## a) Density of states

Using a wavefunction with periodic boundary conditions, one needs  $k_x L_x = 2\pi n_x$ , where  $n_x$  is an integer and  $L_x$  is a crystal dimension in the x-direction. Then any quantity needs to be summed over the states as

$$\sum_{n_x,n_y}$$

which can be changed to an integral as

$$rac{L_x L_y}{\left(2\pi\right)^2}\int dk_x dk_y$$

since a change in  $\Delta n_x$  corresponds to a change  $(L_x/2\pi)\Delta k_x$ . Then changing to polar coordinates  $dk_x dk_y = k dk d\phi$ . Integrating over angle this is

$$\frac{A}{2\pi}\int kdk$$

If one wanted to be able to integrate over energy, use  $E = \hbar v_F k$  to change k and dk to get

$$rac{2\pi A}{\left(hv_{F}
ight)^{2}}\int EdE$$

so that the density of states per unit area is

$$D(E)=rac{2\pi}{\left(hv_{\,F}
ight)^2}\,E$$

This needs to be multiplied by 2 since there is a degeneracy of two conduction and valence bands and 2 since there are two spin states for each, giving

$$D(E) = rac{8\pi}{\left(hv_F
ight)^2} E$$

b) The charge (number) density per area for the capacitor is

$$n = rac{K_o \epsilon_o}{d} \cdot V / q$$

In [125]: q=1.6E-19
n=3.9\*8.85E-14\*20/500E-7/q
print 'n=',n,'electrons/cm2' #per cm2

n= 8.62875e+11 electrons/cm2

The density of states is

$$D(E)=rac{2\cdot 2}{2\pi}~rac{E}{\left(\hbar v_{F}
ight)^{2}}$$

and the density of electrons added is

$$n=\int_0^{E_F}\!dE\,f(E)D(E)$$
 .

where the Fermi factor is unity at T=0 up to  $E_F$  (and nearly the same at RT since it will be found that  $k_BT \ll E_F$ ) so that

$$E_F = {h \sqrt{n \pi} \over 2 \pi} \, v_F$$

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In [126]: h=6.63E-34
vF=1E8
EF=h*sqrt(n*pi)*vF/2/pi
print EF/q, 'V'
0.108583180137 V
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c) To calculate the density of atoms in the lattice, examine the cell defined by  $\vec{a_1}, \vec{a_2}$ . There are 4 corner atoms, each shared by 4 similar cells. In addition there is one basis atom per cell. The area of this cell is  $A = 2 \times (1/2)a\sqrt{3}a/2$ .

```
In [127]: a=2.47E-8
    A=2*2*(1/2)*a*sqrt(3)*a/2
    natoms=2/A
    print natoms,'atoms per cm2'
```

1.89267245551e+15 atoms per cm2  $\,$ 

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In [128]: ratio = n/natoms
print 'number of electrons per atom =','%.3g' %ratio
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number of electrons per atom = 0.000456