EE2003 SEMICONDUCTOR FUNDAMENTALS

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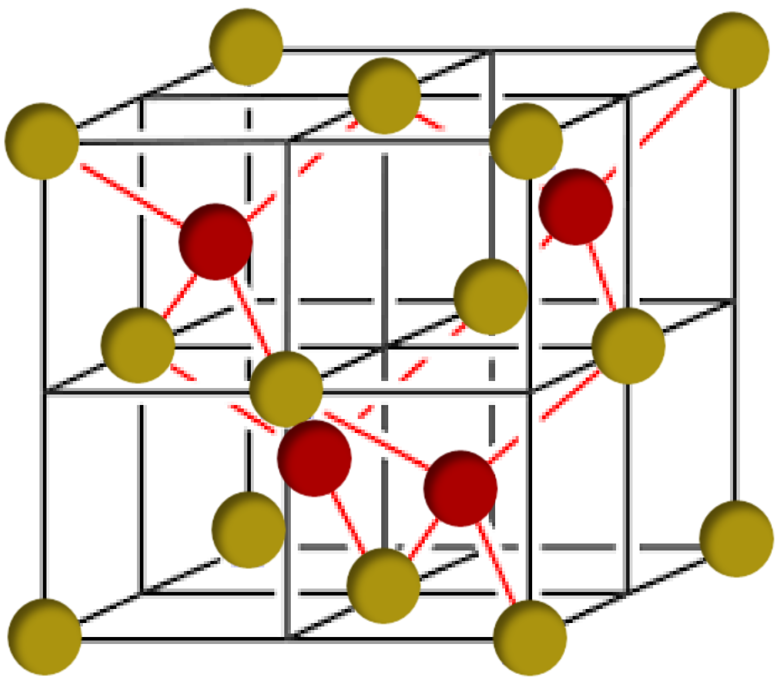
Tutorial 3: Si/GaAs Crystal Structure; Energy Band

Question 1

For the unit cell of the silicon crystal with lattice constant of 5.43 Å,

a) determine the number of atoms in the unit cell,
b) calculate the **shortest distance** between any two atoms,
c) calculate the volume density of silicon atoms (number of atoms/cm^3) in the crystal,
d) calculate the mass density of silicon, given that the **atomic weight** of silicon is 28.09 and **Avogadro's number** is 6.02×10^{23} atoms or molecules/mole.
e) calculate the density of **valence electrons** in silicon.

1(a) determine the number of atoms in the unit cell



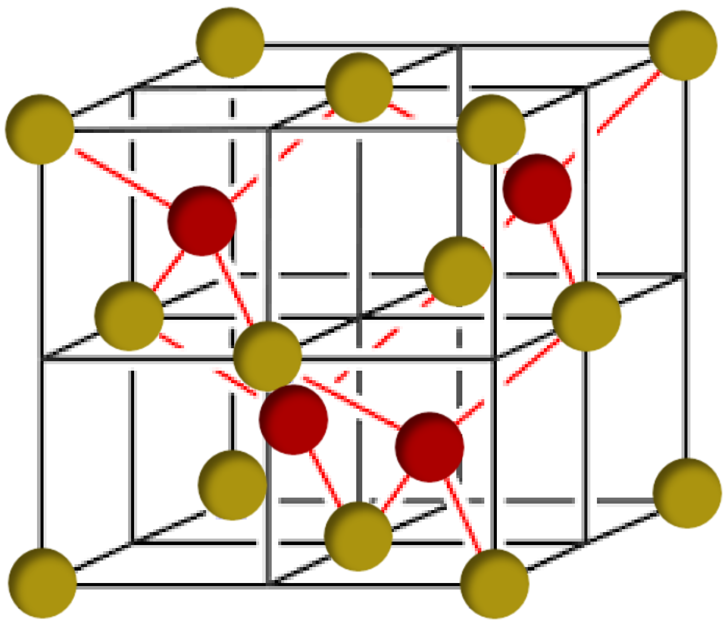
Corners: $\frac{1}{8} \times 8 = 1$

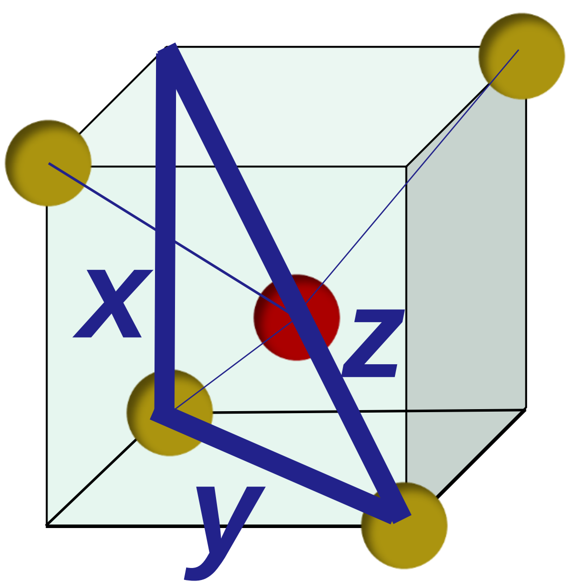
Faces: $\frac{1}{2} \times 6 = 3$

Internal: 4

Total: 8

1(b) calculate the **shortest distance** between two atoms





$$x = \frac{a}{2}$$

$$y = \sqrt{\left(\frac{a}{2}\right)^2 + \left(\frac{a}{2}\right)^2} = \frac{a}{\sqrt{2}}$$

$$z = \sqrt{x^2 + y^2} = \frac{\sqrt{3}}{2}a$$

shortest distance $= \frac{z}{2} = \frac{\sqrt{3}}{4}a$

1(c) calculate the volume density of silicon atoms (number of atoms/cm^3) in the crystal

$$\textbf{Volume density} = \frac{\text{no. of atoms in one unit cell}}{\text{vol. of unit cell}}$$

$$= \frac{8}{\left(5.43 \times 10^{-8}\ \text{cm}\right)^3} = 5 \times 10^{22}\ \text{atoms/cm}^3$$

1(d) calculate the mass density of silicon, given that the **atomic weight** of silicon is 28.09 and **Avogadro's number** is 6.02×10^{23} atoms or molecules/mole.

