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BARRIER HEIGHT OF ANISOTYPE HETEROJUNCTION IN PRESENCE OF INTERFACE STATES AND DEEP LEVEL IMPURITIES

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A theoretical model on the barrier height of anisotype heterojunction is proposed considering the presence of both the interface states and the deep level impurities. The Fermi level pinning in these structure is found to be dependent on the interface state density, the shallow and deep impurity concentrations and the characteristics energy of the two crystallites originally proposed by Tersoff [16-18]. It is seen that, in addition to the interface states, the barrier height of the system is sensitive to the deep level impurities.

1. Introduction

The barrier height is a parameter which plays an important role in the electrical characteristics of various heterojunction devices such as switching devices [1-5], solar cells [6,7] and Junction Field Effect Transistors [8]. Although extensive works have been carried out in the past to realize the mechanism of barrier formation in terms of work function difference and band discontinuties, the present state of knowledge seems to be inadequate when localized states are present in the device. These localized states may be present at the interface of the two crystallites forming from the junction and within the individual crystallites in the form of deep levels. The capacitance-voltage characteristics of Cu_2S/CdS heterojunctions reveal distinct effects of bulk defects [9,10]. The role of deep centres on the barrier height and the open circuit voltage of MIS-devices has been discussed recently by Chattopadhyay and Das [11,12]. Therefore, for any realistic analysis of the barrier height, a combined effect of the above two types of states must be considered. In this communication a theoretical model of the barrier height is proposed by taking into account the above nonidealities in the system.

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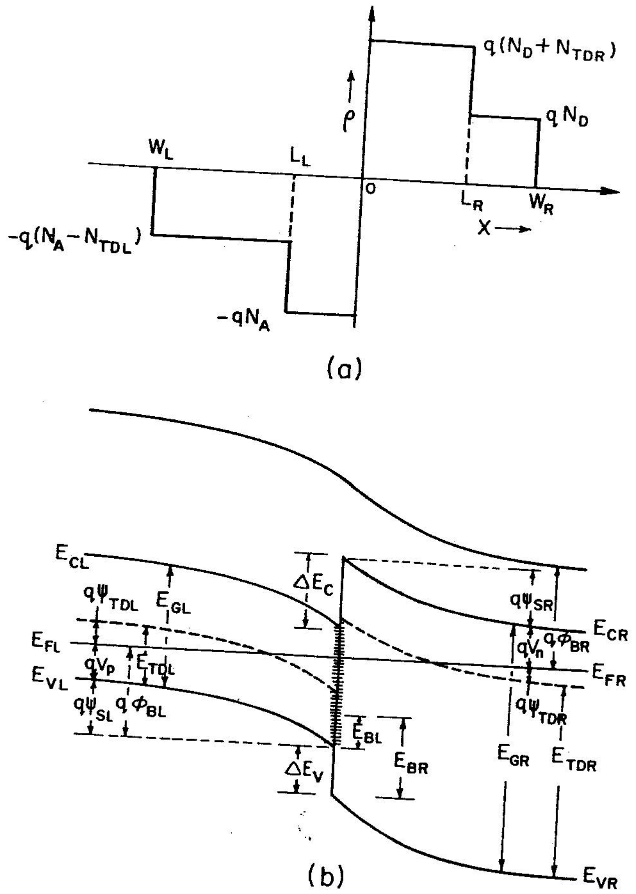

ig. 1. Energy band diagrams of anisotype heterojunction before (A) and after (B) the align-
ent of Fermi levels of the two crystallites.

2. Space charge density

ie calculation of the potential and field distributions in junction devices requires solu-
on of Poisson's equation with appropriate boundary conditions. The analysis seems to
intricate if deep level impurities are present. We adopt here the approach of Ref. 11
investigate how the device properties are influenced by donor like deep centres. Fig.
hows the energy band and charge density diagrams of an anisotype heterojunction in
sence of deep donors, where ΔE_C and ΔE_V are the band discontinuities and $\chi_{L,R}$
the electron affinities of the two crystallites. We have used the subscripts L and
o differentiate the crystallites on the left and right. The presence of deep levels
arates the depletion layers width of the two crystallites into two regions of different

space charge densities. For the crystallite on the left, the space charge densities for the two regions can be written as:

