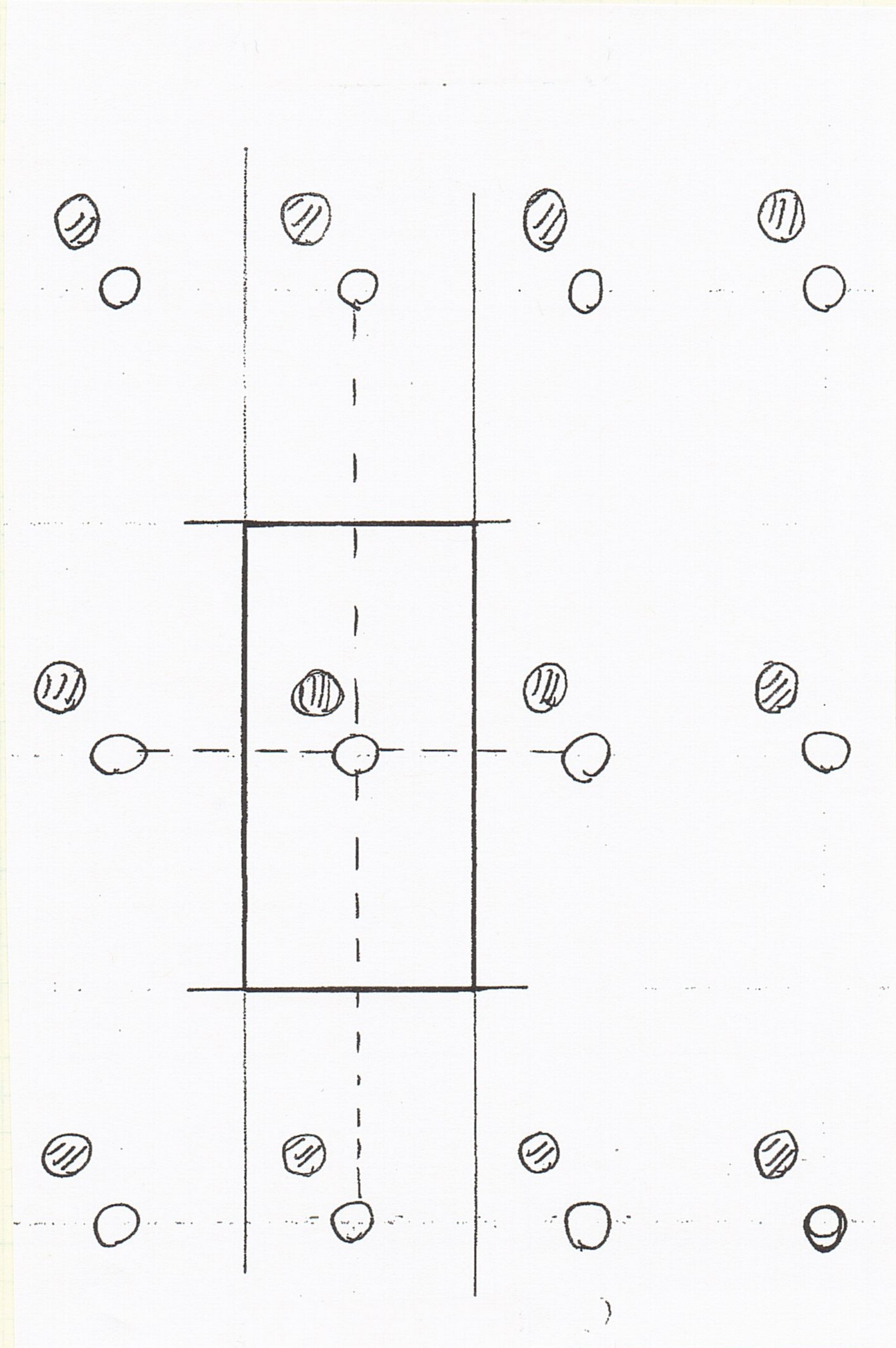
Q1

[Marks]

[1]



[1] The basis is 2.

