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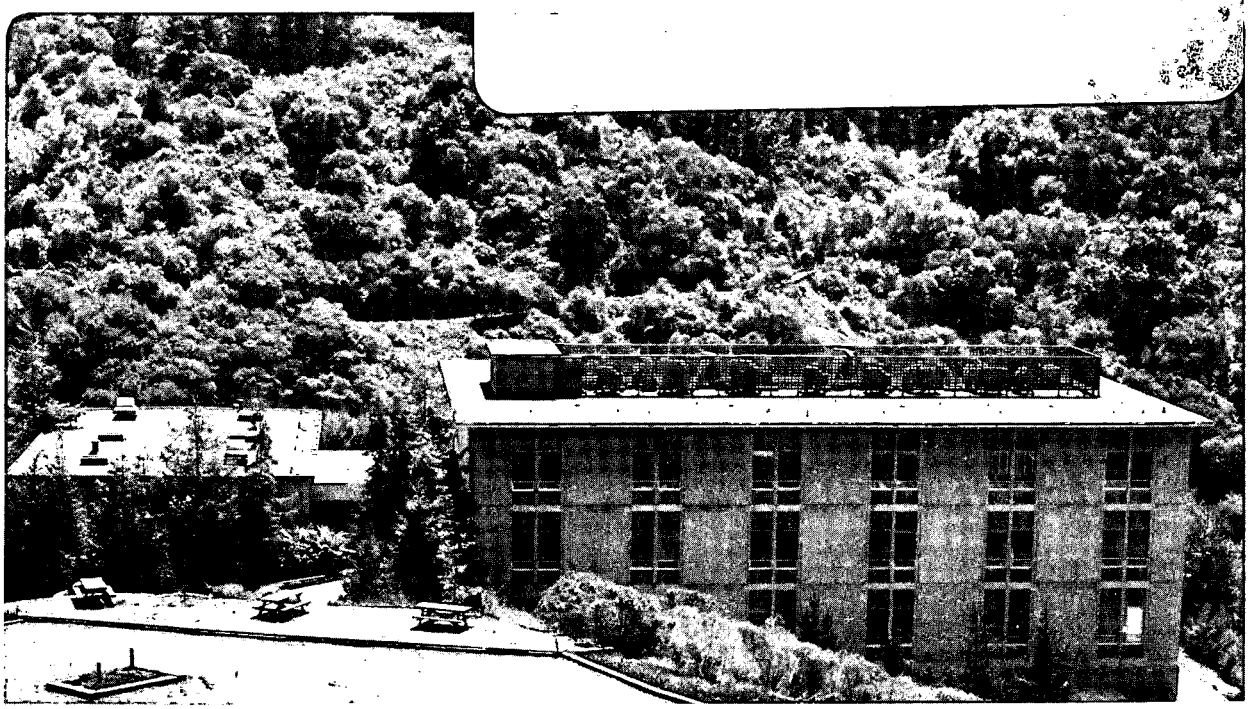

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MECHANISM OF SCHOTTKY BARRIER FORMATION: THE ROLE OF AMPHOTERIC NATIVE DEFECTS

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Abstract

A correlation between the Fermi level pinning deduced from Schottky barrier heights and from electrical properties of irradiated III-V semiconductors is found. The correlation indicates that similar defects are responsible for the Fermi level stabilization in both cases. It is proposed that amphoteric native defects, i.e. the defects which change their electrical characteristics depending on the Fermi level position, play a dominant role in the processes leading to a Schottky barrier formation. A detailed analysis of metal-GaAs contacts shows that in this case the amphoteric defects responsible for the barrier heights are: V_{Ga} (acceptor) and a donor complex $As_{Ga} + V_{As}$. It is shown that for thick metal coverages two barriers are formed. A surface barrier determined by the charge associated with a native defect and the bulk barrier controlled by the bulk doping. The sum of the two barrier heights satisfies the Schottky condition for the interface but it is the bulk barrier that determines the macroscopic electrical properties of the contact. The model explains the evolution of the Fermi level position at the interface observed for metal coverages varying in a broad range of thicknesses. The relationship of the present proposal to previous models of Schottky barriers is discussed.

