Project #4

表面与界面能

铜的表面能

当物体形成表面时，表面上的原子键发生断裂，接近表面的几层原子不再如之前处于平衡状态，从而导致能量的升高，升高的温度便是物体的表面能。

利用 LAMMPS 做出 20*20*40 fcc 的盒子，删去边缘的原子制造出一段真空层；算出此时体系的总能量 E_0，然后从中间把盒子切成两半并移至足够远的距离，此时的体系总能量为 E_{final}，

从而表面能：

$$\gamma_{surface=}\frac{E_{final}-E_0}{2A}$$

A 为表面的面积

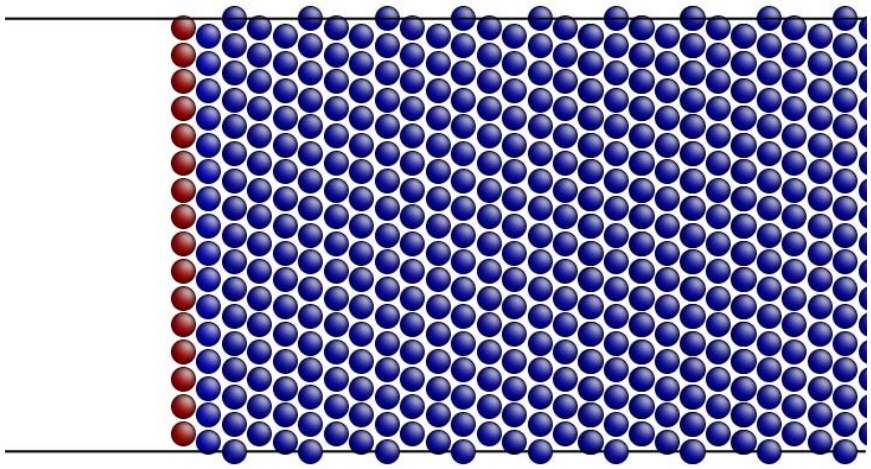
(100) 面与 (111) 面

如下是输入文件 *in.surface_Cu_100*

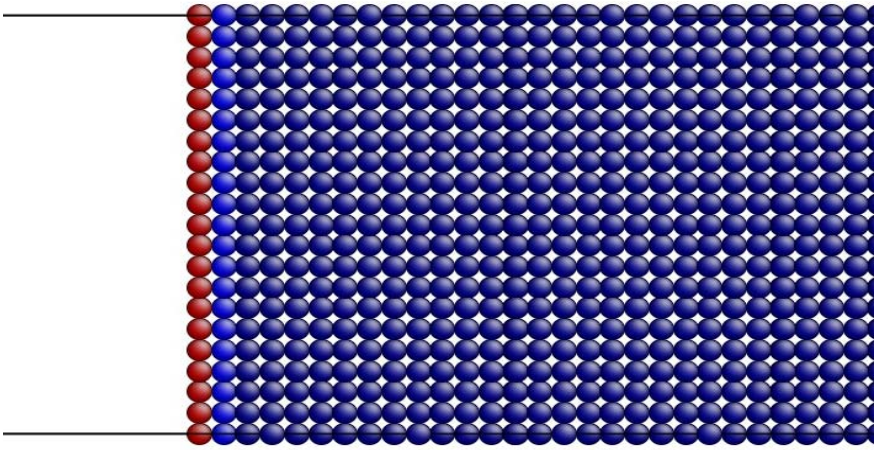
```
# LAMMPS      Cu _Surface_100
units                 metal
boundary              p p p
atom_style            atomic
lattice               fcc 3.61
region                box block 0 20 0 20 0 40
create_box            1 box
create_atoms          1 box
timestep              0.005
thermo                5
pair_style            eam/alloy
pair_coeff          * * jin_copper_lammps.setfl Cu

region              boundary1 block INF INF INF INF 29.9 INF
region              boundary2 block INF INF INF INF INF 9.9
group               boundary1 region boundary1
group               boundary2 region boundary2
group               boundary union boundary1 boundary2
```

```
delete_atoms      group boundary

neighbor          0.6 bin
neigh_modify      every 5 delay 0 check yes

compute           3 all pe/atom
compute           4 all ke/atom
compute           5 all coord/atom 3.0

dump              1 all custom 100 dump.atom id xs ys zs c_3 c_4 c_5
dump_modify       1 format "%d %16.9g %16.9g %16.9g %16.9g %16.9g %g"

min_style         sd
minimize          1.0e-30 1.0e-15 1000 10000
variable          E equal pe
print             "----------------------    E=$E---------------------------"
run               0

region            down    block INF INF INF INF INF 19.94
region            up block INF INF INF    INF    19.95 INF
group             up region up
group             down region down
displace_box      all z delta    0 40 units lattice remap none
displace_atoms up move    0 0 40      units    lattice
minimize          1.0e-30 1.0e-20 10000 100000
print             "-----SURFACE----------E=$E-------------------------------"
```

