Exercise Solid-State Physics (ET2908 and ET3175-D1) 2008-2009Q1: dr. R. Ishihara, DIMES-TC1.06, r.ishihara@tudelft.nl

Solution for Exercise-sheet 5

I. Hydrogen atoms

(I.1) Solution Refer to the answer of the exercise sheet 6.

(I.2)

(a) Write down the electron configuration ($1s^2 2s^2 ...$) of a Si atom.

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

(b) How many 3p states exist in the Si atom and how are they occupied by electrons?

Solution For the 3p, $l = 0$ where $m = 0, \text{or} \pm 1$, hence three orbits. Each orbit can be occupied two electrons having the spin up and down. Therefore total six states exist for the 3p. Two of the three orbits posses one electron for each. The rest does not have any electron.

(c) If many Si atoms are brought close together, the 3p states interact with 3s states. Explain how do the states interact each other and how electrons are distributed over the states.

Solution The 2s orbit is occupied by two electrons. When the Si atoms are brought close together, one electron in the 2s orbit is promoted and jumps into the empty 3p orbit. The four orbits (one 2s and three 3p) having one electron for each reform new four equivalent orbits having one electron for each. (The process is called as sp3 hybridization.) Each orbit shares the electron with another orbit of neighboring atom which shares its own electron as well. The states in the orbit are fully occupied making covalent bonding.

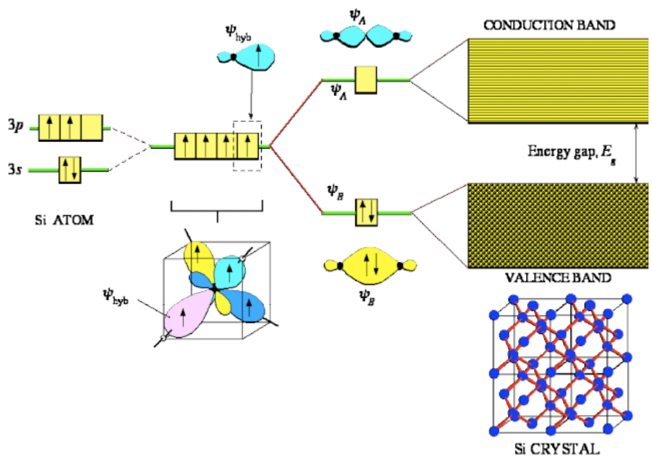

Figure 1: sp3 hybridization and formation of covalent bonding

(I.3)

Solution: By the Kronig-Penny model, the relation between k, total energy E and potential barrier V_0 can be obtained as follows ;

$$P\frac{\sin \alpha a}{\alpha a} + \cos \alpha a = \cos ka \tag{1}$$

where

$$P = \frac{ma}{\hbar^2} V_0 d \tag{2}$$

(ii) The equation can be expressed by

$$\frac{\sin \alpha a}{\alpha a} + \frac{\cos \alpha a}{P} = \frac{\cos ka}{P}. \tag{3}$$

If $V_0 \to \infty$ with a finate value of d, then $P = \infty$. Therefore $\sin \alpha a = 0$, that is, $\alpha a = n\pi (n = \pm 1, \pm 2, ...)$. From the equation,

$$E = \frac{\hbar^2 \pi^2}{2ma^2} n^2 (n = \pm 1, \pm 2, ...). \tag{4}$$

The E can be plotted as a function of k in Fig.1.

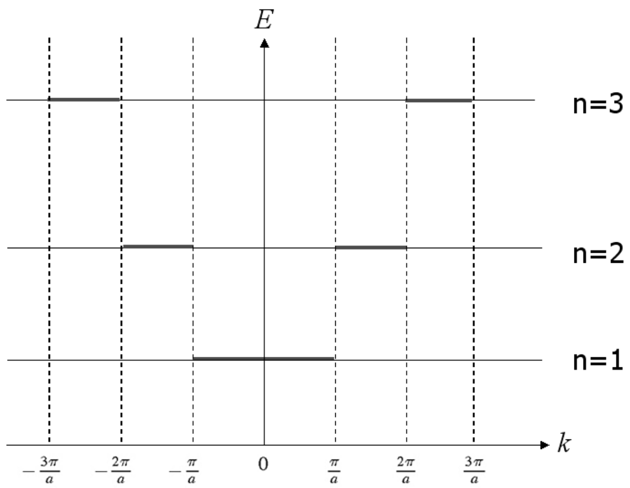

Figure 2: The E-k diagram for infinite high periodic barrier in Kronig-Penny model