Junction analysis and temperature effects in semi-conductor heterojunctions
by Naresh Tandan

A thesis submitted to the Graduate Faculty in partial fulfillment of the requirements for the degree of DOCTOR OF PHILOSOPHY in Electrical Engineering
Montana State University

Abstract:
A new classification for semiconductor heterojunctions has been formulated by considering the different mutual positions of conduction-band and valence-band edges.

To the nine different classes of semiconductor heterojunction thus obtained, effects of different work functions, different effective masses of carriers and types of semiconductors are incorporated in the classification. General expressions for the built-in voltages in thermal equilibrium have been obtained considering only nondegenerate semiconductors. Built-in voltage at the heterojunction is analyzed. The approximate distribution of carriers near the boundary plane of an abrupt n-p heterojunction in equilibrium is plotted. In the case of a p-n heterojunction, considering diffusion of impurities from one semiconductor to the other, a practical model is proposed and analyzed. The effect of temperature on built-in voltage leads to the conclusion that built-in voltage in a heterojunction can change its sign, in some cases twice, with the choice of an appropriate doping level. The total change of energy discontinuities (&ΔEc + ΔEv) with increasing temperature has been studied, and it is found that this change depends on an empirical constant and the 0°K Debye temperature of the two semiconductors. The total change of energy discontinuity can increase or decrease with the temperature. Intrinsic semiconductor-heterojunction devices are studied? band gaps of value less than 0.7 eV. are suggested if such devices are to be used at room temperature. Built-in voltage in the case of intrinsic semiconductor heterojunction devices varies slightly with the temperature. With -proper choice of effective masses, the built-in voltage remains essentially constant with the temperature. The advantages of intrinsic semiconductor devices are discussed. A three-dimensional energy-distance-momentum diagram is described; it suggests a change in the wave vector of a carrier, in transit from one semiconductor to other. Thus, the probability of transition of a carrier across the heterojunction is reduced.

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LIST OF SYMBOLS

Subscript "1" represents narrow-gap semiconductor

Subscript "2" represents broad-gap semiconductor

C	Capacitance in Farad.
E_c	Energy of conduction band gap in eV.
ΔE_c	Energy discontinuity in energy band diagram of a heterojunction (associated with electron affinity difference) in eV.
E_F	Fermi level, n and p semiconductor in eV.
E_{Fi}, E_{FI}	Intrinsic Fermi level in semiconductor in eV.
E_g	Energy band gap in eV.
E_v	Energy of valence-band edge in eV.
ΔE_v	Energy discontinuity in the valence-band energy diagram of a heterojunction in eV.
h	Planck's constant in Joule-sec.
$\hbar$	$\frac{h}{2\pi}$
J_n	Electron current density in A cm^{-2}.
J_p	Hole current density in A cm^{-2}.
K	Momentum wave vector.
k	Boltzmann's constant in eV° k^{-1}.
m_e^*	Electron effective mass Kg.
m_{de}^*	Density-of-state effective mass for electron in Kg.

m^*_{dh}	Density-of-state effective mass for holes in Kg.
m^*_{lh}	Light hole mass in Kg.
m^*_{hh}	Heavy hole mass in Kg.
m^*_l	Effective mass along the longitudinal ellipsoidal energy surface in Kg.
m^*_t	Effective mass along the transverse ellipsoidal energy surface in Kg.
m^*_h	Effective mass of hole.
N_a, N_A	Acceptor density in cm^{-3}.
N_C	Effective density of energy states at the conduction band edge in cm^{-3}.
N_d, N_D	Donor density in cm^{-3}.
N_V	Effective density of energy states at the valence-band edge in cm^{-3}.
n_o, n	Free electron density in the conduction band in cm^{-3}.
n_d	Unionized donors in cm^{-3}.
n_i	Intrinsic carrier concentration in a semiconductor cm^{-3}.
p_o, p	Hole density in cm^{-3}.
P_a	Unionized acceptors in cm^{-3}.
q	Charge of an electron, 1.6×10^{-19} conlomb.
T	Absolute temperature in °K.
V_{BHT}	Built-in voltage in heterojunction in volts.