1 mole of Si has 6.02×10^{23} atoms (Avogadro's number)

1 mole of Si has a mass of 28.09 g (atomic weight)

1 atom of Si has a mass of $$\frac{28.09}{6.02\times10^{23}}\ \mathrm{g}$$

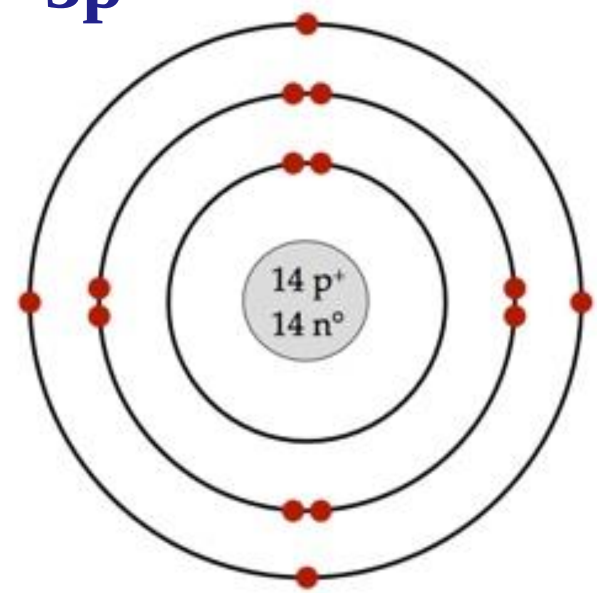
1 cm^3 of Si has a mass of $$\frac{28.09}{6.02\times10^{23}}\times5\times10^{22}=2.33\ \mathrm{g}$$

Mass density of Si is 2.33 g cm^{-3}

1(e) calculate the density of **valence electrons** in silicon

$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^2$

1 atom of Si has 4 valence electrons



Silicon

1 cm^3 of Si has 5×10^{22} atoms

1 cm^3 of Si has $4\times5\times10^{22} = 2\times10^{23}$ valence electrons

Density of valence electrons is 2×10^{23} valence electrons

Question 2

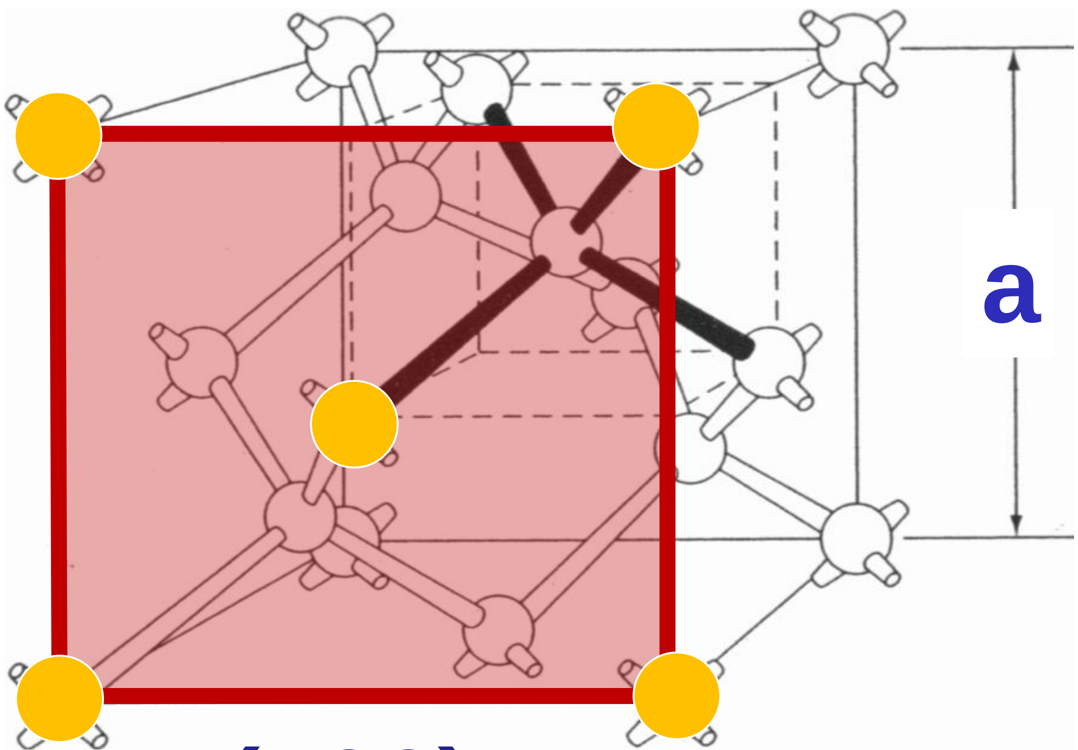
Refer to Figure 2.7 (the diamond structure for Si) of your lecture notes.

(a) The surface of a Si wafer is a (100) plane. Sketch the placement of Si atoms on the surface of the wafer.

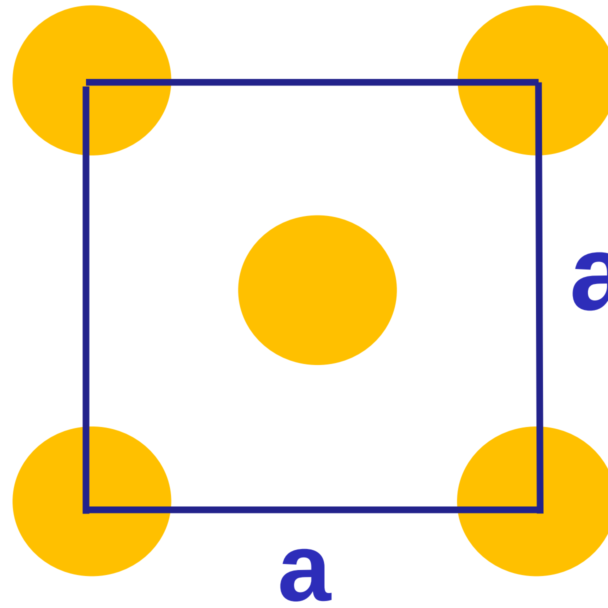
(b) Determine the number of atoms per cm^2 at the surface of the wafer. Take Si lattice constant as 5.43Å.

(c) Repeat parts (a) and (b), this time taking the surface of the Si wafer to be a (110) plane.

