FYS43010 Problem 2 solution suggestion tgf

MAPLE WORKSHEET

```
> restart;
> with(geom3d):
```

Note there are 8 atoms pr. unit cell in the diamond lattice, so..
We define eight points in the unit cell, and call the points UC1 to UC8.

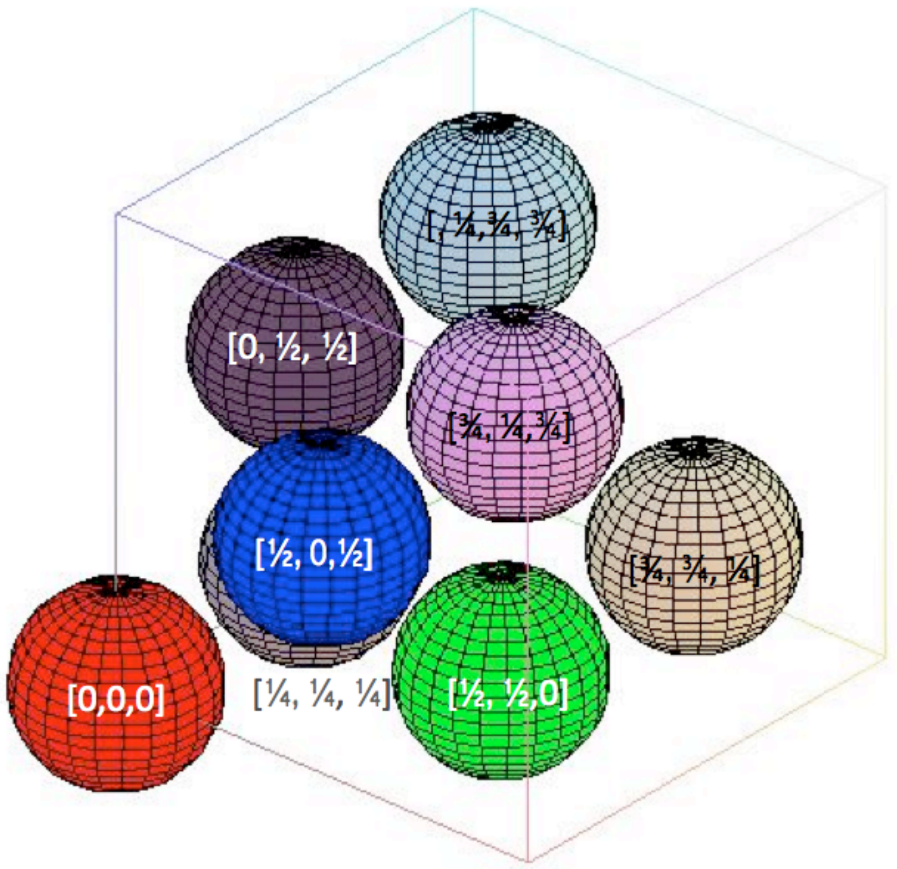
```
> point(UC1,[0,0,0]):
> point(UC2,[0.5,0.5,0]):
> point(UC3,[0.5,0,0.5]):
> point(UC4,[0,0.5,0.5]):
> point(UC5,[0.25,0.25,0.25]):
> point(UC6,[0.75,0.75,0.25]):
> point(UC7,[0.75,0.25,0.75]):
> point(UC8,[0.25,0.75,0.75]):
```

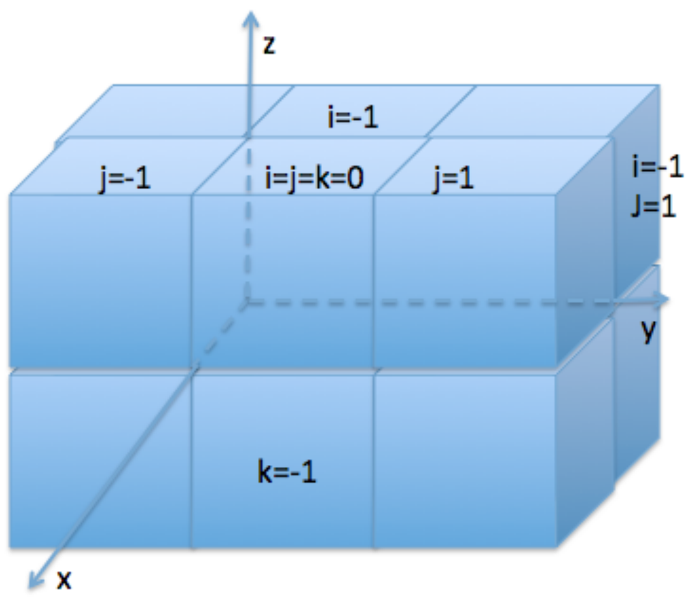
In order to make a drawing of atoms, we define
the radius of the atoms , r0, we define a cube, ACUBE, around a point , APT
the size of the cube is the same as the unit cell ...

```
> r0:=0.2:
> point(APT,[0.5,0.5,0.5]):
> cube(ACUBE,APT,1/2*sqrt(3)):
> sphere(sph1,[UC1,r0],[x,y,z]):
> sphere(sph2,[UC2,r0],[x,y,z]):
> sphere(sph3,[UC3,r0],[x,y,z]):
> sphere(sph4,[UC4,r0],[x,y,z]):
> sphere(sph5,[UC5,r0],[x,y,z]):
> sphere(sph6,[UC6,r0],[x,y,z]):
> sphere(sph7,[UC7,r0],[x,y,z]):
> sphere(sph8,[UC8,r0],[x,y,z]):
```

