 2 atom type(s)  Number of atom for each type:  Type No.  1 1  2 2  Total No. atom: 3  A off\_centre = (x,y,z) as new origine  0.6666666 0.333333 0  9  SUPERCEL  3.32706928250000  3.32706928252858  Found 2 atom type(s)  Number of atom for each type:  Type No.  1 1  2 2  Total No. atom: 3  B off\_centre = (x,y,z) as new origine  0.333333 0.6666666 0  lattice mismatch is: -4.110330969640696E-002  combination of A and B:MoS2 \_SUPERCEL  delta A distance is : 3.01219692109860  delta B distance is : 3.34618175320219    **2D/2D异质结中级版本：**  **运行lattaice\_match\_hex.x,得到多个旋转矩阵组合，如下**  **Graphene**  **2.46772360800000**  **2.46772360804625**  **MoS2**  **3.19031572340000**  **3.19031572343695**  **lattice mismatch is: -0.226495487609582**  **2.325026057720425E-002 1 3 2 0**  **1 3 0| 2 0 0**  **-3 -2 0| 0 2 0**  **0 0 1| 0 0 1**  **2.325026057720425E-002 1 3 2 2**  **1 3 0| 2 2 0**  **-3 -2 0| -2 0 0**  **0 0 1| 0 0 1**  **2.325026057720425E-002 2 3 2 0**  **2 3 0| 2 0 0**  **-3 -1 0| 0 2 0**  **0 0 1| 0 0 1**  **2.325026057720425E-002 2 3 2 2**  **2 3 0| 2 2 0**  **-3 -1 0| -2 0 0**  **0 0 1| 0 0 1**  **2.325026057720425E-002 3 1 2 0**  **3 1 0| 2 0 0**  **-1 2 0| 0 2 0**  **0 0 1| 0 0 1**  **2.325026057720425E-002 3 1 2 2**  **3 1 0| 2 2 0**  **-1 2 0| -2 0 0**  **0 0 1| 0 0 1**  **2.325026057720425E-002 3 2 2 0**  **3 2 0| 2 0 0**  **-2 1 0| 0 2 0**  **0 0 1| 0 0 1**  **2.325026057720425E-002 3 2 2 2**  **3 2 0| 2 2 0**  **-2 1 0| -2 0 0**  **0 0 1| 0 0 1**  选取第一个晶格变换对：  Graphene: TRAN\_A1=  MoS2： TRAN\_B1=  运行vaspkit,输入400，得到POSCAR  检查此时得到的POSCAR基矢是不是标准形式，如不是，则进一步运行vaspkit并输入923，得到标准化的POSCAR.  将 POSCAR 复制SUPERCELL\_A.vasp和SUPERCELL\_B.vasp  运行heterojunction\_building.x,将在屏幕上显示如下提示内容，按要求输入参数设置：  input the height of vallcum:  15  input the distance between nearby layers  3  SUPERCEL  6.52898311610000  6.52898311619230  Found 1 atom type(s)  Number of atom for each type:  Type No.  1 14  Total No. atom: 14  A off\_centre = (x,y,z) as new origine  0 0 0  9  SUPERCEL  6.38063144680000  6.38063144687391  Found 2 atom type(s)  Number of atom for each type:  Type No.  1 4  2 8  Total No. atom: 12  B off\_centre = (x,y,z) as new origine  0 0 0  lattice mismatch is: 2.325031159328295E-002  combination of A and B:SUPERCEL\_SUPERCEL  delta A distance is : 0.000000000000000E+000  delta B distance is : 3.01219692109860      **2D/2D异质结复杂版本：**  产生旋转矩阵**：**  为了使异质结界面两侧的结构具有相同的夹角，将六角的石墨烯转化为直角的晶格。