

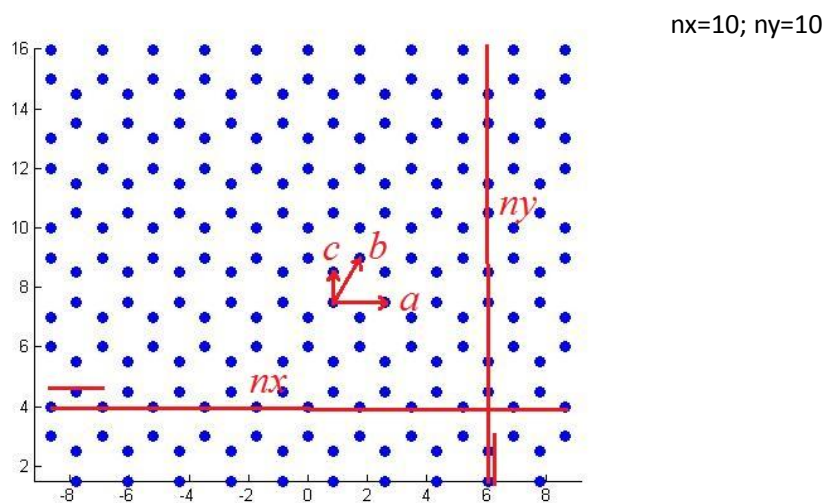
Nanotube with arbitrary radius construction in MATLAB

Summary on code

1. Basic information input:

```
a=[sqrt(3),0];           #base 1
b=[sqrt(3)/2,1.5];       #base 2
c=[0,1];                 #vector from one atom A to atom B
k=1;                     #counter for later
nx=20;ny=20;             #width of graphene is nx, length is ny, unit is one
                           hexagon
```

Sketch graph

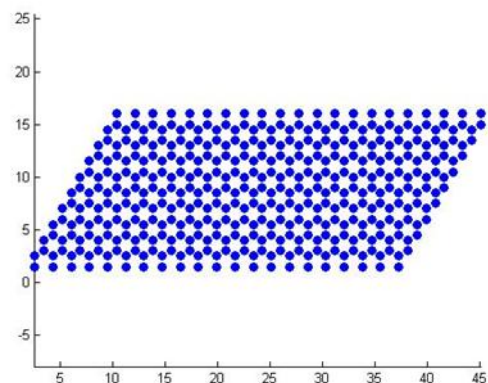


2. generate graphene

```
for i=1:2*nx+1
    for j=1:ny
        x(k)=a(1)*i+b(1)*j;
        y(k)=a(2)*i+b(2)*j;
        k=k+1;
    end
end

for i=1:2*nx+1
    for j=1:ny
        x(k)=c(1)+a(1)*i+b(1)*j;
        y(k)=c(2)+a(2)*i+b(2)*j;
        k=k+1;
    end
end

%cut a square area
cc=1;
```



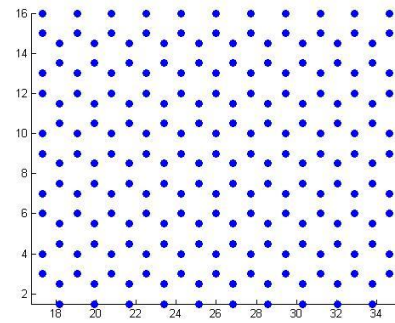
```

for i=1:k-1
    if x(i)>=nx*a(1) & x(i)<=2*nx*a(1)

cx(cc)=x(i);cy(cc)=y(i);cc=cc+1;
    end
end

%move the center of this piece to x=0
cx=cx-(min(cx)+max(cx))/2;

```

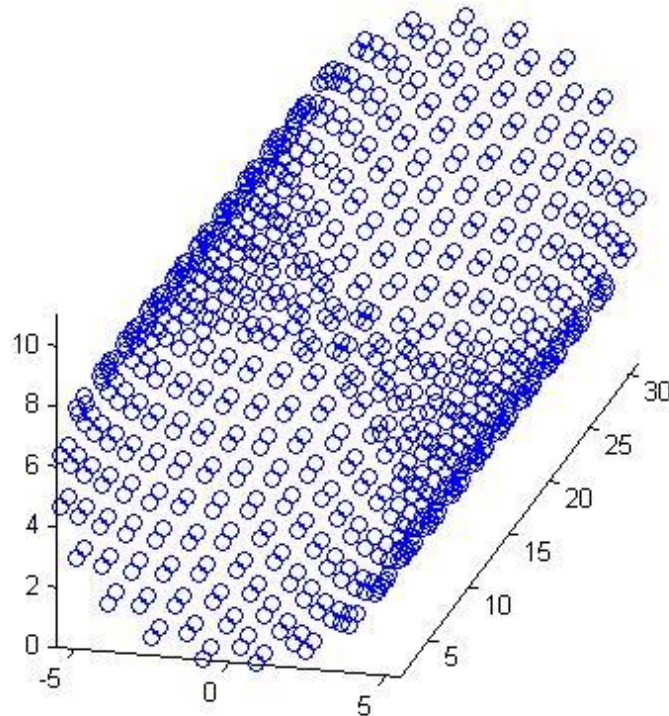


3.roll the sheet up

```

r=(max(cx)-min(cx))/(2*pi); #calculate the radium
for ccc=1:cc-1                #keep y, relocate x and z of every atom
    theta=cx(ccc)/r;
    ntx(ccc)=r*sin(theta);nty(ccc)=cy(ccc);ntz(ccc)=r-r*cos(theta);
end

```



4.output POSCAR

```

fid=fopen('POSCAR','wt');
for i=1:cc-1

```

```
        fprintf(fid,'%d %d %d\n',ntx,nty,ntz);  
end  
fclose(fid);
```