So, let us just draw the atoms of our unit cell and the actual unit cell

```
draw([sph1(color=red),sph2(color=green),sph3(color=blue),sph4(color=violet),sph5
,sph6,sph7,sph8,ACUBE( style=WIREFRAME)],view=[-0.2..1.2,-0.2..1.2,-
0.2..1.2],orientation=[-54,71]);
```

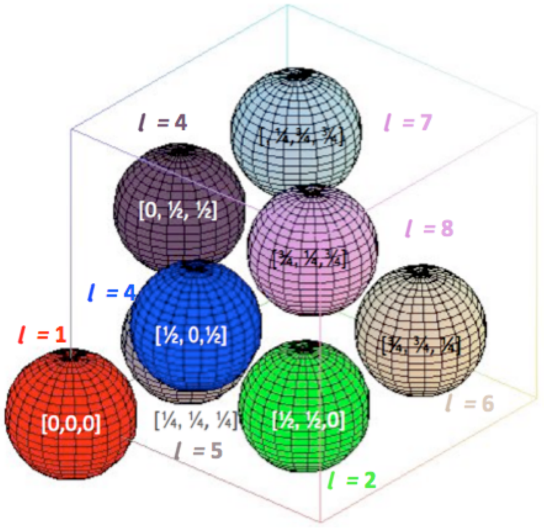

[¼, ¾, ¾]
[0, ½, ½]
[¾, ¼, ¾]
[½, 0, ½]
[¾, ¾, ¼]
[0,0,0]
[¼, ¼, ¼]
[½, ½, 0]


z
i=-1
j=-1
i=j=k=0
j=1
i=-1
J=1
y
k=-1
x

```
> point(Origo,[0,0,0]):
> coords:='coords':
```

We will make a loop where we translate the unit cell by one unit every time around the loop, We then measure the distance from the eight points in the unit cell to origo

```
> cellnum:=0:atnum:=0:thelist:='thelist':
> for i from -2 to 1 do
>   for j from -2 to 1 do
>    for k from -2 to 1 do
>     cellnum:=cellnum+1;
>     for l from 1 to 8 do
>       atnum:=8*(cellnum-1)+l;
>        if l=1 then point(coords,[i,j,k])
>        elif l=2 then point(coords,[i+0.5,j+0.5,k])
>        elif l=3 then point(coords,[i,j+0.5,k+0.5])
>        elif l=4 then point(coords,[i+0.5,j,k+0.5])
>
>        elif l=5 then point(coords,[i+0.25,j+0.25,k+0.25])
>        elif l=6 then point(coords,[i+0.75,j+0.75,k+0.25])
>        elif l=7 then point(coords,[i+0.25,j+0.75,k+0.75])
>        elif l=8 then point(coords,[i+0.75,j+0.25,k+0.75])
>      end if;
>      d:=distance(coords,Origo);
>      thelist[atnum]:=evalf(d);
>     od; # l
>    od; # k
>   od; # j
> od;# I
```



Now we have 512 distances in the variable ‘thelist’. This is unsorted, so.. we sort the list,

```
> sortedlist:=sort([seq(thelist[j],j=1..512)]):
```