Plane	**(100)**	**(111)**
Surface energy(mJ / m^2 **)**	**1330**	**1228**



Plane (111)



Plane (100)

镁的 hcp/fcc 界面能

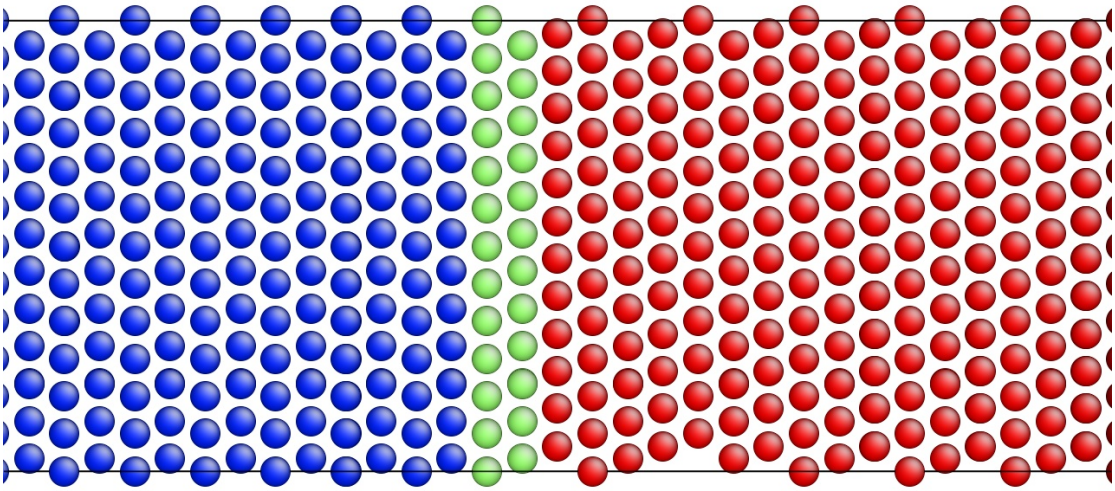
计算镁的 hcp/fcc 界面能比较有趣。正如我们所知，镁是 hcp 结构的金属，它是按 ABABABABAB⋯ 所排列的；当我们进行一系列移动之后得到 ABABCABCAB⋯ ，从而产生镁的 hcp/fcc 界面。