I. Introduction

The physical processes leading to the formation of a Schottky barrier (SB) have been a subject of intensive studies for over four decades.[1,2] Numerous physical models aimed at explaining the characteristics of metal-semiconductor interfaces have been proposed.[3-8] Insensitivity of SB heights to the metal work functions has led to the generally accepted assumption that defect states pinning the Fermi energy must exist at the interface.

Although many native defect systems[9,10] were proposed to be responsible for the pinning, there was never any direct evidence for the existence of such defects at the interface. Furthermore, a number of recent experiments on the dependence of the Fermi level position on metal layer thickness also have shown that in some instances the Fermi level is not pinned at the interface.[11,12] The results of these experiments seemed to put into question the universality of the defect model.

This paper shows how many of these apparently contradictory experimental findings can be explained in terms of a new model of SB formation. The model is based on the existence of amphoteric native defects which are shown to be responsible for the Fermi level pinning at metal-semiconductor interfaces, as well as for Fermi level stabilization in irradiated III-V materials. The model is applied to a detailed description of the physical processes leading to barrier formation on the most extensively studied metal-GaAs system.

II. Amphoteric native defects

It has been known for a long time that the stability of electrically active defects depends on the position of the Fermi level.[13] Thus it has been found that amphoteric impurities have a tendency to preferentially

occupy minority sites because this leads to a lower total formation energy.[14] This type of behavior can be found also among native defects in compound semiconductors. In some cases small structural transformations result in a complete change of the electrical characteristics of the defect. A good example is the gallium vacancy V_{Ga} in GaAs.[15] The vacancy is a stable acceptor in n-type material and transforms to a $As_{Ga} + V_{As}$ donor complex in p-type material. This behavior stems from a large electronic contribution to the defect reaction $V_{Ga} + As_{As} \leftrightarrow As_{Ga} + V_{As}$. The introduction of such defects will compensate both n- and p-type materials. Eventually, the Fermi level will be stabilized at the energy at which equilibrium for the defect reaction $V_{Ga} + A_{As} \leftrightarrow As_{Ga} + V_{As}$ is attained.

An example of the physical system in which transformations of native defects results in the stabilization of the Fermi level is a semiconductor with native defects intentionally introduced by either electron, neutron, or γ-ray irradiation. In compound semiconductors radiation creates vacancy-interstitial pairs on both anion and cation sublattices. The defects undergo transformations leading to an energetically stable configuration with the Fermi level position determined by the balance between donor and acceptor-like defects. If this equilibrium Fermi level position is located near the middle of the band-gap the effect of radiation will be to compensate p- as well as n-type material. However, if the equilibrium Fermi level position is located closer to the conduction or valence band edge, irradiation will result in an increase of free electron or hole concentrations, respectively. In most of the III-V semiconductors, radiation induces Fermi level shift towards mid-gap.[16] There are, however, remarkable exceptions, namely InAs,[17] which becomes strongly

n-type, and InSb and GaSb which show an increase of free hole concentration upon irradiation.[16] Summarizing we observe that in irradiated III-V semiconductors the Fermi level is stabilized near the conduction band for InAs, it is close to the valence band edge in GaSb and InSb, and it is located deeper in the band-gap for all the other III-V materials.

Examination of the SB heights for III-V semiconductors shows that there exists a striking correlation between trends in Fermi energy pinning positions at metal-semiconductor interfaces and bulk position of the Fermi level in irradiated material. Measurements of SB heights point out that for InAs the Fermi energy is pinned at ~ 0.13 eV above the conduction band edge[18] whereas it is located at ~ 0.1 and ~ 0.03 eV above the valence band edge for GaSb and InSb, respectively.[19] For all the other III-V materials the Fermi energy deduced from SB heights is separated at least by 0.4 eV from the valence and conduction band edges. The surprising correlation between the Fermi level position found in semiconductors modified by completely different effects suggests that we should examine if there exists a common physical phenomenon leading to Fermi level stabilization at metal-semiconductor interfaces and in irradiated semiconductors. Since ample experimental evidence has been accumulated which shows that native defects are responsible for Fermi level stabilization in irradiated materials one could conclude that similar defects may play a dominant role in the formation of the SBs on III-V and elemental semiconductors. In order to obtain a more detailed picture of the physical processes leading to formation of the barriers, additional information on the thermodynamic properties of the most abundant native defects is needed. In the following it is shown that the current knowledge on native defects in GaAs enables us to formulate a microscopic model of Schottky barriers for this material.