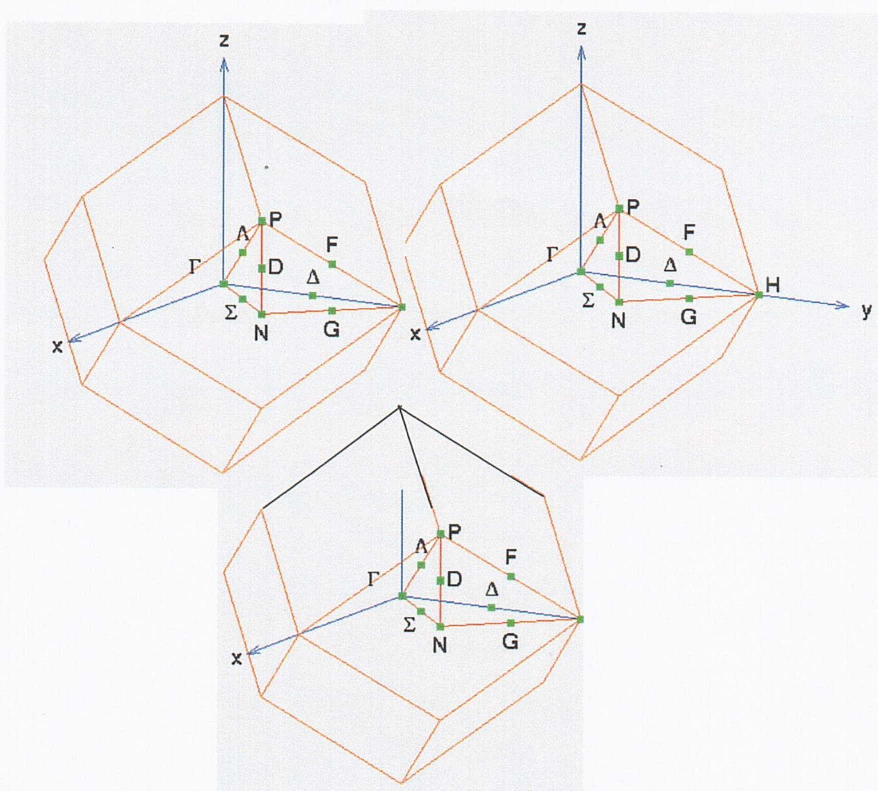
(2)

[1 for one cell]

[½ for reference]

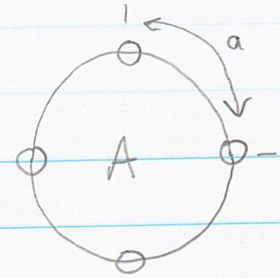
[½ for showing nesting]

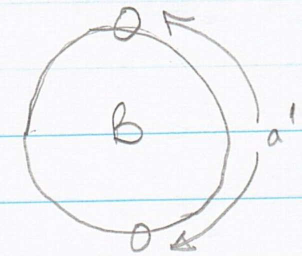
Nesting of FCC unit cells (http://cst-www.nrl.navy.mil/users/mehl/phonons/bcc/)



Each cell is a rhomic duodecahedron

Q3 Consider cyclic representation:





A	B
$N = 4$	$N' = 2$
$Na = 4a$	$N'a' = 2a' = 2 \times 2a = 4a$

Allowed values of k: $k_A = \frac{2\pi n}{Na}$, $k_B = \frac{2\pi n}{N'a'}$

for $-\frac{\pi}{a} \leq k_A \leq \frac{\pi}{a}$ | $-\pi/a' \leq k_B \leq \frac{\pi}{a'}$

range of n is: $-\frac{N}{2} \leq n \leq \frac{N}{2}$ | $-N'/2 < n < N'/2$

\# distinct k-values / band: N | N' states / band

Allow for spin (2 states / k-value): $\underline{2N}$ | $\underline{2N'}$ states / band

$$\# \text{ electrons} = \# \text{ primitive cells} \times \frac{\text{atoms}}{\text{prim cell}} \times \frac{\text{val. electrons}}{\text{atom}}$$

[1 for reasoning]

$= N \times 1 \times 1 = N$ | $= N' \times 2 \times 1 = 2N'$

$$\# \text{ filled bands} = \frac{\text{electrons}}{\text{states / band}}$$

$= \frac{N}{2N}$ | $\frac{2N'}{2N'}$

half-full | full

[1 for B]

metal | semiconductor (or insulator)