Si Unit Cell



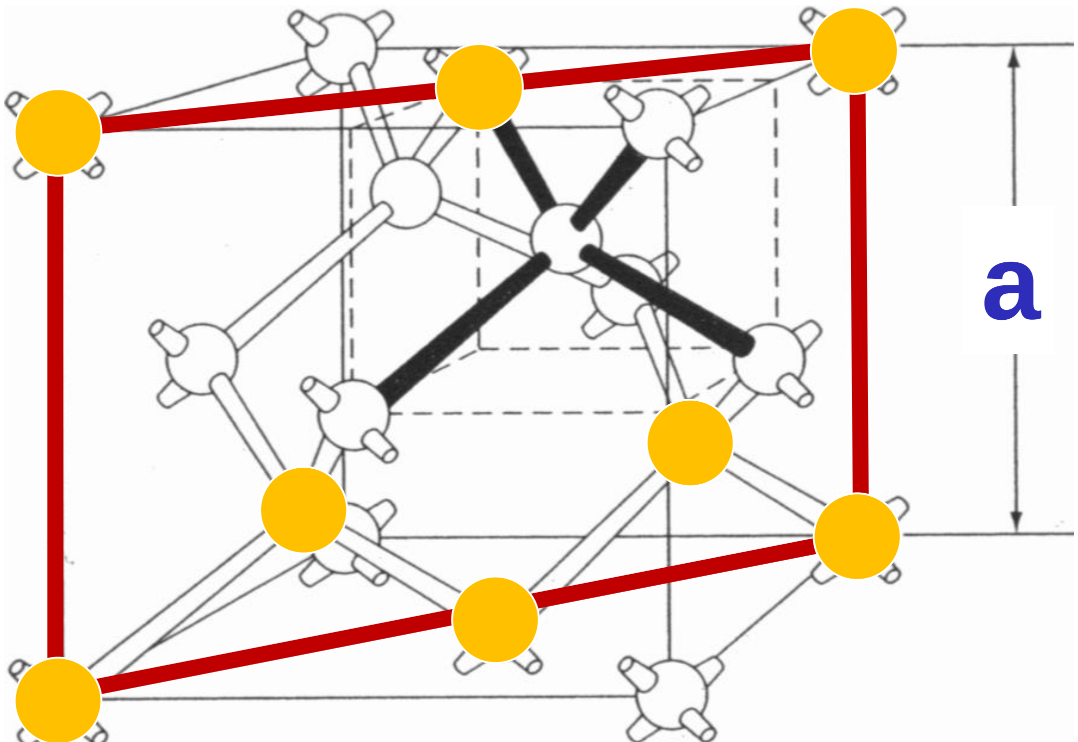
(100)



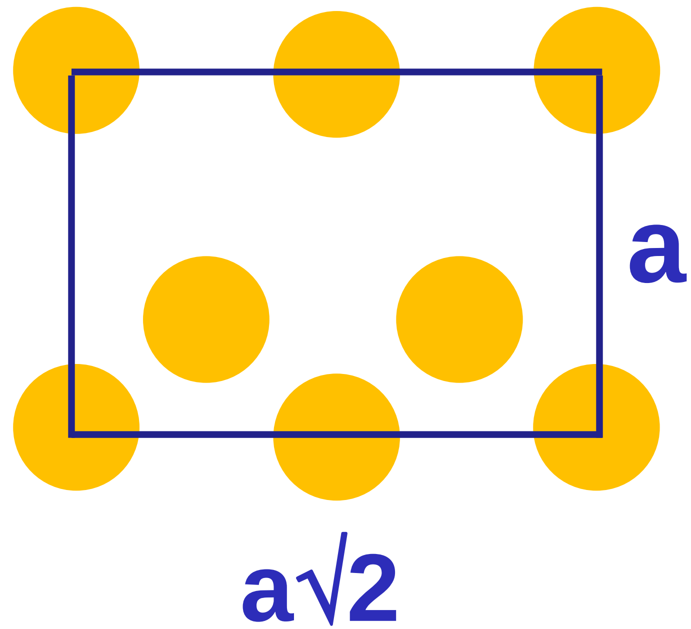
Area of plane: a^2

No. of atoms on the plane: 2

Si Unit Cell



(110)