III. Schottky barriers on GaAs

Recent theoretical studies of defects in GaAs have shown [15,20,21] that two simple amphoteric native defect systems exist in GaAs. In arsenic rich material a deviation from stoichiometry is accommodated by gallium vacancies V_{Ga} or donor complexes $As_{Ga} + V_{As}$. In gallium rich material arsenic vacancies V_{As} or acceptor complexes (Ga_{As}, V_{Ga}) are formed. In both cases the complexes are formed by a simple displacement of the arsenic (gallium) atom in between two nonequivalent sites. For our purpose the most important property of these defects is a strong dependence of the defect reactions $V_{Ga} + As_{As} \leftrightarrow As_{Ga} + V_{As}$ and $V_{As} + Ga_{Ga} \leftrightarrow Ga_{As} + V_{Ga}$ on the Fermi energy.[15] In n-type material V_{Ga} or $Ga_{As} + V_{Ga}$ acceptors are stable, whereas in p-type V_{As} or $As_{Ga} + V_{Ga}$ are preferentially formed. This characteristic amphoteric behavior of the native defects is a core component of the proposed model of SB formation.

The chemical and physical processes occurring at the interface during metal deposition or oxidation affect semiconductor stoichiometry close to the interface. There is substantial evidence that an arsenic rich layer close to the interface is formed in GaAs.[22,23] Therefore, our considerations will be limited to the discussion of the arsenic rich material. It should be noted, however, that a similar approach can be used to consider gallium rich interfaces. The defects accommodating excess arsenic at the interface are V_{Ga} and/or $As_{Ga} + V_{As}$. It has been found from the calculations of the defect energy levels [15,21] that for $E_F \lesssim E_V + 0.5$ eV $(As_{Ga}, V_{As})^{3+}$ is formed and for $E_F \gtrsim E_V + 0.7$ eV, $(V_{Ga})^{3-}$ is stable. Formation of these defects will induce a Fermi energy shift towards the mid-gap in both cases. If the concentration of defects is large enough the Fermi level will be stabilized

at about ~ E_v + 0.6 eV when both donors and acceptors are formed and compensate each other.

In the case of stabilized Fermi energy the reaction $V_{Ga} + As_{As} \leftrightarrow As_{Ga} + V_{As}$ which is a first step in gallium vacancy diffusion can easily occur. Thus the defects which are originally created close to the interface can under these conditions migrate into the bulk. In the case of n-type GaAs the electric field in the depletion layer will enhance migration of negatively charged gallium vacancies. However, since the defect transformations are controlled by the Fermi level position the diffusion into the bulk will be suppressed when the Fermi level rises above E_v + 0.7 eV. Assuming a bulk doping level of ~ 10^{17} cm^{-3} and parabolic potential distribution in the depletion layer one obtains D ≈ 70Å for the maximum defect penetration depth. This means that the majority of defects are in a bulk-like environment and may be quite insensitive to chemical and/or physical processes occurring at the very interface.

From the above considerations one may conclude that for submonolayer coverage, and for large enough concentrations of defects the Fermi level at the interface is pinned at the same energy for p- and n-type material. The pinning position is determined by the equilibrium between native donors and acceptors and depends on additional factors such as metal reactivity and/or electronegativity which can affect a subtle balance between donors and acceptors. Experimental data show that for a majority of metals the Fermi level is pinned in the energy range E_v + 0.5 eV to E_v + 0.7 eV independently of the material type and doping level.[24] This indicates that a substantial concentration of defects is formed during a room temperature metal deposition. For example, for heavily doped, 10^{18} cm^{-3} GaAs more than ~10^{12} cm^{-2} of triply ionized defects is required to assure Fermi level pinning in the interfacial layer.