$$\begin{aligned} \rho_L &= -qN_A, & 0 < x < L_L, \\ &= -q(N_A - N_{TDL}), & L_L < x < W_L, \end{aligned} \tag{1}$$

where N_A and N_{TDL} are respectively the densities of shallow acceptors and deep donors. The above two regions are separated at $x = L_L$ where the potential is defined as

$$\Psi_{TDL} = (E_{TDL} - E_F)/q \tag{2}$$

The space charge density developed in the crystallite can be obtained following our previous work [11] given by

$$Q_{SCL} = -[2q\epsilon_s(N_A\Psi_{SL} - N_{TDL}\Psi_{TDL})]^{1/2}. \tag{3}$$

The Fermi level position in the bulk may be calculated using charge neutrality condition given by

$$E_{FL} = E_{VL} + kT\ln\left[A_0A_1 + \{(A_0A_1)^2 + A_2\}^{1/2}\right], \tag{4}$$

where

$$\begin{aligned} A_0 &= 1/(2gN_A), \\ A_1 &= N_{VL}g - (N_A + N_{TDL})\exp(E_{TDL}/kT), \\ A_2 &= N_{VL}\exp(E_{TDL}/kT)/N_A g, \end{aligned}$$

and g is the ground state degeneracy factor for donor states, the value of which may be taken as 2 for donor states [13]. In a similar manner, the expression for the space charge density and Fermi level position for the crystallite on the right can be obtained given by

$$Q_{SCR} = [2q\epsilon_s\{(N_D + N_{TDR})\Psi_{SR} - N_{TDR}\Psi_{TDR}\}]^{1/2} \tag{5}$$

and

$$E_{FR} = E_{CR} - kT\ln\left[B_1/2B_2 + \{(B_1/2B_2)^2 + B_3/B_2\}^{1/2}\right], \tag{6}$$

where

$$\begin{aligned} B_1 &= N_{CR}\exp(E_{TDR} - E_{GR})/kT - N_{DR}g, \\ B_2 &= (N_{DR} + N_{TDR})\exp(E_{TDR} - E_{gR})/kT, \\ B_3 &= N_{CR}g. \end{aligned}$$

3. Interface state charge density

As described above, the localized states in the bulk of the semiconductor modify the space charge density determined by the parameters N_{TD} and E_{TD}. The modification of the space charge density is also expected if localized states are present at the interface of the heterojunction. However, in this case, the modification of the space charge density comes through an indirect way namely, due to charge conservation of the whole system. The interface of a layered structure has been previously modelled in a number of works. Bardeen [14] described interface of metal-semiconductor contact in terms of neutral energy and interface states and proposed possibility of Fermi level pinning at the neutral energy. Subsequently, Tejedor et al [15] discussed the significance of the neutral energy in their interface state model. Recently, there has been further progress in the interpretation of Bardeen pinning in metal-semiconductor contact and heterojunction mainly due to a series of works published by Tersoff [16-18]. According to Tersoff's model there exists a mid gap energy determined by the bulk properties of the semiconductor where Fermi level is pinned. For a heterojunction, the mid gap energies of the constituting semiconductors tend to be aligned and thus resulting in so called band discontinuties. The calculation of Tersoff [17] shows excellent agreement between the theory and experiment. The above description seems to be valid for intrinsic semiconductor. However, when the semiconductors forming the junction are extrinsic, a deviation from the above picture is expected. One can model such a junction by assuming that, due to Fermi level alignment, the states between the Tersoff's mid gap energy and the Fermi energy are filled with electrons and a net negative charge density at the junction. One can apply the rule that $E_{BR} = E_{BL} + \Delta E_V$ where E_{BL} and E_{BR} are the mid gap energies associated with the two semiconductors and ΔE_V is the valence band discontinuity. The charge density at the interface can be calculated with reference to either E_{BL} or E_{BR} and in both the cases, one expects the same result. Therefore, the interface state charge density of the heterojunction under consideration becomes

$$Q_{ITL} = -q^2 D_{ITL} \left[\Psi_{SL} + V_P - E_{BL}/q\right] \tag{7}$$

with respect to semiconductor on the left and

$$Q_{ITR} = -q^2 D_{ITR} \left[E_{GR}/q - \Psi_{SR} - V_N - E_{BR}/q\right] \tag{8}$$

