Module 2 Unit 1

SEMICONDUCTORS – NOTES (SUPPLEMENTAL)

(As per SVU-R2020 Scheme & Syllabus)

Formation of energy bands in solids

The energy levels of electrons bound to the nucleus in any atom are essentially discrete, which follows from atomic theory. The typical energy configuration for any element say for example, silicon $(Z = 14)$ is given by, 1s², 2s², 2p⁶, 3s², 3p². We consider two such Si atoms far away i.e. isolated from each other to start with. Now, let the two atoms come close to each other so that they interact meaning an electron from one atom is influenced by the electrostatic potential of the nucleus of other atom also. Then, the two Si atoms are no longer isolated and they form a single system. In such an interacting system, now there cannot be two electrons (one from each of the Si atoms) having the same energy as per Pauli's exclusion principle. The bond formation between two atoms leads to splitting of the energy levels. In case of Si, 3s and 3p level split first and initially form a hybrid state (SP³ hybridization), which splits further at the distance equal to the bond length.

In general, a solid may be considered as an assembly of a large number of atoms (say N) closely packed with each other. In such an interacting system, each energy level (particularly, the outer energy levels) splits N-fold giving a band of closely spaced energies as shown in figure above. The formation of energy bands is different in each solid and it is highly complicated. In different solids, the energy bands may be overlapping each other or they may remain separated by small or large gaps. The overlapping or separation between valence band and conduction band is of particular importance as it ultimately decides the electrical, thermal and optical properties of materials. The classification of solids based on energy bands is shown in figure below.

Insulators e.g. Glass

Solids having partially overlapping conduction band (CB) and valence band (VB) or very small gap inbetween are termed conductors. Solids having small energy gap typically between 1 to 3 eV are termed as semiconductors while Solids having large energy gap typically greater than 5 eV are termed as isolators. The dependence of electrical conductivity on this energy band gap is exponential. To give you a feel of it, it may require only a few nano to microvolt to get a few milliampere current from metals. For getting the same current, it would require a few volts for a semiconductor while even by applying few thousands of volts, insulators may not still allow the current to flow.

Doping, intrinsic and extrinsic semiconductors

Doping: A carefully engineered process of adding specific amount of foreign atoms into host semiconductor. Usual range of doping in Si for most of the applications is 10^{15} to 10^{19} /cm³. Typical methods used for doping are high temperature (800-900°C) diffusion using vapours of dopants or ion implantation at room temperature using bombardment of dopant ions of a few keV energy.

Intrinsic semiconductor: Semiconducting element in which, the electrical conduction is possible only by breaking covalent bonds between host atoms is called as intrinsic semiconductor. With each bond broken, we get an electron-hole pair for electrical conduction.

Extrinsic semiconductor: Semiconducting elements in which, electrical conduction is carried predominantly by electrons or holes obtained from donor or acceptor impurities are called as extrinsic semiconductors. The number of electrons or holes obtained is large as compared to number of electron-hole pairs obtained by breaking bonds.

Charge carriers in intrinsic semiconductor:

Following diagram shows typical bonding structure of silicon; a prototype semiconductor. A particular electron "A" is a part of one of the covalent bonds. The same is indicated in an equivalent energy band diagram. It takes 1.1 eV of energy (at RT) to break a covalent bond in Si. When we do that, electron A becomes free and a vacancy bearing positive charge is created due to incomplete bond. This is regarded as "hole".

The same is indicated in the energy band picture by showing electron "A" making a "jump" from VB to CB. Thus, it takes a minimum of 1.1 eV to create free electron-hole pair for conduction in intrinsic silicon. This value varies depending upon semiconductors e.g. in GaAs, it is 1.4 eV.

Charge carriers in extrinsic n-type semiconductor:

When we dope a pure semiconductor such as silicon with pentavalent impurity such as phosphorous, all four covalent bonds are completed. It takes very small amount of energy (merely 0.05 eV) to remove the fifth electron from the impurity. Electron-holes pairs are still created by breaking bonds between silicon atoms but now their proportion is very low (at RT). Thus for electrons, there are two sources: one, from host atoms by bond breaking and second, from donors but for holes, there is only one source that is bond breaking. Therefore, electrons become excess in number in n-type material and they are called as "majority carriers" while holes are called as "minority carriers".

The addition of impurity is shown by indicating a "donor" level just below the CB in the energy band diagram

Charge carriers in extrinsic p-type semiconductors:

When we dope a pure semiconductor such as silicon with trivalent impurity such as boron, only three silicon atoms around it can form bonds with it and the forth bond is incomplete. But this is not a hole. When an electron shared by a neighbouring pair of silicon atoms jumps to boron to complete the forth covalent bond between boron and silicon, it leaves behind "uncompensated" silicon atom with deficit of one electron from its valence level. This is regarded as hole. Since the silicon atom is uncompensated, it acquires a net positive charge, which is assigned to the hole. In semiconductors at RT, such processes occur at all times and it can be called as "bond exchange". Although it appears like breaking the bond between two host atoms, it doesn't take full 1.1 eV of energy but it happens at merely 0.05 eV of energy. This is the energy required to create a "free hole".

Electron-holes pairs are still created by breaking bonds between silicon atoms but now their proportion is very low (at RT) Thus for holes, there are two sources: one, from host bond breaking and second, bond exchange with acceptors but for electrons, there is only one source that is bond breaking. Therefore, holes become excess in number in p-type material and they are called as "majority carriers" while electrons are called as "minority carriers". The addition of impurity is shown by indicating a "acceptor" level just above the VB in the energy band diagram

Direct and Indirect bandgap semiconductors:

Direct band gap semiconductor

Indirect band gap semiconductor

In direct bandgap semiconductors, when an electron makes a transition from CB to VB or vice versa, its momentum is readily conserved since there is no change in k value (k is related with momentum). In indirect bandgap semiconductors, however, large change in k value is required for electron to make transition between bands. Here, a third particle called "phonon" is required for conservation of momentum. Phonons are quanta of lattice vibrations (the same way photons are quanta of light). Phonons possess small enenrgy but large momentum. In particular, during transition of electrons from CB to VB, energy is released in the form of emission of a photon of energy equal to the difference between CBM and VBM. For direct bandgap semiconductors, this process takes place efficiently (with quantum efficiency > 80%) whereas for indirect bandgap semiconductors, the efficiency is poor (<

10%) due to the requirement of phonons. For this reason, light emitting devices such as LEDs are always made from direct bandgap materials like GaAs whereas Si cannot make an efficient LED or laser diode.

Abobe problem is not very critical during upward transition i.e. absorption as electrons in the VB of indirect bandgap materials can absorb higher energy photons to transfer into VB. Hence, although Si and Ge cannot be used for making sources of light (LEDs), they are very much useful as detectors of light (photodiodes).

Continuity equation: One of the most important equations of semiconductor physics is the continuity equation. It states that "when equilibrium state is disturbed, excess carriers are generated in the semiconductor but at any instance, the rate at which, carrier concentration is changing with time is counterbalanced by spatial variation of the current density". In simple words, it means that if excess carriers are injected into the semiconductor, they flow out so that an electric current is established. The continuity equation is a direct consequence of the law of conservation of charge since the equation demands that there is no indefinite sourcing or sinking of charges. In mathematical form,

∂n $\frac{\partial \mathbf{n}}{\partial \mathbf{t}} = \frac{1}{\mathbf{q}}$ q ∂J_n $\frac{\partial J_n}{\partial x}$ + (G_n – R_n); where, G_n and R_n is called rate of generation and recombination of charge carriers. A similar equation holds for holes with a negative sign for first term of the RHS.

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