V_{BHM}	Built-in voltage in homojunction in volts.
x	Distance in cm.
γ	Emitter injection efficiency.
ε	Dielectric constant of the semiconductor in F cm^{-1}.
μ_n	Mobility of electrons in cm^2 v^{-1} sec^{-1}.
μ_p	Mobility of holes in cm^2 v^{-1} sec^{-1}.
ϕ_m	Work function of a semiconductor in eV.
χ_e	Electron affinity of a semiconductor in eV.
χ_h	$(\chi_e + E_g)$ in eV.
$\psi(x)$	Electrostatic potential difference as a function of distance in volts.
σ	Conductivity in mhos.
θ	Debye temperature.

ABSTRACT

A new classification for semiconductor heterojunctions has been formulated by considering the different mutual positions of conduction-band and valence-band edges. To the nine different classes of semiconductor heterojunction thus obtained, effects of different work functions, different effective masses of carriers and types of semiconductors are incorporated in the classification. General expressions for the built-in voltages in thermal equilibrium have been obtained considering only nondegenerate semiconductors. Built-in voltage at the heterojunction is analyzed. The approximate distribution of carriers near the boundary plane of an abrupt n-p heterojunction in equilibrium is plotted. In the case of a p-n heterojunction, considering diffusion of impurities from one semiconductor to the other, a practical model is proposed and analyzed. The effect of temperature on built-in voltage leads to the conclusion that built-in voltage in a heterojunction can change its sign, in some cases twice, with the choice of an appropriate doping level. The total change of energy discontinuities ($\Delta E_C + \Delta E_V$) with increasing temperature has been studied, and it is found that this change depends on an empirical constant and the 0°K Debye temperature of the two semiconductors. The total change of energy discontinuity can increase or decrease with the temperature. Intrinsic semiconductor-heterojunction devices are studied; band gaps of value less than 0.7 eV. are suggested if such devices are to be used at room temperature. Built-in voltage in the case of intrinsic semiconductor heterojunction devices varies slightly with the temperature. With proper choice of effective masses, the built-in voltage remains essentially constant with the temperature. The advantages of intrinsic semiconductor devices are discussed. A three-dimensional energy-distance-momentum diagram is described; it suggests a change in the wave vector of a carrier, in transit from one semiconductor to other. Thus, the probability of transition of a carrier across the heterojunction is reduced.

Chapter 1

INTRODUCTION

Historical Review

A semiconductor heterojunction is a junction between two dissimilar semiconductors where the crystal structure is continuous across the interface. Semiconductor heterojunction research is an important area of device study which has evolved from the research of the last decade. The barriers introduced into the energy-band diagram by the energy-gap difference of two semiconductors allows a new degree of freedom to the device designer. For example, in GaAs injection lasers [1], the addition of $Al_xGa_{1-x}As$ confinement barriers has resulted in a major reduction in 300°K threshold current densities. Electrooptical effects in heterojunctions that are promising include infrared to visible upconversion systems [2], the window effect [3], solar cells [4] and photo transistors [5]. High yield photo cathodes [6], cold cathodes [7] and electron multipliers [8] of the negative-electron affinity type represent yet other families of devices where heterojunctions are involved.

The heterojunction structure was first considered by Preston [9]. Gubanov [10] produced an analysis of

heterojunctions with n-n, p-p and p-n combinations. Shockley [11] proposed a circuit device incorporating a change in the magnitude of the forbidden gap in the transition region of p-n junction. Kroemer [12] proposed the use of a heterojunction as a wide-gap emitter to increase the injection efficiency of transistors. The Anderson theory [3] is discussed in the following section and a brief summary of other theories is discussed on page 7.