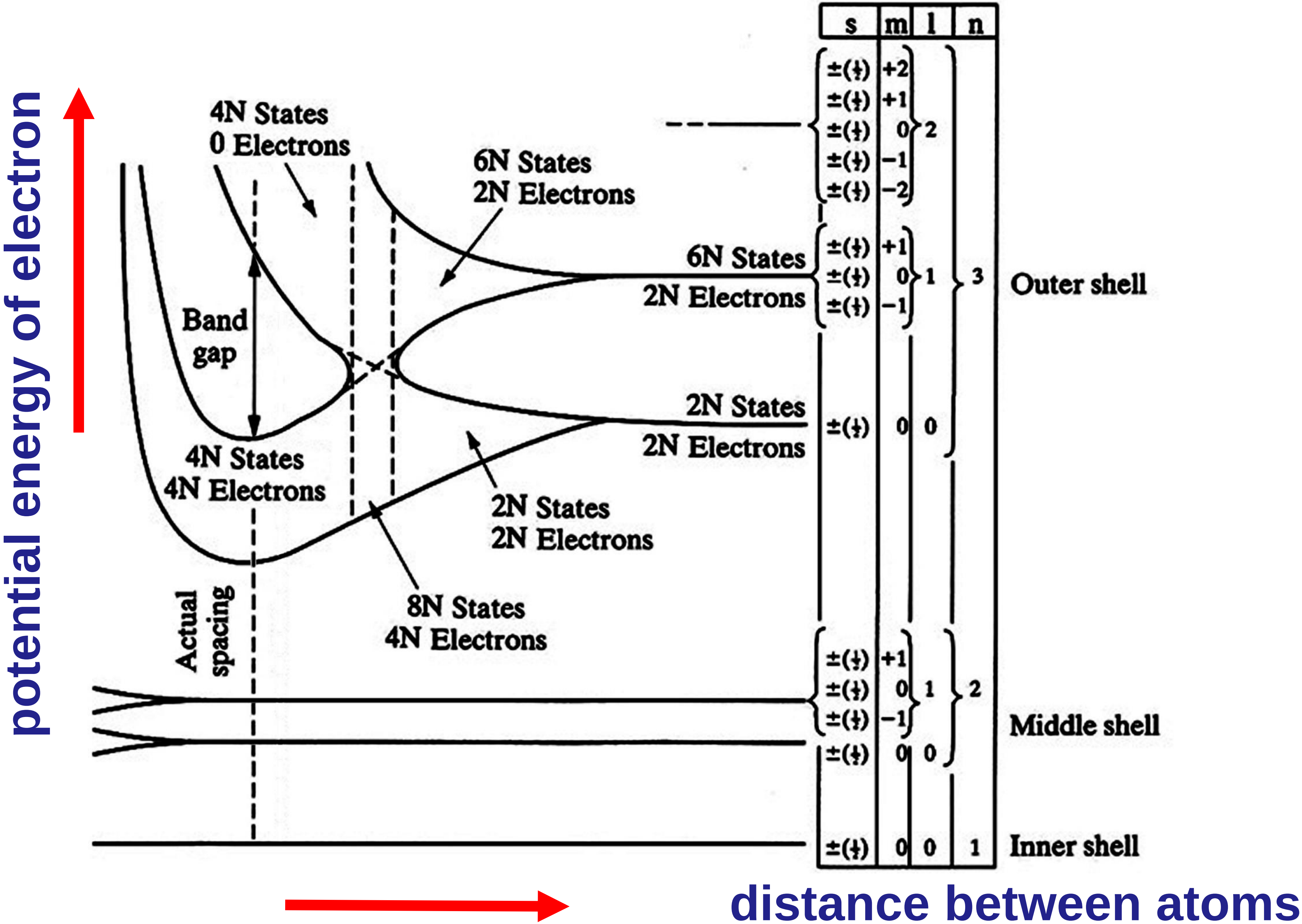


Area of plane: $a^2\sqrt{2}$

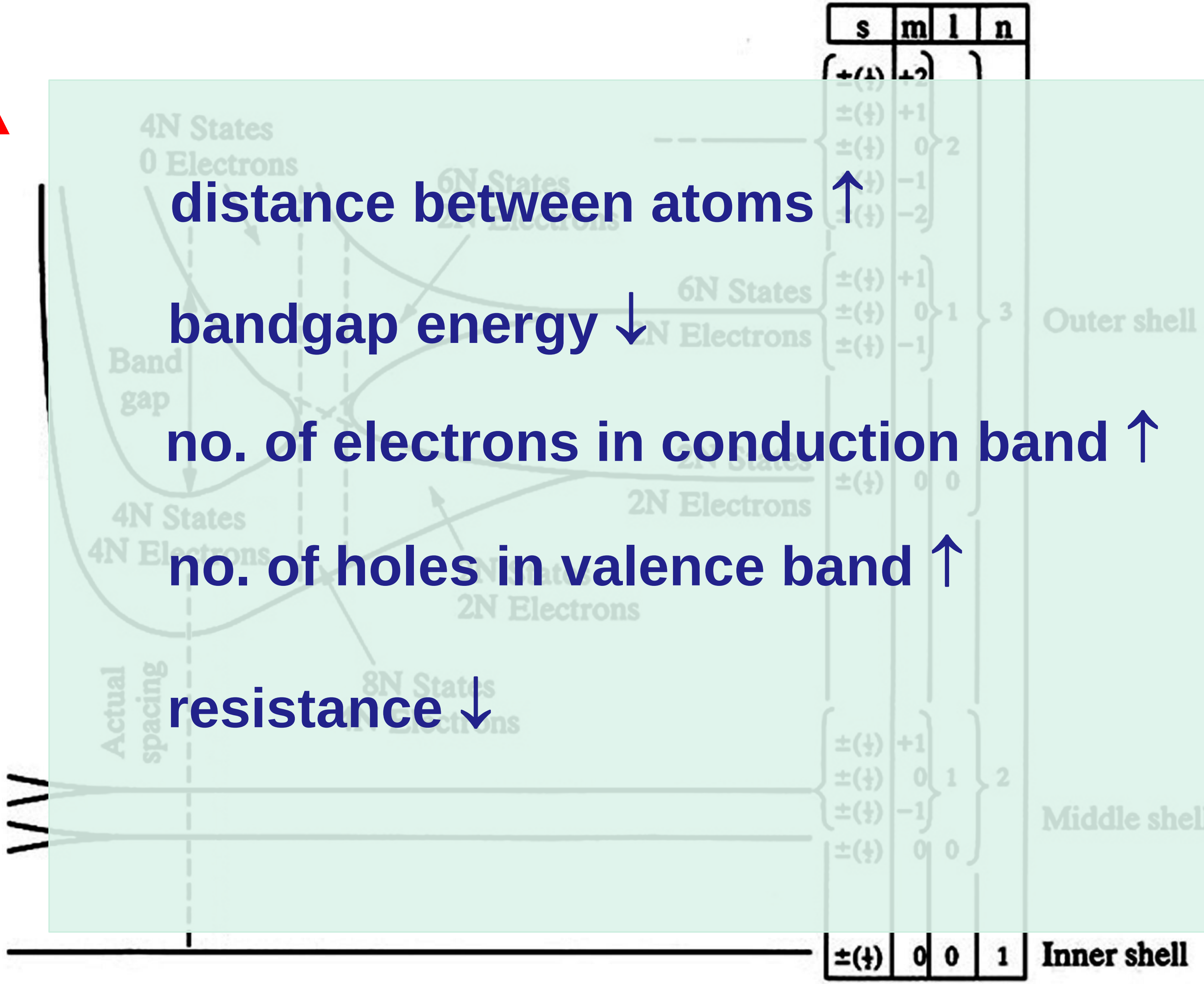
No. of atoms on the plane: 4

Question 3

In Fig. 2.1, the formation of energy bands and forbidden band of silicon are depicted. If the equilibrium lattice spacing were to change by a small amount, discuss how you would expect the electrical properties of silicon to change. Explain why the energy bandgap decreases as temperature increases.


potential energy of electron
distance between atoms
4N States
0 Electrons
6N States
2N Electrons
Band gap
4N States
4N Electrons
6N States
2N Electrons
2N States
2N Electrons
2N States
2N Electrons
8N States
4N Electrons
Actual spacing
s
m
l
n
Outer shell
Middle shell
Inner shell

potential energy of electron



distance between atoms ↑

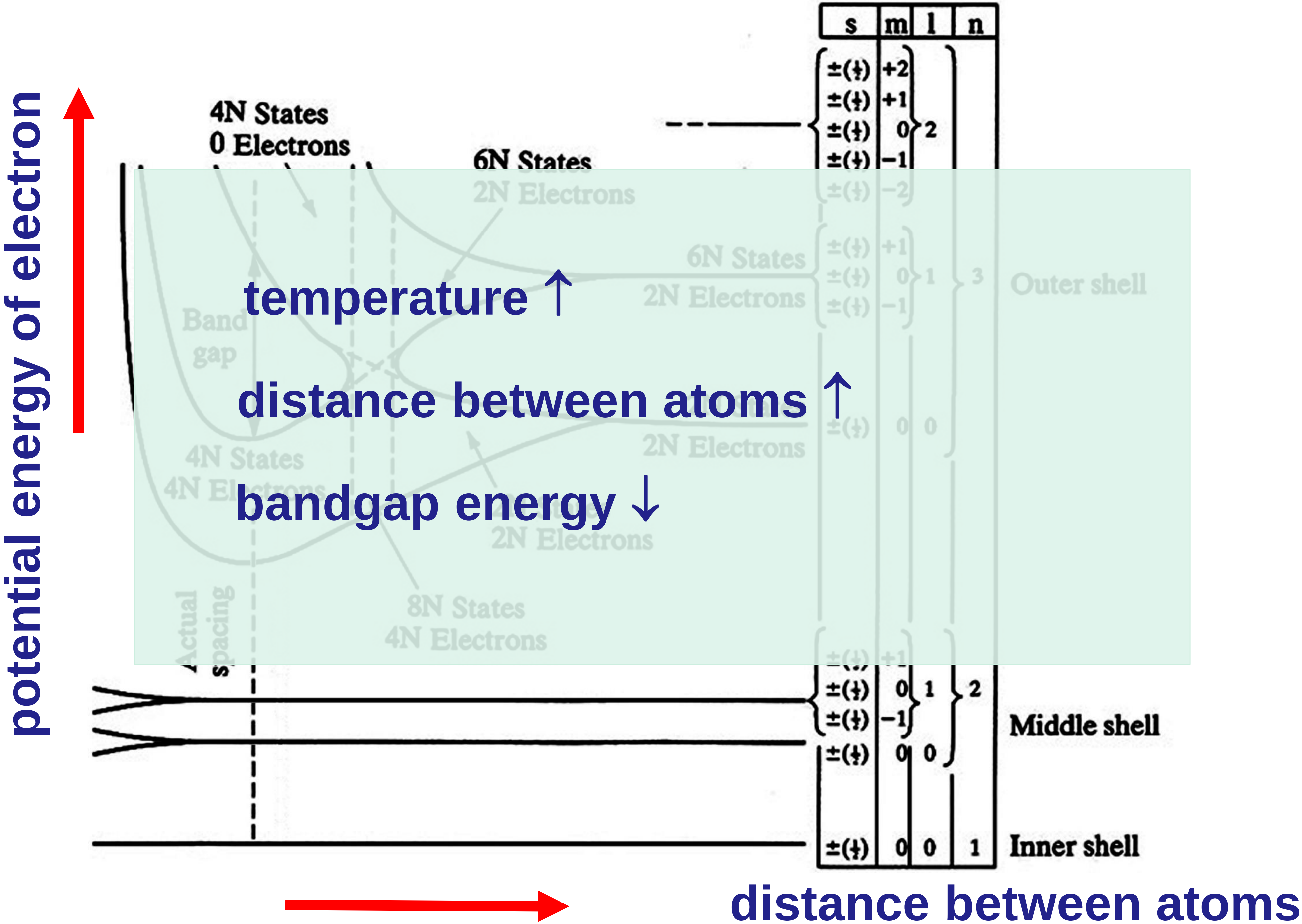
bandgap energy ↓

no. of electrons in conduction band ↑

no. of holes in valence band ↑

resistance ↓

distance between atoms


potential energy of electron
4N States
0 Electrons
6N States
2N Electrons
6N States
2N Electrons
Band gap
2N Electrons
4N States
4N Electrons
2N Electrons
8N States
4N Electrons
Actual spacing
s
m
l
n
Outer shell
Middle shell
Inner shell
temperature ↑
distance between atoms ↑
bandgap energy ↓
distance between atoms

Question 4

Considering the *E*-*k* diagram in Fig. 2.2 for Si and GaAs:

(a) Which material has a lower electron effective mass in the conduction band?

(b) Which of these would you expect to produce photons (light) more efficiently through electron-hole recombination?

(c) Consistent with your answer to part (b), what would you expect the energy of the emitted photons to be? What would be their wavelength in µm? You can use E_g(Si) = 1.11 eV, and E_g (GaAs) = 1.43 eV.

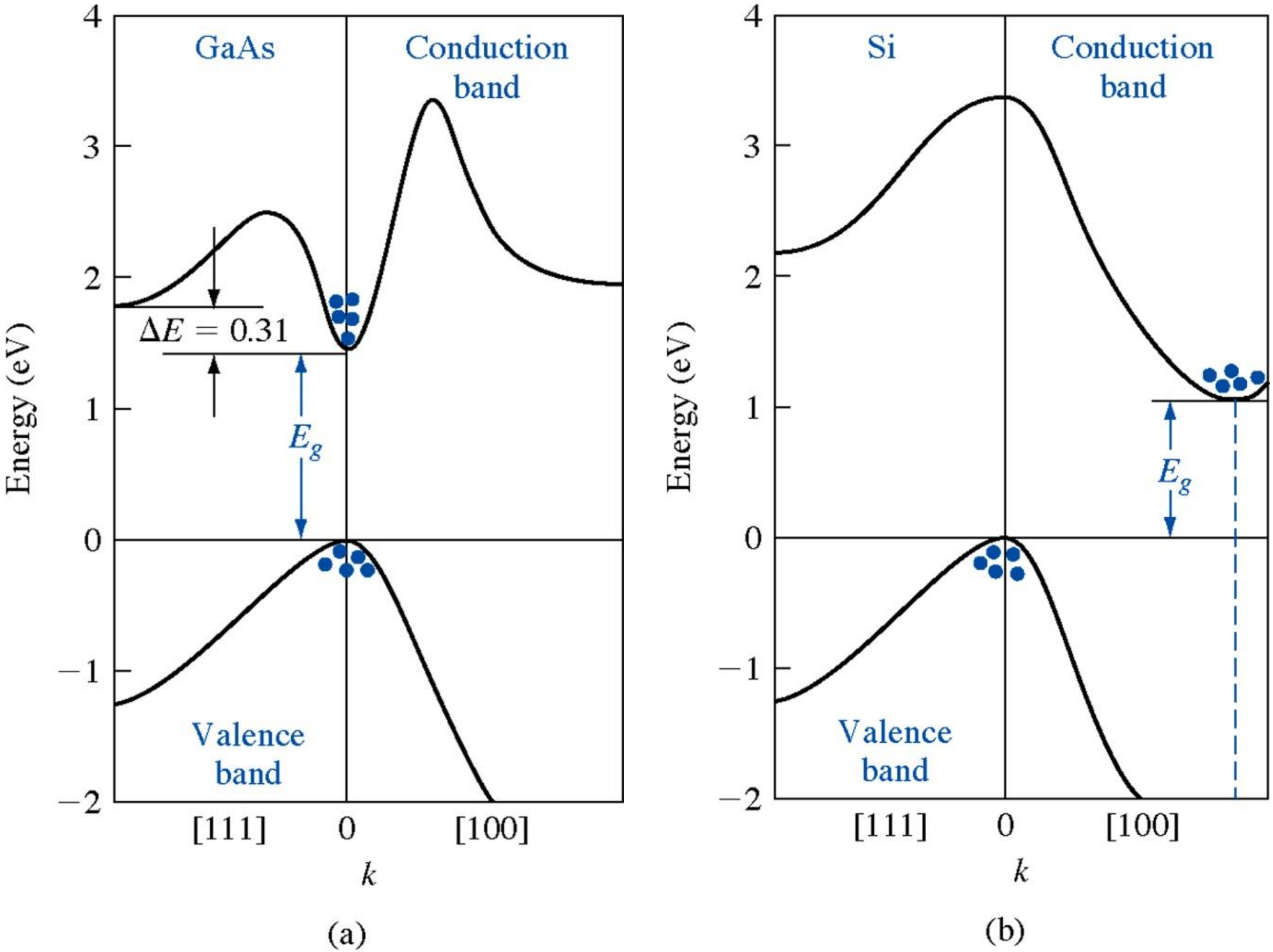


Fig. 2.2 Energy band structure of (a) GaAs and (b) Si.

How is effective mass related to the *E – k* diagram?

$$m^* \propto \left(\frac{d^2E}{dk^2} \right)^{-1}$$

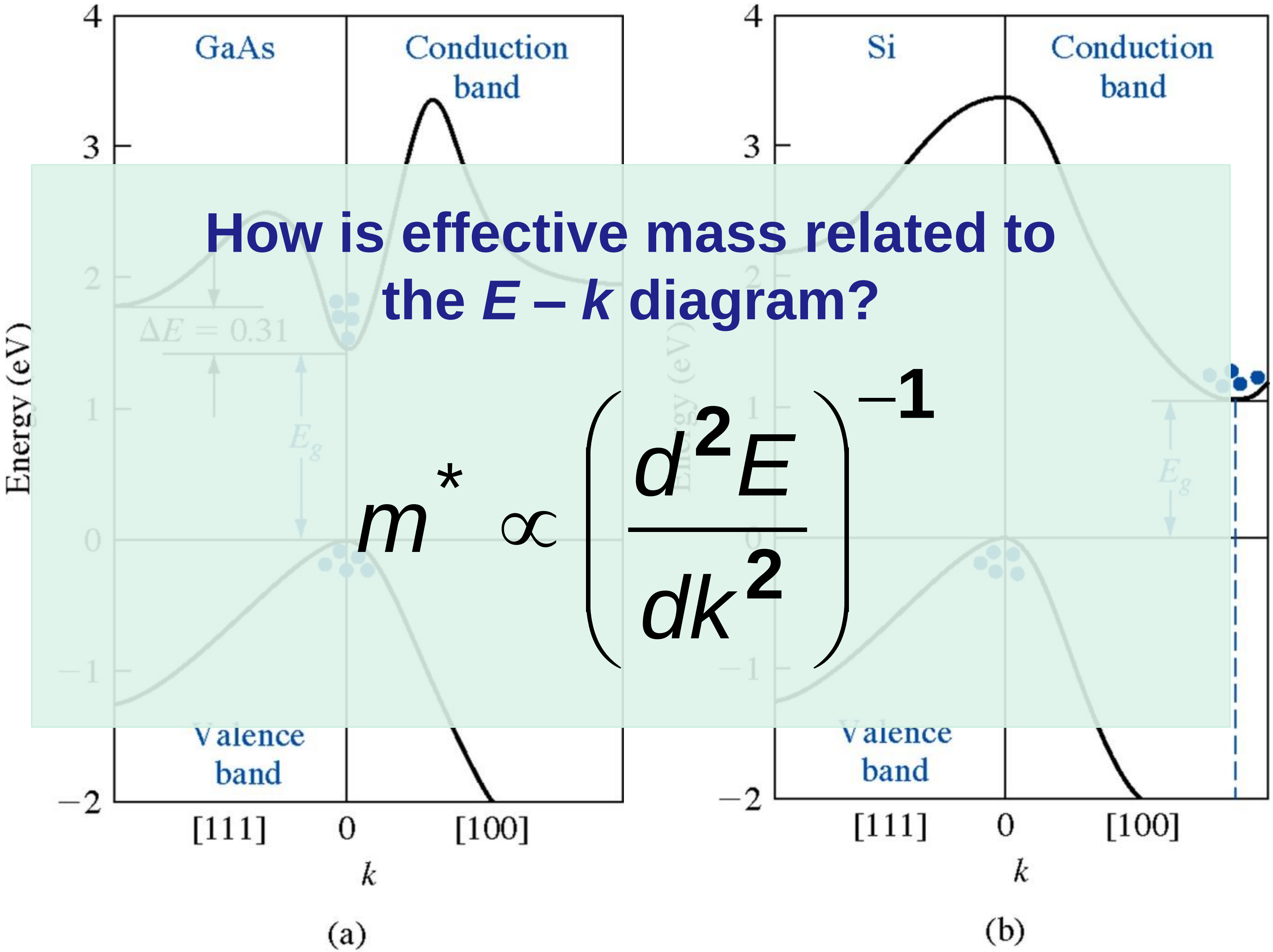
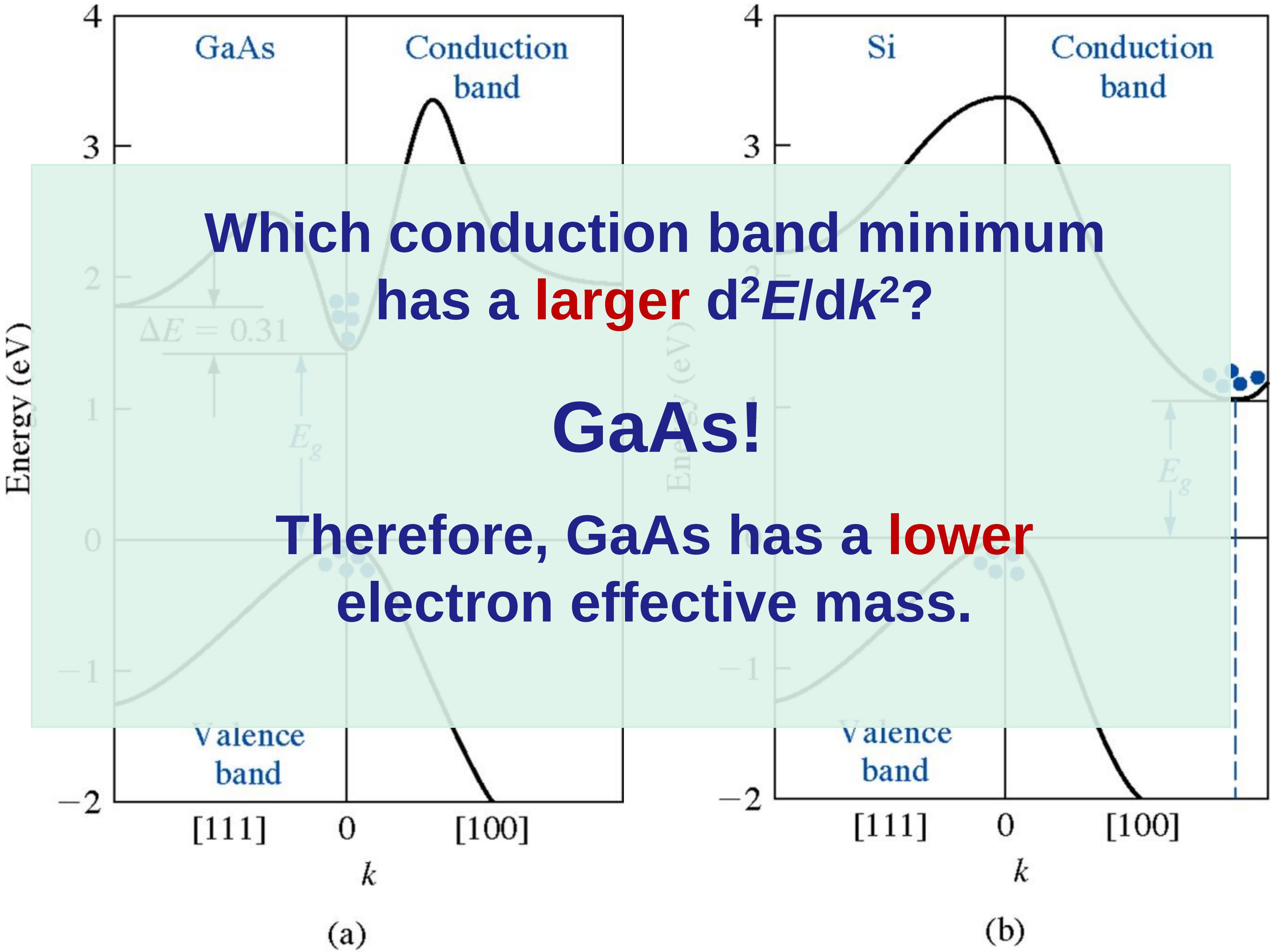


Fig. 2.2 Energy band structure of (a) GaAs and (b) Si.



Which conduction band minimum has a larger d^2E/dk^2?

GaAs!

Therefore, GaAs has a lower electron effective mass.

Fig. 2.2 Energy band structure of (a) GaAs and (b) Si.

Which material emits light when an electron recombines with a hole?

GaAs!

Because GaAs is a direct bandgap semiconductor.

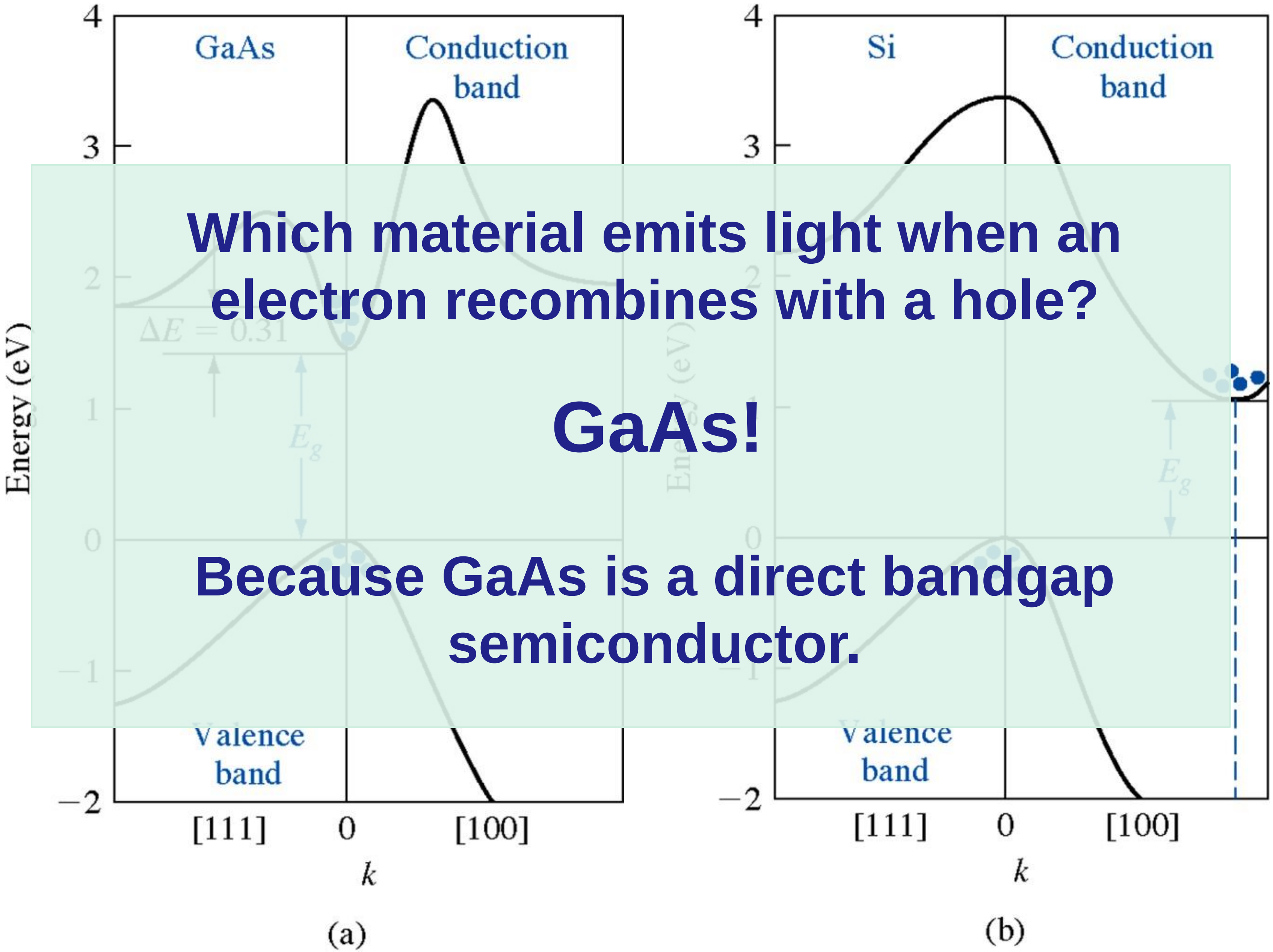
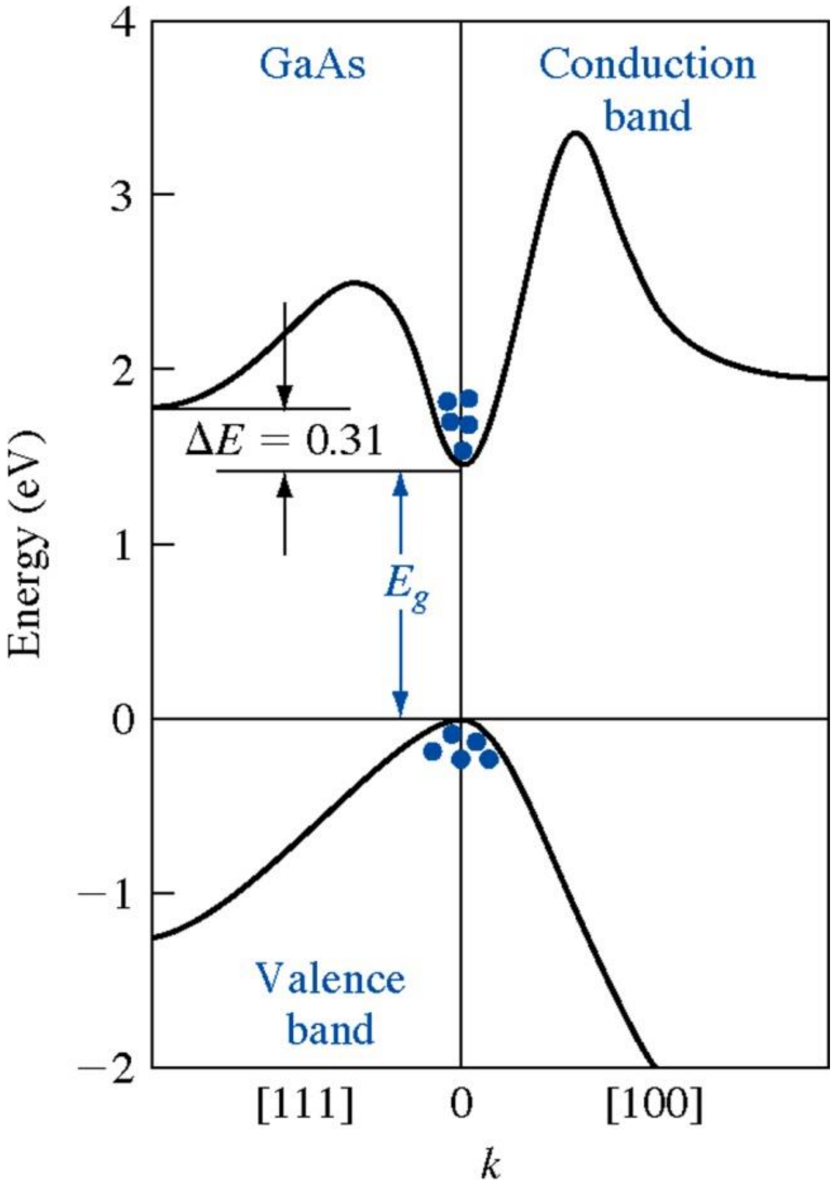


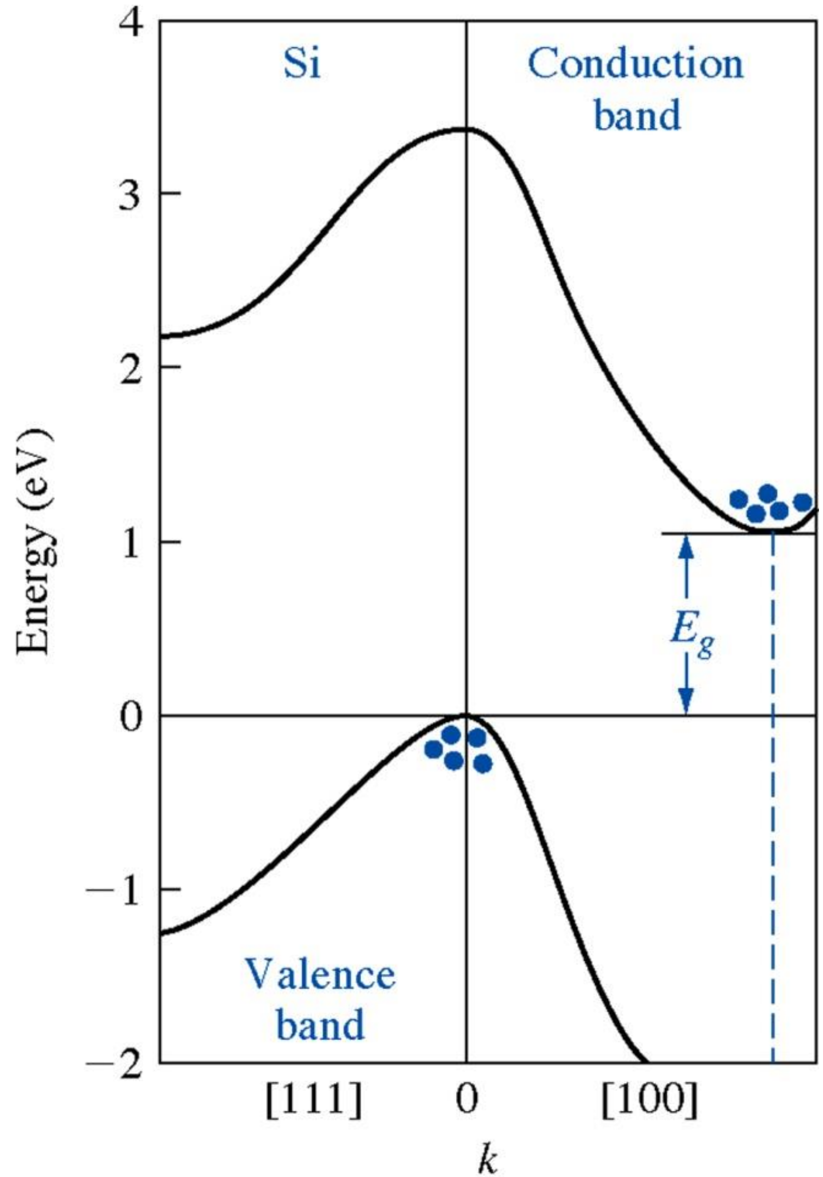
Fig. 2.2 Energy band structure of (a) GaAs and (b) Si.



direct bandgap

- electrons and holes have the same wave vector
- hence, they can readily recombine
- energy difference is converted into light

- electrons have a different wave vector from the holes
- hence, they cannot readily recombine
- Phonons (lattice vibrations) needed to change the electron wave vector to become the same as the holes
- Due to this interaction between electrons and phonons, energy difference is converted into heat



indirect bandgap

$$E_{ph} = E_g = hf = \frac{hc}{\lambda}$$

$$\lambda = \frac{hc}{E_g} = \frac{\mathbf{6.63 \times 10^{-34} \times 3 \times 10^{8}}}{\mathbf{1.43 \times 1.6 \times 10^{-19}}} = \mathbf{0.87\ \mu m}$$

h **– Planck's constant**

c **– speed of light**

f **– frequency**

λ **– wavelength of light**