with respect to-the semiconductor on the right, where $D_{ITL,R}$ represents densities of nterface states defined in $\mathrm{cm}^{-2}\ \mathrm{eV}^{-1}$. The equivalence of the quantities Q_{ITL} and Q_{ITR} can be proved considering the correlation between the potentials Ψ_{SL} and Ψ_{SR} an be obtained from an analysis of the energy band diagram given by

$$\Psi_{SR} + \Psi_{SL} = \chi_L + E_{GL} - V_P - \chi_R - V_N. \tag{9}$$

ne can also obtain from the band diagrams

$$\chi_L = \chi_R + \Delta E_C \tag{10}$$

d

$$E_{GR} = \Delta E_C + \Delta E_V + E_{GL}. \tag{11}$$

ostituting eqn. (10) in (9) one obtains

$$\Psi_{SR} + \Psi_{SL} = \Delta E_C + E_{GL} - V_P - V_N. \tag{12}$$

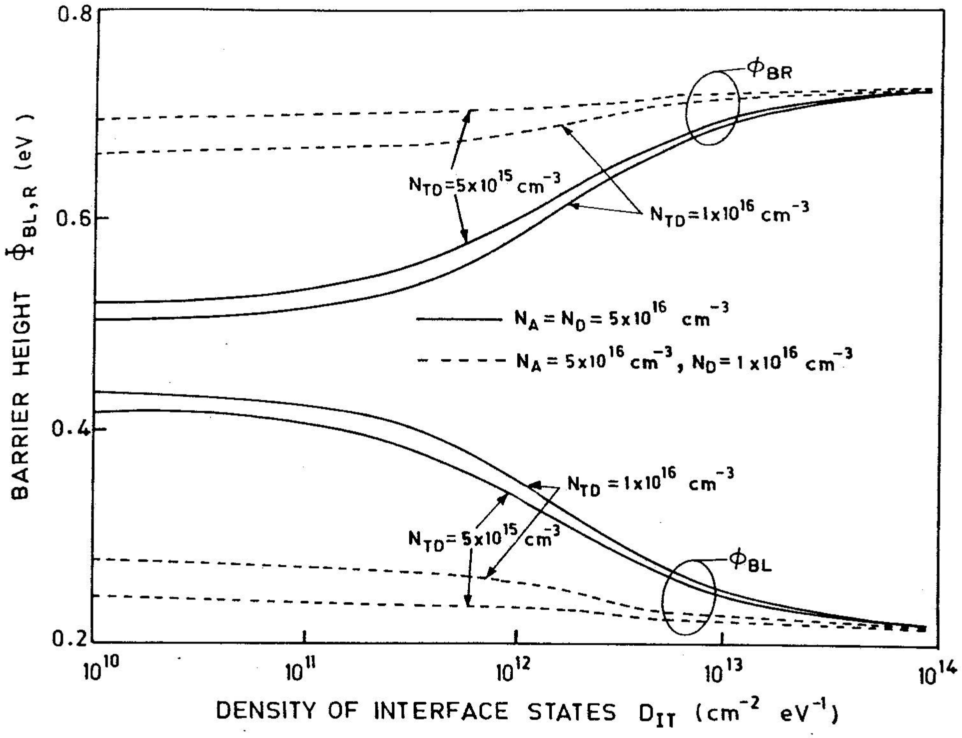

Fig. 2. The variation of barrier heights Φ_{BL} and Φ_{BR} as a function of the density of interface states (D_{IT}). Parametric values: $E_{BL} = 0.22$ eV, $E_{BR} = 0.4$ eV, $E_C = 0.28$ eV, $E_V = 0.18$ eV, E_{GL}(Ge) = 0.18 eV and E_{GL}(Si) = 1.12 eV. $E_{TDR} = 0.80$ eV and $E_{TDL} = 0.30$ eV. In the calculation it is assumed that $D_{ITL} = D_{ITR} = D_{IT}$.

It can be readily shown with the help of eqns. (10), (11) and (12) that the expression for Q_{ITR} is exactly the same as that of Q_{ITL}. Therefore, one can proceed with any one of eqns. (7) and (8). Hence, in the subsequent discussions, a term Q_{IT} is used instead of Q_{ITL} or Q_{ITR}.