Q4

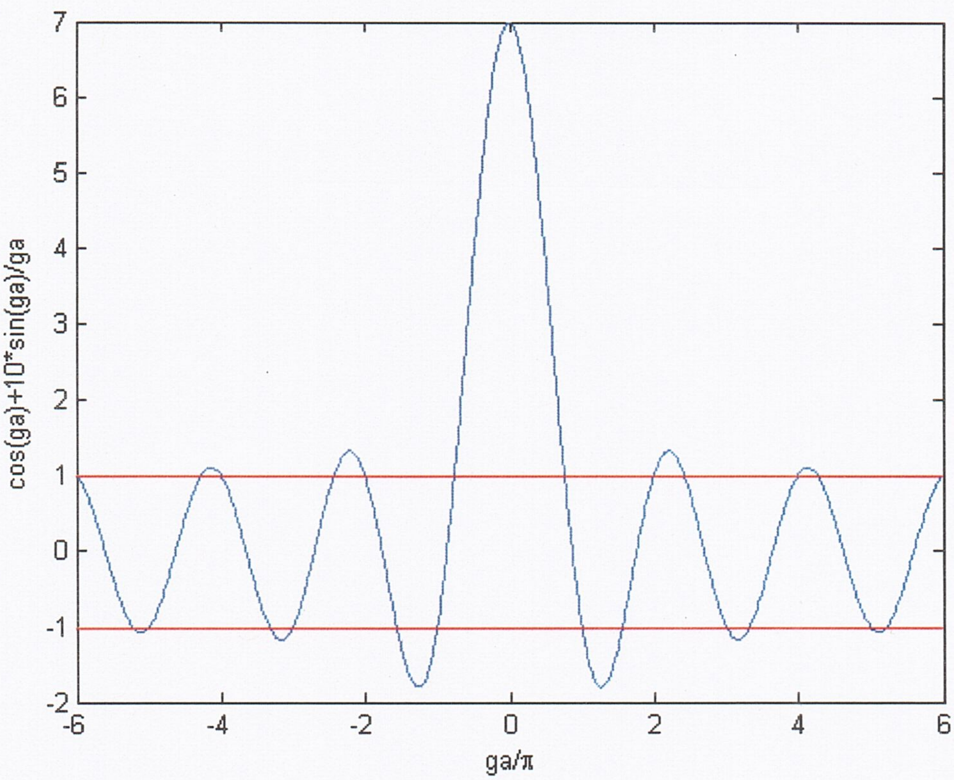
```
% Plotting Fig. 2.4
% EECE 480, September 2011

clear;

hbar=1.054573e-34; %[J-s]
m0=9.109390e-31;   %[kg]
mstar=1;
A=6;
ga=linspace(-6*pi,6*pi,1000);
rhs=cos(ga)+A.*sin(ga)./ga;

plot(ga./pi,rhs,ga./pi,ones(length(ga)),'r', ga./pi,-ones(length(ga)),'r');
xlabel('ga/\pi');  ylabel('cos(ga)+10*sin(ga)/ga');
```

[1 for code]



[2 for figure correctly labelled]

Q5 The material has $N \times 4 \times 2 = 8N$ electrons

[1 for # filled bands] $\therefore$ First 4 bands are filled at 0 K, and the bandgap is between band # 4 and band # 5

[1 for identifying Eg] From the plot from Q4, the top of band 4 occurs at $g = 4\pi/a$.

[1 for g values] To find the bottom of band # 5, solve (2.17) iteratively to find a solution slightly greater than $4\pi/a$.

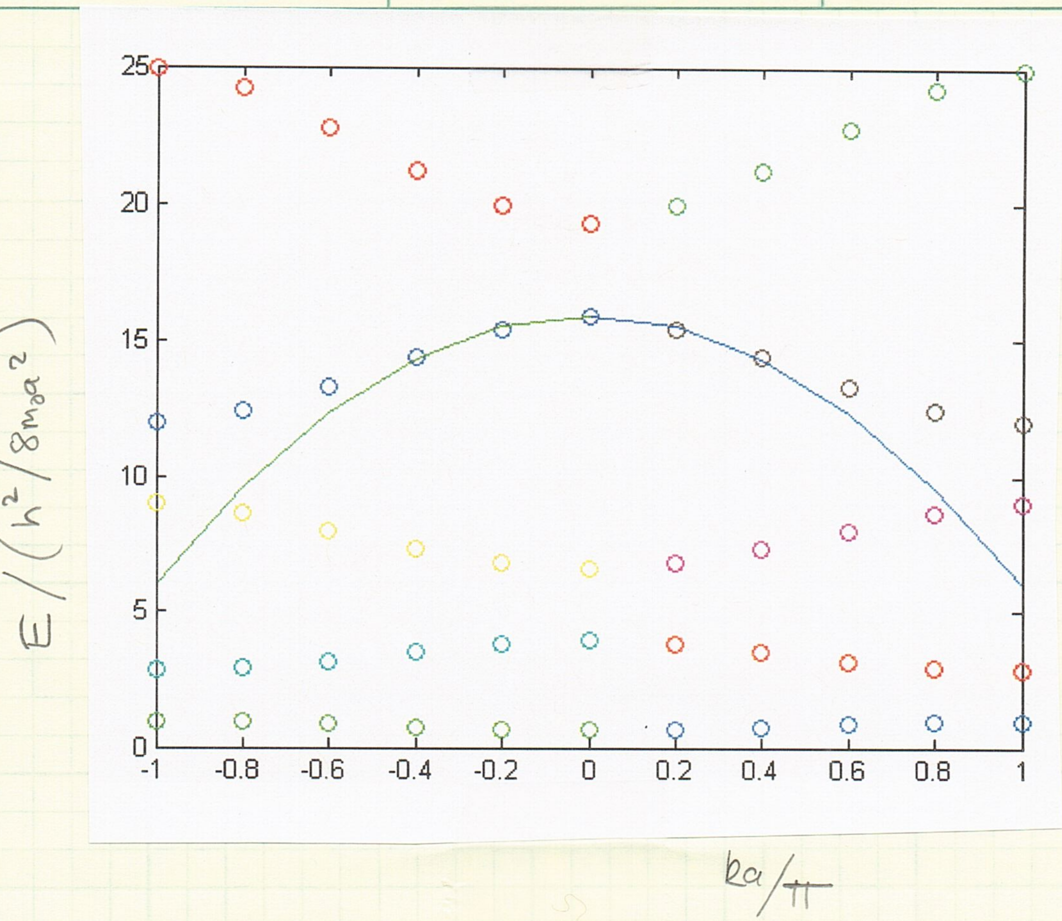
The solution is $g = 4.2679\,\pi/a$.