Anderson's Theory. The energy-band model of an ideal abrupt heterojunction without interface states was proposed by Anderson based on the previous work of Shockley. This model is important as it can adequately explain most of the transport processes, and only a slight modification [13] of the model is needed to account for non-ideal cases such as interface states. Consider the energy-band profile of the two isolated semiconductors as shown in Figure 1. The two semiconductors are assumed to have different band gaps (E_{g_1},E_{g_2}), different dielectric constants (ε_1,ε_2), different work function (ϕ_{m_1},ϕ_{m_2}), and different electron affinities (χ_{1e},χ_{2e}). The work function is defined as the energy required to remove an electron from the Fermi level (E_F) to a position just outside of

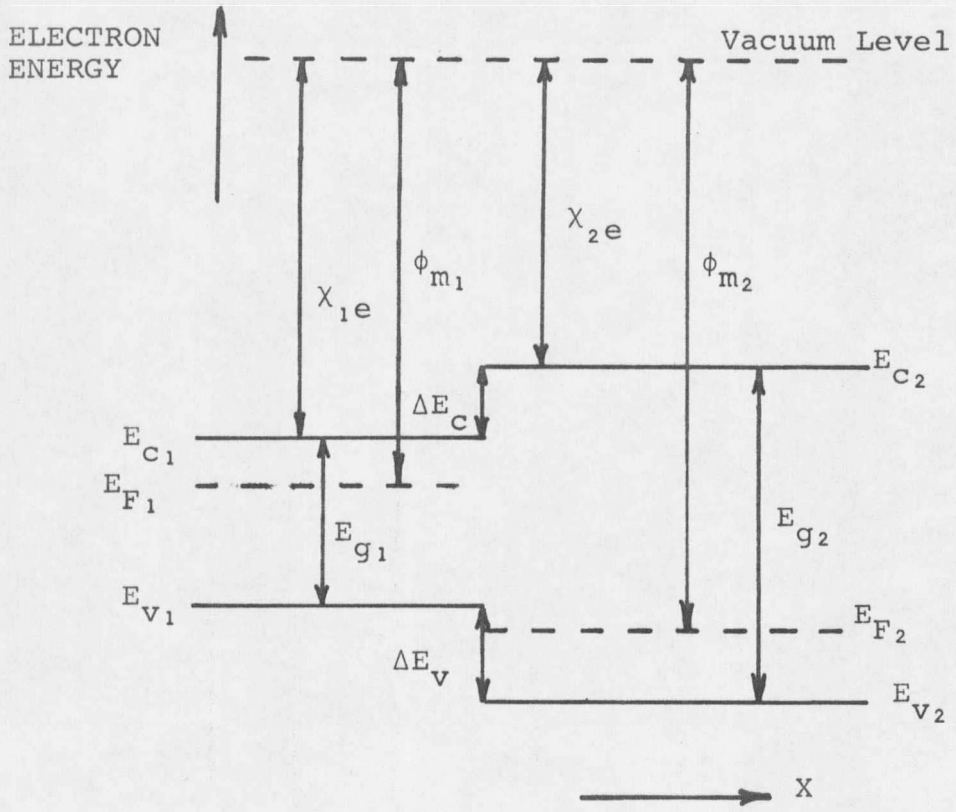

Figure 1. Energy-band diagram for two isolated semiconductors in which space charge neutrality is assumed to exist in every region.

the material. The bottom of the conduction-band is represented by E_c and the top of the valence-band is represented by E_v. The subscripts 1 and 2 refer to the narrow-gap and wide-gap semiconductors, respectively. Electron affinity is defined as the energy required to remove an electron from the bottom of conduction-band to a position just outside of the material. It is assumed that space charge neutrality exists in every region and thus band edges ($E_{c_1}, E_{c_2}, E_{v_1}, E_{v_2}$) are shown to be horizontal. The difference in energy of the conduction-band edges in the two materials is represented by ΔE_c and that in the valence-band edges is ΔE_v.

A junction formed between an n-type narrow-gap semiconductor and a p-type wide-gap semiconductor is considered. The energy-band profile of such a junction at equilibrium is shown in Figure 2.