4. Barrier height

The barrier height of the system can be obtained from the solution of the charge neutrality equation given by

$$Q_{SCL} + Q_{SCR} + Q_{IT} = 0, \tag{13}$$

where space charge densities $Q_{SCL,R}$ in the two crystallites are given by eqns. (3) and (5) and the interface state charge density Q_{IT} can be calculated with the help of eqn. (7) or (8). Considering the values of ΔE_C, ΔE_V and E_{BL} and E_{BR} from ref. 16 and the values of E_{TDL} and E_{TDR} to be 0.3 and 0.8 eV respectively, we calculate the barrier height of the system $\Phi_{BL,R} = \Psi_{SL,R} + V_{P,N}$ as a function of interface state density at temperature $T = 300$ K. The results of the calculation are plotted in Fig. 2 as a function of interface state density for two cases when (i) the doping of the two crystallites are same ($N_A = N_D = 5 \times 10^{16}$ cm^{-3}, represented by continuous line curves) and (ii) for different doping ($N_A = 5 \times 10^{16}$ cm^{-3}, $N_D = 1 \times 10^{16}$ cm^{-3}, represented by dashed line curves). The effect of N_{TD} on the barrier height is also shown in Fig. 2.

5. Discussion

Fig. 2 shows the variation of barrier heights of Ge-Si systems as a function of interface state density. When the doping concentrations of the two crystallites are the same, the variation of Φ_{BL} and Φ_{BR} are opposite. At low value of D_{IT}, the Fermi levels of the two crystallites are not pinned. However, as the density of states increases, the barrier height Φ_{BR} gradually increases until it becomes pinned at the characteristic energy E_{BR}. The barrier height of the other crystallite on the left decreases with D_{IT} and ultimately becomes fixed at E_{BL}. As apparent from the figure that the barrier heights $\Phi_{BL,R}$ for unequal doping concentration also exhibit opposite nature of variation with interface state density, but with certain changes in their absolute values compared to the case when the doping concentrations are equal. The deep level impurities in effect decrease the barrier for the crystallite on the right while they increase the barrier for the crystallite on the left. It may be mentioned, that in calculating barrier height we have considered two specific values of E_{TDL} and E_{TDR}. These values may depend on the impurities actually present in the host crystal. The type of the impurity states and their energetic location in the band gap are available in the literature [19]. Therefore, to enable the model calculation in a realistic case, the prior knowledge on the deep level parameters is required. In fact, these parameters can be measured directly by DLTS technique.

The calculated values of the barrier height may be used to obtain the saturation current density of Ge-Si system. Depending on the potential barrier and the band discontinuities, the current transport across a Ge-Si system may be either due to flow of electrons from Si to Ge or holes from Ge to Si side. Under thermoionic emission model, the saturation current density can be represented by $J_{OL,R} = A^*T^2 \exp -(q\Phi_{BL,R}/kT)$. With $A^* = 120$ A cm^{-2} K^{-2}, $T = 300$ K and $\Phi_{BR} = 0.628$ eV, the value of J_{OR} comes out to be 3.43×10^4 A cm^{-2}. Such a value is consistent with the observed experimental I-V characteristics of Ge(p)-Si(n) heterojunction at $T = 298$ K [20]. Note that the above value of barrier height can be realized through interface states and doping levels of the system. With reference to Fig. 2, it may be concluded that, the value of interface state charge density required to fix a value of $\Phi_{BR} = 0.628$ eV is nearly 3.2×10^{-7} C cm^{-2}. It may be mentioned that the density of states under the present interface state model is much different from that of dangling bond concept. For Ge-Si system the density of dangling bonds have been estimated to be 1.1×10^{14} cm^{-2} [20] and the corresponding value of trapped charge density is about 1.76×10^{-5} C cm^{-2}. The mismatch in the quantitative values of trapped charge densities results from the basic definitions of the density of states, of the respective interface state models. In the present case, it is defined per unit energy interval per unit area. Similar definition of density of states has been adopted by Card [21] and considered its value varying from $10^{10} - 5 \times 10^{11}$cm^{-2} eV^{-1}.

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