In order to consider thick metal coverages we shall utilize the fact that the native defects are distributed in a thin layer within D < 100Å of the interface. With increasing metal coverage, after a well-defined metal layer has been formed, the Fermi energy at the interface is determined by the internal metal work function φ_m^I.[25] Three different cases, corresponding to distinct ranges of the value of metal work function, are possible for n-type GaAs: (1) $\varphi_m^I - \chi_S > E_g - 0.5$ eV; (2) $\varphi_m^I - \chi_S < E_g - 0.7$ eV; and (3) $E_g - 0.7$ eV $< \varphi_m^I - \chi_S < E_g - 0.5$ eV, where $E_g = 1.42$ eV is the GaAs band gap and χ_S is the GaAs electron affinity. In the first case [schematically shown in Fig. 1(b)], the Fermi energy at the interface falls below E_v + 0.5 eV level, therefore $(As_{Ga},V_{As})^{3+}$ donors are formed to accommodate excess arsenic. A depletion layer is created. The thickness of the layer d is determined by the $As_{Ga} + V_{As}$ donor concentration N_D and by the condition that, at the edge of the depletion layer, the Fermi energy moves above E_v + 0.5 eV. As it was discussed above, in such a case $As_{Ga} + V_{As}$ donors will be partly transformed into V_{Ga} acceptors, and the material will become compensated. The position of the Fermi energy for $d < x < D$ will be controlled by the charge balance between deep donors and acceptors and the net concentration of shallow donors (n-type material). For $x > D$ a depletion layer, controlled by the bulk doping N_d, is formed with the barrier height $E_g - 0.7 < \phi_{Bb}^n < E_g - 0.5$. A different situation occurs for the second case when the Fermi energy at the interface is located above the E_v + 0.7 eV level, i.e. $\varphi_m^I - \chi_S < E_g - 0.7$ eV shown in Fig. 1(c). Such a location of the Fermi energy will induce formation of the acceptor defects $(V_{Ga})^{3-}$ and therefore a p-type-like depletion layer of a thickness d will be formed at the

interface. As shown in Fig. 1(c), in this range the Fermi energy moves rapidly with respect to the conduction band until it falls below $E_v + 0.7$ eV where again the material is becoming compensated. As in the previous case for $x > D$ a barrier ϕ^n_{Bb}, controlled by the bulk doping N_d, is formed. Finally, for the third case $E_g - 0.7$ eV $< \varphi^I_m - \chi_S < E_g - 0.5$ eV, shown in Fig. 1(d), the Fermi energy at the interface is located at the level at which both the deep donors and acceptors are formed, resulting in compensated layer of the thickness D. Beyond the gallium depleted layer, i.e. for $x > D$, a thick depletion layer controlled by bulk doping N_d is formed.

A very important result of this analysis is that in all three cases, independent of the value of metal work function, the height of the bulk barrier ϕ^n_{Bb} lies in the range 0.72 eV to 0.92 eV. Identical analysis for metal-(p-type GaAs) contacts provide similar results with the bulk barrier ϕ^p_{Bb} controlled by bulk doping of concentration N_a. The height of the barrier lies in the energy range 0.5 eV $\leq \phi^p_{Bb} <$ 0.7 eV. It is therefore clear that the thin, arsenic rich layer at the GaAs surface acts as a buffer layer accommodating a part of the potential difference $^I_m - \chi_S$, so that the Fermi level is pinned in a narrow range of energies.

The final position of the Fermi level in the compensated layer depends on a number of factors such as distribution of the native defects in the interfacial layer and the range of the solid phase metal-semiconductor reactions at the interface. The intrinsic parameter which is related to internal work function[25] and which affects the final pinning energy is the metal electronegativity X_m measured with respect to the "effective" electronegativity of GaAs X^{eff}_{GaAs}. For metals with $X_m > X^{eff}_{GaAs}$ the electronegativity difference will induce a downward shift of the Fermi

energy towards E_v + 0.5 eV in the compensated region $d < x < D$ and for metals with $X_m > X^{eff}_{GaAs}$ the Fermi energy will be shifted towards the level E_v + 0.7 eV. The special case occurs for $X_m \approx X^{eff}_{GaAs}$ when the Fermi level is pinned at the energy ~ E_v + 0.6 eV.

The above considerations give a general rule for prediction of SB height for different metals, providing the effective electronegativity of GaAs is known. In Fig. 2 experimental data for SBs for metals with different electronegativities are shown. As predicted by the present model, a distinct transition from almost equal Schottky barriers $\phi^n_{Bb} \approx \phi^p_{Bb} = 0.7$ eV for low electronegativities to $\phi^n_{Bb} \approx 0.9$ and $\phi^p_{Bb} \approx 0.5$ for large electronegativies is observed. The transition occurs at about $X_m \approx 1.8$, which happened to be close to the average electronegativity of Ga (1.6) and As (2.0). The lines represent values of the bulk barrier heignts predicted by the model. Considering limited accuracy of the barrier height measurements and uncertainties in definition of electronegativity, the agreement is quite satisfactory. Deviations of the barrier heights from the predicted values observed for some metals may be attributed to the solid phase reactions at the interface. Also the metals on the low electronegativity side may preferentially react with arsenic leading to a gallium rich interface. In this case the defect reaction $V_{As} + Ga_{Ga} \leftrightarrow Ga_{As} + V_{Ga}$ has to be considered. Although the main conclusion of the model remains unchanged the actual pinning positions can be slightly different in this case.

There are two reasons why the surface barrier ϕ^n_{Bs} does not affect the electrical characteristics of the Schottky contacts. Firstly, the large concentration of defect states in the barrier facilitates a direct tunneling to the metal. Secondly, transport through the barrier is controlled by the

field emission[26] rather than thermionic emission. It can be shown that for the native defect concentration $N_D \gtrsim 3 \times 10^{19}$ cm^{-3} the thin barrier contribution to the total barrier determined from the I-V characteristics is negligible.

A crucial conclusion derived from the present model is that for thick metal coverages the Fermi level at the interface is unpinned and satisfies the Schottky condition $\phi^n_{Bs} + \phi^n_{Bb} = \phi^I_m - \chi_S$ although the macroscopic barrier measured by the I-V technique is determined by the native defect pinning of the Fermi energy (Bardeen limit).

One of the major differences between the present model and the previously proposed defect models[3-8,30] lies in the predicted evolution of the surface Fermi level pinning position with the metal layer thickness. Thus, an experimental verification of our model would require measurements of the surface Fermi level for metal thicknesses beyond several monolayers. Although such experiments are difficult and frequently provide ambiguous results [24] there are a number of reports which clearly support our model.

Recent Soft X-ray Photoemission Spectroscopy (SXPS) measurements of the Fermi level position on metal $In_xGa_{1-x}As$ structures have shown that for a metal layer thickness exceeding ~ 10Å, the Fermi energy at the interface is stabilized.[12] The stabilization energy depends on the deposited metal and was found to correlate with the "effective" work function of a reacted interface layer. In particular these results have shown that the interface pinning energy at Au-$In_xGa_{1-x}As$ contacts differs very much from the pinning position deduced from the Schottky barrier height measured using C-V characteristics.[18] The present model provides a simple explanation of this apparent contradiction. In the case of a well-defined metal overlayer the surface sensitive SXPS technique measures the sum of the surface and the

bulk barriers $\phi^n_{Bs} + \phi^n_{Bb} = \varphi_m - \chi_S$, where φ^I_m is the metal work function (or "effective" work function[12]). On the other hand results of ref. 18 represent the bulk barrier ϕ^n_{Bb} which is determined by the defect pinning position.

Existence of the interface barrier ϕ_{Bs} predicted by the present model has been confirmed for Au-GaAs and Ag-GaAs contacts using electric field induced Raman scattering (EFIRS).[11] This technique provides information on an average electric field in a thin (~85Å) layer at the interface. The measurements have shown an abrupt increase of the electric field for the metal layer thickness exceeding ~ 10Å when a well-defined metal layer is formed.