The electrostatic potential difference between any two points can be represented by the vertical displacement of the band edges between these two points in a semiconductor. An electrostatic field can be represented by the slope of the edges on a band diagram. The total built-in voltage (V_{BHT}) is equal to the sum of the partial built-in

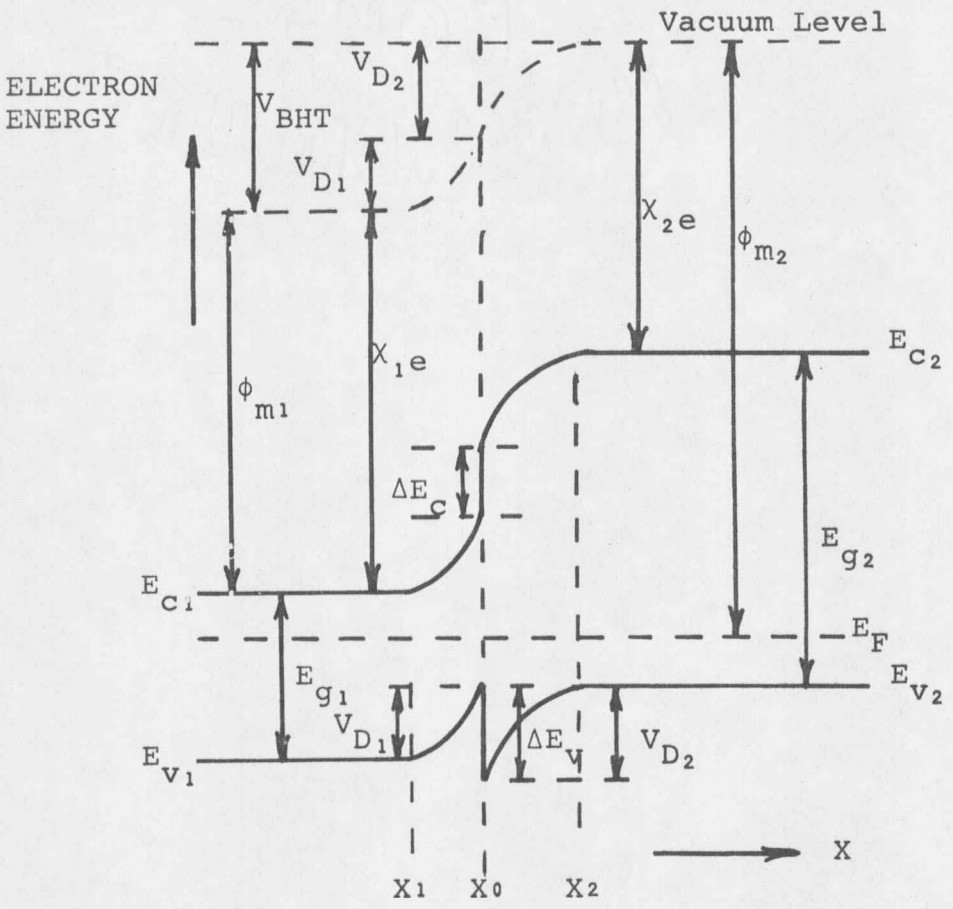

Figure 2. Energy-band diagram of n-p heterojunction in thermal equilibrium.

voltages ($V_{D_1} + V_{D_2}$), where V_{D_1} and V_{D_2} are the electrostatic potentials supported at equilibrium by semiconductors 1 and 2, respectively. Since the Fermi level must coincide on both sides in equilibrium and the vacuum level is everywhere parallel to the band edges and is continuous, the discontinuity in the conduction band edges (ΔE_c) and valence-band edges (ΔE_v) is invariant with doping in those cases where E_g and χ are not functions of doping (i.e., nondegenerate semiconductors). A degenerate semiconductor is one in which Fermi level lies in the conduction or in the valence-band. It is assumed that the electron density is zero for $X>X_1$, and the hole density is zero for $X<X_2$. Then at any point in the transition region, the space charge density is merely equal to the donor or acceptor density.

$$p_1 = q\, N_{D_1} \qquad X_1 \leq X \leq X_0$$

$$p_2 = q\, N_{A_2} \qquad X_0 \leq X \leq X_2$$

where N_{D_1} is the donor concentration in semiconductor 1 and N_{A_2} is the acceptor concentration in semiconductor 2. The solution of Poisson's equation in the one dimensional case with appropriate doping levels gives the solution for an abrupt junction as follows [3]: