PHYSICS OF SEMICONDUCTOR DEVICES

Jean-Pierre Colinge
Cynthia A. Colinge

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by

J. P. Colinge
Department of Electrical and Computer Engineering
University of California, Davis

C. A. Colinge
Department of Electrical and Electronic Engineering
California State University

KLUWER ACADEMIC PUBLISHERS
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ce (period = $a+b$), the $\frac{2\pi}{+b}$. The $E(k)$ curve can iodicity of $\frac{2\pi}{a+b}$, which one-dimensional crystal

ited to k-values ranging rmation. This particular ouin zone. The second rom $\frac{\pi}{a+b}$ to $\frac{2\pi}{a+b}$, the $\frac{2\pi}{a+b}$ to $\frac{3\pi}{a+b}$, etc.

tions (Expression 1.1.12) or k:

$\pm 1, \pm 2, \pm 3, ...)$ (1.1.30)

crystal (or the number of he length of the crystal is first Brillouin zone, the k- given by the following is excluded because it is a

orresponding values for n s of k to consider are:

$), -N/2)$ (1.1.31)

st Brillouin zone, which ice cells. For every wave ch energy band. By virtue band can thus contain a

rillouin zone is equal to sity of k-values in the first

values
e zone

$$= \frac{N}{2\pi/(a+b)} = \frac{N(a+b)}{2\pi} = \frac{L}{2\pi} \qquad (1.1.32)$$

In the case of a three-dimensional crystal, energy band calculations are, of course, much more complicated, but the essential results obtained from the one-dimensional calculation still hold. In particular, there exist permitted energy bands separated by forbidden energy gaps. The 3-D volume of the first Brillouin zone is $8\pi^3 N/V$, where V is the volume of the crystal, the number of wave vectors is equal to the number of elementary crystal lattice cells, N. The density of wave vectors is given by:

$$n(\mathbf{k}) = \text{density of } \mathbf{k} = \frac{\text{number of } \mathbf{k}\text{-vectors}}{\text{volume of the zone}} = \frac{NV}{8\pi^3 N} = \frac{V}{8\pi^3} \qquad (1.1.33)$$

1.1.4. Valence band and conduction band

Chemical reactions originate from the exchange of electrons from the outer electronic shell of atoms. Electrons from the most inner shells do not participate in chemical reactions because of the high electrostatic attraction to the nucleus. Likewise, the bonds between atoms in a crystal, as well as electric transport phenomena, are due to electrons from the outermost shell. In terms of energy bands, the electrons responsible for forming bonds between atoms are found in the last occupied band, where electrons have the highest energy levels for the ground-state atoms. However, there is an infinite number of energy bands. The first (lowest) bands contain core electrons such as the 1s electrons which are tightly bound to the atoms. The highest bands contain no electrons. The last ground-state band which contains electrons is called the *valence band*, because it contains the electrons that form the -often covalent- bonds between atoms.

The permitted energy band directly above the valence band is called the *conduction band*. In a semiconductor this band is empty of electrons at low temperature ($T=0K$). At higher temperatures, some electrons have enough thermal energy to quit their function of forming a bond between atoms and circulate in the crystal. These electrons "jump" from the valence band into the conduction band, where they are free to move. The energy difference between the bottom of the conduction band and the top of the valence band is called "forbidden gap" or "bandgap" and is noted E_g.

In a more general sense, the following situations can occur depending on the location of the atom in the periodic table (Figure 1.11):

A: The last (valence) energy band is only partially filled with electrons, even at $T=0K$.

B: The last (valence) energy band is completely filled with electrons at $T=0K$, but the next (empty) energy band overlaps with it (*i.e.*: an empty energy band shares a range of common energy values; $E_g < 0$).

C: The last (valence) energy band is completely filled with electrons and no empty band overlaps with it ($E_g > 0$).

In cases A and B, electrons with the highest energies can easily acquire an infinitesimal amount of energy and jump to a slightly higher permitted energy level, and move through the crystal. In other words, electrons can leave the atom and move in the crystal without receiving any energy. A material with such a property is a *metal*. In case C, a significant amount of energy (equal to E_g or higher) has to be transferred to an electron in order for it to "jump" from the valence band into a permitted energy level of the conduction band. This means that an electron must receive a significant amount of energy before leaving an atom and moving "freely" in the crystal. A material with such properties is either an *insulator* or a *semiconductor*.

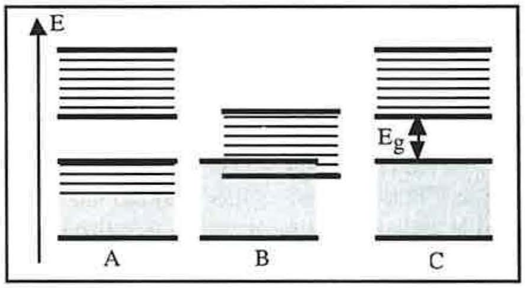

Figure 1.11: Valence band (bottom) and conduction band in a metal (A and B) and in a semiconductor or an insulator (C).[6]

The distinction between an insulator and a semiconductor is purely quantitative and is based on the value of the energy gap. In a semiconductor E_g is typically smaller than 2 eV and room-temperature thermal energy or excitation from visible-light photons can give electrons enough energy for "jumping" from the valence into the conduction band. The energy gap of the most common semiconductors are: 1.12 eV (silicon), 0.67 eV (germanium), and 1.42 eV (gallium arsenide). Insulators have significantly wider energy bandgaps: 9.0 eV (SiO_2), 5.47 eV (diamond), and 5.0 eV (Si_3N_4). In these materials room-temperature thermal energy is not large enough to place electrons in the conduction band.