Another experiment which had no clear interpretation and which can be understood within the framework of our model is the most recent measurement of the dependence of surface cathodoluminescence on gold layer thickness on GaAs.[31] In this experiment two emission lines with the low photon energy edges at ~ 0.7 eV and 0.9 eV are observed for low metal coverages. The intensity of the emission line at 0.9 eV decreases with increasing metal layer thickness and disappears completely for a 15Å thick coverage. Such behavior is very consistent with the predictions of the present model. At low coverages the Fermi level is pinned at the energy ~ E_v + 0.6 eV with V_{Ga} and $As_{Ga} + V_{As}$ present. Thus two emission lines due to the electron transitions from the conduction band to defect levels $(V_{Ga})^{1-}$ + cb(e) $\rightarrow$ $(V_{Ga})^{2-}$ + hν at hν ≈ 0.9 eV and $(As_{Ga},V_{As})^{3+}$ + cb(e) $\rightarrow$ $(As_{Ga}V_{Ga})^{2+}$ + hν at hν ≈ 0.7 eV are seen. For thicker metal overlayers the Fermi energy at the surface falls below E_v + 0.5 eV (see fig. 1b), therefore only the $As_{Ga} + V_{As}$ donor is a stable defect and the V_{Ga} related emission at 0.9 eV disappears.

IV. Relationship to other models

A distinct correlation between the Fermi energy determined from electrical measurements of the SB heights and Fermi level behavior in irradiated III-V semiconductors strongly indicates that amphoteric native defects play a major role in the mechanism of SB formation and that the model proposed for GaAs can be extended to other III-V semiconductors. The suggestion is supported by calculated trends in the energy levels for vacancies and antisites in III-V compounds.[32] The predicted trends (although not the actual defect level energies) agree with experimentally observed variations of the barrier heights. Obviously the native defects considered in this paper will follow these trends since they also can be represented by dangling bond type defects.

Much more puzzling and probably even more significant is the correlation of the native defect pinning energy with a calculated branch point energy E_B [5,33] which has been used as a reference energy for the metal induced gap states (MIGS) model of SBs. Since E_B can be interpreted as the energy separating bonding states from antibonding states,[34] one could argue that introduction of native defects which have deep energy levels in the band gap and can undergo transformation changing their electrical properties will lead to the energetically most favorable state with all bonding states occupied and antibonding states empty.[35] Such argument would explain an overall movement of the Fermi energy towards E_B in semiconductors in which native defects are created either by irradiation or by metal deposition. In GaAs the Fermi level stabilization energy for the defects considered in this paper is $\sim E_v + 0.6$ eV and agrees with $E_B \simeq E_v + 0.5$ eV.[33] Calculations of the energy of defect reactions for major defects in other III-V materials will be needed to verify universality of this argument.

V. Summary

It is found that amphoteric native defects are responsible for Fermi level stabilization in irradiated III-V semiconductors and Fermi level pinning at metal-semiconductor interfaces. A detailed Schottky barrier formation mechanism developed for metal-GaAs contacts accounts very well for basic characteristics of the barriers and their dependence on metal electronegativity. Also, it explains an apparently contradictory data on SB height and surface Fermi level pinning obtained for thick metal coverages.