Then we write out the five shells which is what was asked for

```
> shnum:=0:d:=0:cntr:=0: print(shellnum,numinshell, shelldistance);
> for j from 1 to 512 do
>   if ((sortedlist[j]-d)>=0.01)
>          then
>               if shnum<6 then
>                   x:=sqrt(convert(d^2,rational));
>                   print(shnum,cntr, x*a=d*a,  d*0.553*nm);
>               end if;
>               shnum:=shnum+1;
>               d:=sortedlist[j];
>               cntr:=0;
>   end if:
>   cntr:=cntr+1:
>   od:
```

shellnum, numinshell, shelldistance

$$0, 1, 0 = 0, 0.$$

$$1, 4, \frac{1}{4}\sqrt{3}\ \mathrm{a} = 0.4330127019\ \mathrm{a},\ 0.2394560242\ \mathrm{nm}$$

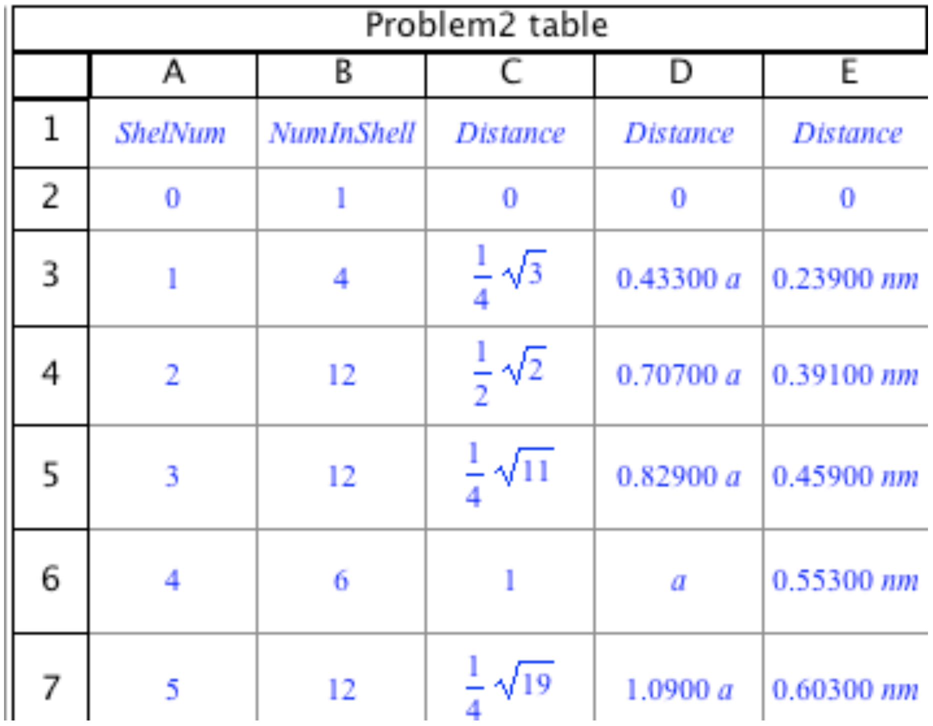
$$2, 12, \frac{1}{2}\sqrt{2}\ \mathrm{a} = 0.7071067812\ \mathrm{a},\ 0.3910300500\ \mathrm{nm}$$

$$3, 12, \frac{1}{4}\sqrt{11}\ \mathrm{a} = 0.8291561976\ \mathrm{a},\ 0.4585233773\ \mathrm{nm}$$

$$4, 6, \mathrm{a} = 1.\ \mathrm{a},\ 0.553\ \mathrm{nm}$$

$$5, 12, \frac{1}{4}\sqrt{19}\ \mathrm{a} = 1.089724736\ \mathrm{a},\ 0.6026177790\ \mathrm{nm}$$

If we had removed the condition if shnum<6 and always taken the action
we would have gotten more shells out.
Then for the high number shells the numbers in the shell is incorrect,
but it is OK for shellnum 1 to 5, and we can make it OK for higher by including more cells to test, i.e. increase the range of the variables i, j, k in the loop.



Problem2 table

	A	B	C	D	E
1	*ShelNum*	*NumInShell*	*Distance*	*Distance*	*Distance*
2	0	1	0	0	0
3	1	4	$\frac{1}{4}\sqrt{3}$	$0.43300\,a$	$0.23900\,nm$
4	2	12	$\frac{1}{2}\sqrt{2}$	$0.70700\,a$	$0.39100\,nm$
5	3	12	$\frac{1}{4}\sqrt{11}$	$0.82900\,a$	$0.45900\,nm$
6	4	6	1	a	$0.55300\,nm$
7	5	12	$\frac{1}{4}\sqrt{19}$	$1.0900\,a$	$0.60300\,nm$