from (2.6) $\Delta E = E_g = \dfrac{h^2}{8m_0a^2}\left[(4.2679)^2 - (4)^2\right]$

[1 for answer] for $a = 0.75\,\text{nm}$, $\underline{E_g = 1.49\ \text{eV}}$

Q6

[1½ for plot]

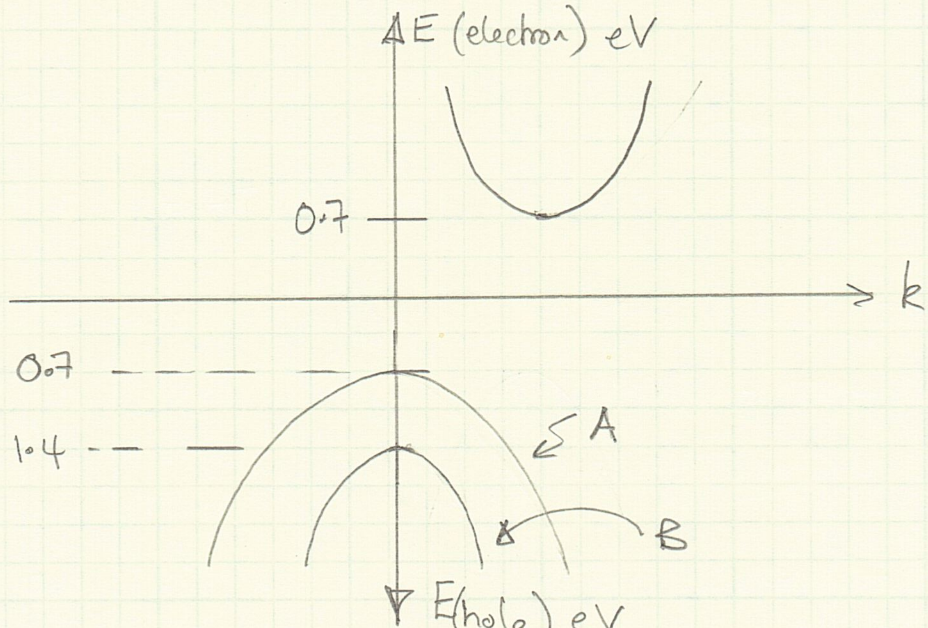


[1½ for m_n^*]

The fit shown here is for $m_h^* = 0.1\, m_0$

Q7

[1 for correct E-k plots]



$E_g(A) = 1.4\text{eV}$, $\underline{\underline{E_g(B) = 2.1\text{ eV}}}$

[1 for answers] $m^* = \left[\frac{1}{\hbar^2}\frac{d^2E}{dk^2}\right]^{-1}$ $m_A^* \propto (2\alpha)^{-1}$, $m_B^* \propto (4\alpha)^{-1}$ $\therefore$ $\underline{\underline{m_A^* > m_B^*}}$

Q8.

[1 for reasoning]

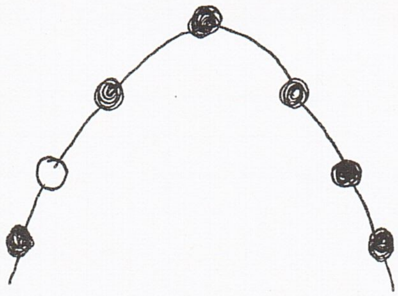


Fig. 2.10b

$$F_{x,ext} = \hbar \frac{\Delta k_x}{\Delta t} \quad (2.25)$$

$$= +q\,\mathcal{E}_x \quad \text{for a hole}$$

$$\therefore \Delta k_x = \frac{q\,\mathcal{E}_x}{\hbar}\,\Delta t$$

i.e., hole moves to more positive k_x

[1 for answer]