其转换矩阵为  # TRANSFORMATION MATRIX  1 1 0  -1 1 0  0 0 1  运行vaspkit,输入400，得到POSCAR，将POSCAR复制为03\_Graphene\_POSCAR\_rect，采取与上面类似的步骤：  运行./lattice\_match\_rect.x 得到如下结果：  !black\_p  3.30999994280000  4.38000011440000  SUPERCEL  2.46772360804625  4.27422266811989  5.987846047899037E-003 2.474776222330966E-002 3 1  4 1  name = TRAN\_A1  ntot is 1  3 0 0| 4 0 0  0 1 0| 0 1 0  0 0 1| 0 0 1  5.987846047899037E-003 2.474776222330966E-002 3 2  4 2  name = TRAN\_A2  ntot is 2  3 0 0| 4 0 0  0 2 0| 0 2 0  0 0 1| 0 0 1  5.987846047899037E-003 2.474776222330966E-002 3 3  4 3  name = TRAN\_A3  ntot is 3  3 0 0| 4 0 0  0 3 0| 0 3 0  0 0 1| 0 0 1  5.987846047899037E-003 2.474776222330966E-002 3 4  4 4  name = TRAN\_A4  ntot is 4  3 0 0| 4 0 0  0 4 0| 0 4 0  0 0 1| 0 0 1  5.987846047899037E-003 2.474776222330943E-002 3 5  4 5  name = TRAN\_A5  ntot is 5  3 0 0| 4 0 0  0 5 0| 0 5 0  0 0 1| 0 0 1  选取如下旋转矩阵  Black\_P: TRAN\_A1=  MoS2： TRAN\_B1=  运行vaspkit,输入400，得到POSCAR  检查此时得到的POSCAR基矢是不是标准形式，如不是，则进一步运行vaspkit并输入923，得到标准化的POSCAR.  将 POSCAR 复制SUPERCELL\_A.vasp和SUPERCELL\_B.vasp  运行heterojunction\_building.x,将在屏幕上显示如下提示内容，按要求输入参数设置：    input the height of vallcum:  15  input the distance between nearby layers  3  SUPERCEL  9.92999982840000  4.38000011440000  Found 1 atom type(s)  Number of atom for each type:  Type No.  1 12  Total No. atom: 12  A off\_centre = (x,y,z) as new origine  0 0 0  9  SUPERCEL  9.87089443218501  4.27422266811989  Found 1 atom type(s)  Number of atom for each type:  Type No.  1 16  Total No. atom: 16  B off\_centre = (x,y,z) as new origine  0 0 0  lattice mismatch is: 5.987846047899037E-003  combination of A and B:SUPERCEL\_SUPERCEL  delta A distance is : 2.05805933086422  delta B distance is : 0.000000000000000E+000      **金属/半导体异质结：**  MoS2  3.19031572340000  3.19031572343695  Ni\(1\1\  2.47900009160000  2.47900009159173  lattice mismatch is: 0.286936508881249  2.716741433508774E-002 2 0 1 3  2 0 0| 1 3 0  0 2 0| -3 -2 0  0 0 1| 0 0 1  2.716741433508774E-002 2 0 2 3  2 0 0| 2 3 0  0 2 0| -3 -1 0  0 0 1| 0 0 1  2.716741433508774E-002 2 0 3 1  2 0 0| 3 1 0  0 2 0| -1 2 0  0 0 1| 0 0 1  2.716741433508774E-002 2 0 3 2  2 0 0| 3 2 0  0 2 0| -2 1 0  0 0 1| 0 0 1  2.716741433508774E-002 2 2 1 3  2 2 0| 1 3 0  -2 0 0| -3 -2 0  0 0 1| 0 0 1  2.716741433508774E-002 2 2 2 3  2 2 0| 2 3 0  -2 0 0| -3 -1 0  0 0 1| 0 0 1  2.716741433508774E-002 2 2 3 1  2 2 0| 3 1 0  -2 0 0| -1 2 0  0 0 1| 0 0 1  2.716741433508774E-002 2 2 3 2  2 2 0| 3 2 0  -2 0 0| -2 1 0  0 0 1| 0 0 1  MoS2: TRAN\_A1=  Ni111： TRAN\_B1=  运行vaspkit,输入400，得到POSCAR  检查此时得到的POSCAR基矢是不是标准形式，如不是，则进一步运行vaspkit并输入923，得到标准化的POSCAR.  