如下是输入文件 *in.hcp_fcc_vac*

```
# LAMMPS    hcp_fcc_Mg

units             metal
boundary          p p p
atom_style        atomic
lattice           custom 4.5198 a1 1.224744871391589049 0 0 a2 0 0.7071067811865475244    0
a3 0 0 1.1476 basis 0.0 0.0 0.0 basis 0.5 0.5 0.0 basis      0.33333333333333333333 0.0 0.5 basis
0.83333333333333333333 0.5 0.5
region            box block 0 6 0 6 0 36
create_box        1 box
create_atoms      1 box
pair_style        eam/alloy
pair_coeff        * * mg.eam.alloy Mg
neighbor          0.8 bin
neigh_modify      every 5 delay 0 check yes
thermo            10
variable          N equal atoms
variable          E equal pe

region            boundary1 block INF INF INF INF 26.9 INF
region            boundary2 block INF INF INF INF INF 8.9
group             boundary1 region boundary1
group             boundary2 region boundary2
group             boundary union boundary1 boundary2
delete_atoms      group boundary

label             dj
variable          x index 17.9 18.9 19.9 20.9 21.9 22.9 23.9 24.9 25.9
region            up_$x block INF INF INF INF $x INF
group             up_$x region up_$x
displace_atoms up_$x move
-0.333333333333333333333333333333333333333333333333333333333333333 0 0 units lattice
next              x
jump              in.hcp_fcc_vac dj

timestep          0.01
```

```
region          part block INF INF INF INF    12    24
group           part region part
compute         3 all pe/atom
compute         4 all ke/atom
compute         5 all coord/atom 3.0
dump            1 part custom 100 dump.atom id xs ys zs c_3 c_4 c_5
dump_modify     1 format "%d %16.9g %16.9g %16.9g %16.9g %16.9g %g"
min_style       sd
minimize        1.0e-30 1.0e-15 10000 100000
shell           mkdir dump_fcc_hcp
shell           mv dump.atom dump_fcc_hcp/dump.atom
print           "----------fcc_hcp---------------N=$N    E=$E-----------------------"

delete_atoms    group all
lattice         none
lattice         custom 4.5198 a1 1.224744871391589049 0 0 a2 0 0.7071067811865475244    0
a3 0 0 1.1476 basis 0.0 0.0 0.0 basis 0.5 0.5 0.0 basis      0.33333333333333333333 0.0 0.5 basis
0.83333333333333333333333333333333333333333333333333 0.5 0.5
create_atoms    1 box
group           boundary1 region boundary1
group           boundary2 region boundary2
group           boundary union boundary1 boundary2
delete_atoms    group boundary
undump          1
dump            1 all custom 100 dump_hcp.atom id xs ys zs c_3 c_4 c_5
dump_modify     1 format "%d %16.9g %16.9g %16.9g %16.9g %16.9g %g"
min_style       sd
minimize        1.0e-30 1.0e-15 10000 10000
print           "----------hcp---------------N=$N    E=$E-----------------------"
shell           mkdir dump_hcp
shell           mv dump_hcp.atom dump_hcp/dump.atom


delete_atoms    group all
lattice         none
lattice         custom 4.5198 a1 1.224744871391589049 0 0 a2 0 0.7071067811865475244    0
a3 0 0 1.1476 basis 0.0 0.0 0.0 basis 0.5 0.5 0.0 basis      0.33333333333333333333 0.0 0.5 basis
0.83333333333333333333 0.5 0.5
create_atoms    1 box
group           boundary1 region boundary1
group           boundary2 region boundary2
group           boundary union boundary1 boundary2
delete_atoms    group boundary
```

```
label           ddj
variable        y index 9.9 10.9 11.9 12.9 13.9 14.9 15.9 16.9 17.9 18.9 19.9 20.9 21.9 22.9 23.9
24.9 25.9
region          up_fcc_$y block INF INF INF INF $y INF
group           up_fcc_$y region up_fcc_$y
displace_atoms up_fcc_$y move
-0.333333333333333333333333333333333333333333333333333333333333333 0 0 units lattice
next            y
jump            in.hcp_fcc_vac ddj
undump          1
dump            1 all custom 1000 dump_fc.atom id xs ys zs c_3 c_4 c_5
dump_modify     1 format "%d %16.9g %16.9g %16.9g %16.9g %16.9g %g"

min_style       sd
minimize        1.0e-30 1.0e-15 10000 100000

shell           mkdir dump_fcc
shell           mv dump_fcc.atom dump_fcc/dump.atom
print           "----------fcc-------------N=$N    E=$E----------"
```



根据公式：

$$\gamma = \frac{E_t - \frac{1}{2}(E_{hcp} + E_{fcc})}{2A}$$

可以得到：$\gamma = 27.058(mJ/m^2)$，这与之前所得到结果比较吻合。