将 POSCAR 复制SUPERCELL\_A.vasp和SUPERCELL\_B.vasp  运行heterojunction\_building.x,将在屏幕上显示如下提示内容，按要求输入参数设置：  input the height of vallcum:  15  input the distance between nearby layers  3  SUPERCEL  6.38063144680000  6.38063144687391  Found 2 atom type(s)  Number of atom for each type:  Type No.  1 4  2 8  Total No. atom: 12  A off\_centre = (x,y,z) as new origine  0 0 0  9  SUPERCEL  6.55881774245181  6.55881774246744  Found 1 atom type(s)  Number of atom for each type:  Type No.  1 49  Total No. atom: 49  B off\_centre = (x,y,z) as new origine  0 0 0  lattice mismatch is: -2.716744124455517E-002  combination of A and B:SUPERCEL\_SUPERCEL  delta A distance is : 3.01219692109860  delta B distance is : 12.1444045088111      **3D/3D异质结：**  产生旋转矩阵  ./read\_rect.x  cubic-GaN  1.00000000000000  4.58800000000000 0.000000000000000E+000 0.000000000000000E+000  0.000000000000000E+000 4.58800000000000 0.000000000000000E+000  0.000000000000000E+000 0.000000000000000E+000 43.8154000000000  4.58800000000000  4.58800000000000  cubic-GaN  5.06400000000000  5.06400000000000  3.543218235161372E-002 3.543218235161372E-002 8 8  7 7  name = TRAN\_A1  ntot is 1  8 0 0| 7 0 0  0 8 0| 0 7 0  0 0 1| 0 0 1  3.543218235161372E-002 3.543218235161372E-002 8 8  7 7  name = TRAN\_A2  ntot is 2  8 0 0| 7 0 0  0 8 0| 0 7 0  0 0 1| 0 0 1  3.543218235161372E-002 1.925355450236976E-002 8 9  7 8  name = TRAN\_A3  ntot is 3  8 0 0| 7 0 0  0 9 0| 0 8 0  0 0 1| 0 0 1  9.399684044233803E-002 0.164861205145565 8 9  8 7  name = TRAN\_A4  ntot is 4  8 0 0| 8 0 0  0 9 0| 0 7 0  0 0 1| 0 0 1  3.543218235161372E-002 6.670177286291157E-003 8 10    GaN: TRAN\_A1=  HfO2： TRAN\_B1=  运行vaspkit,输入400，得到POSCAR  检查此时得到的POSCAR基矢是不是标准形式，如不是，则进一步运行vaspkit并输入923，得到标准化的POSCAR.  将 POSCAR 复制SUPERCELL\_A.vasp和SUPERCELL\_B.vasp  运行heterojunction\_building.x,将在屏幕上显示如下提示内容，按要求输入参数设置：  input the height of vallcum:  15  input the distance between nearby layers  2  SUPERCEL  36.7040000000000  36.7040000000000  Found 2 atom type(s)  Number of atom for each type:  Type No.  1 1280  2 1280  Total No. atom: 2560  A off\_centre = (x,y,z) as new origine  0 0 0  9  SUPERCEL  35.4480000000000  35.4480000000000  Found 2 atom type(s)  Number of atom for each type:  Type No.  1 588  2 1176  Total No. atom: 1764  B off\_centre = (x,y,z) as new origine  0 0 0  lattice mismatch is: 3.543218235161372E-002  combination of A and B:SUPERCEL\_SUPERCEL  delta A distance is : 21.7815116480000  delta B distance is : 13.9173289128000      该部分还需要进一步优化，获得最小超元胞。 | |
| 程序实现原理简述（建议以算法流程图的形式呈现）：  读入两种结构的晶格参数  通过旋转矩阵构造超元胞，寻找晶格匹配的基矢：输入元胞基矢是（a1,b1）和 (a2,b2),构造超元胞（m\*a1,n\*b1）和 (i\*a2,j\*b2),计算新超元胞的基矢长度，  对0<m<10,0<n<10,通过循环判断是否满足应变小于设定值  六角  立方ma,nb  满足应变条件，输出晶格近似匹配的m,n,I,j数值，并计算出旋转矩阵组  利用旋转矩阵，运行vaspkit得到新的超元胞SUPERCELL\_A.vasp和SUPERCELL\_B.vasp，并将这两个文件合为一个结构（heterojunction\_building.f实现） | |