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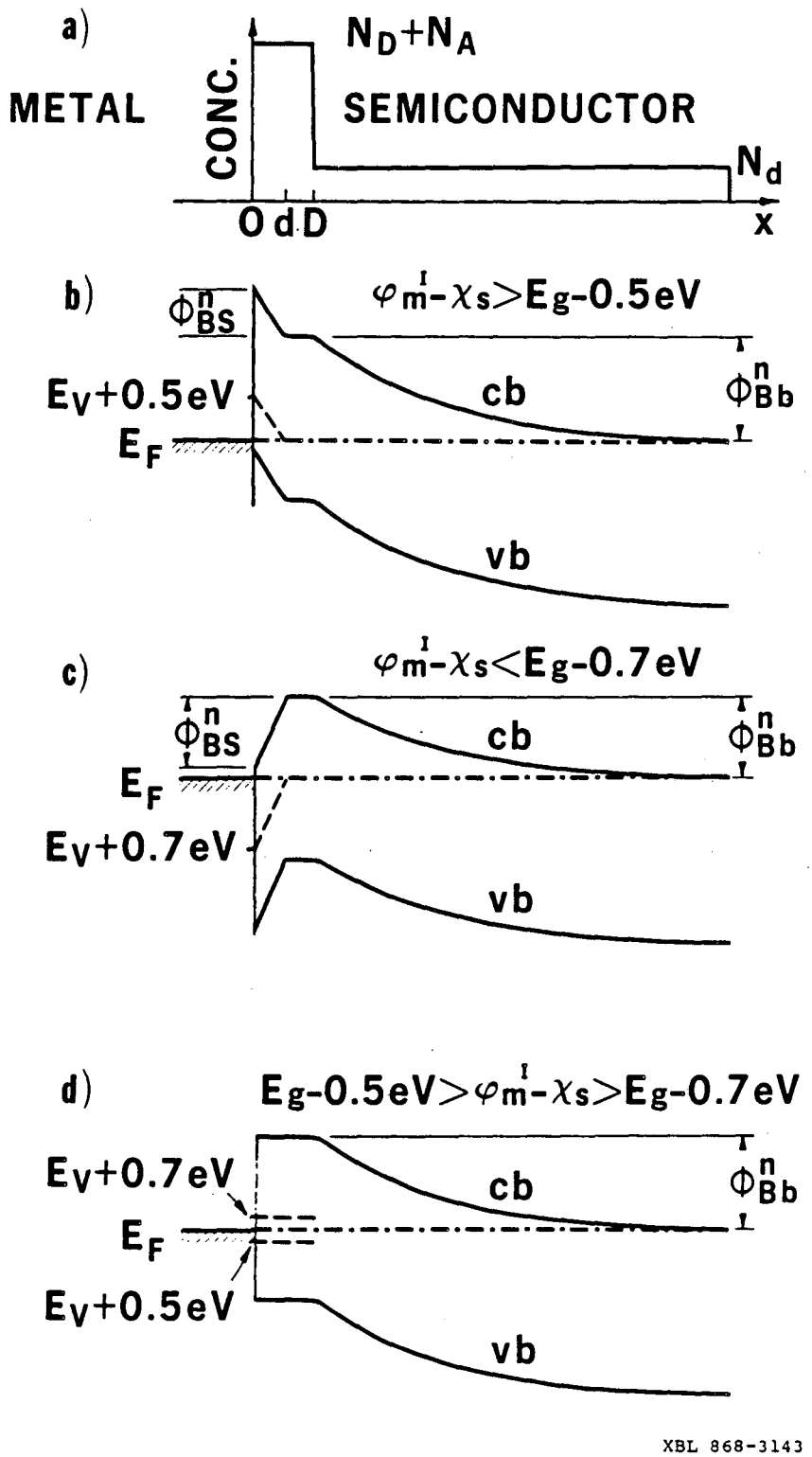
Figure captions

Fig. 1 a) Profiles of native defects N_A,N_D and bulk impurity N_d concentrations. b), c) and d) Band diagrams of Schottky contacts for metals with different work functions.

Fig. 2 Schottky barrier heights for n-type and p-type GaAs as functions of metal electronegativity. Experimental data come from ref. 27 (Mg), ref. 28 (Hf), all the other metals ref. 29.


a)
METAL
CONC.
N_D+N_A
SEMICONDUCTOR
N_d
O d D
x
b)
Φ^n_{BS}
$\varphi_m^I-\chi_s>E_g-0.5eV$
$E_V+0.5eV$
cb
Φ^n_{Bb}
E_F
vb
c)
$\varphi_m^I-\chi_s<E_g-0.7eV$
Φ^n_{BS}
cb
Φ^n_{Bb}
E_F
$E_V+0.7eV$
vb
d)
$E_g-0.5eV>\varphi_m^I-\chi_s>E_g-0.7eV$
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cb
Φ^n_{Bb}
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Figure 1.

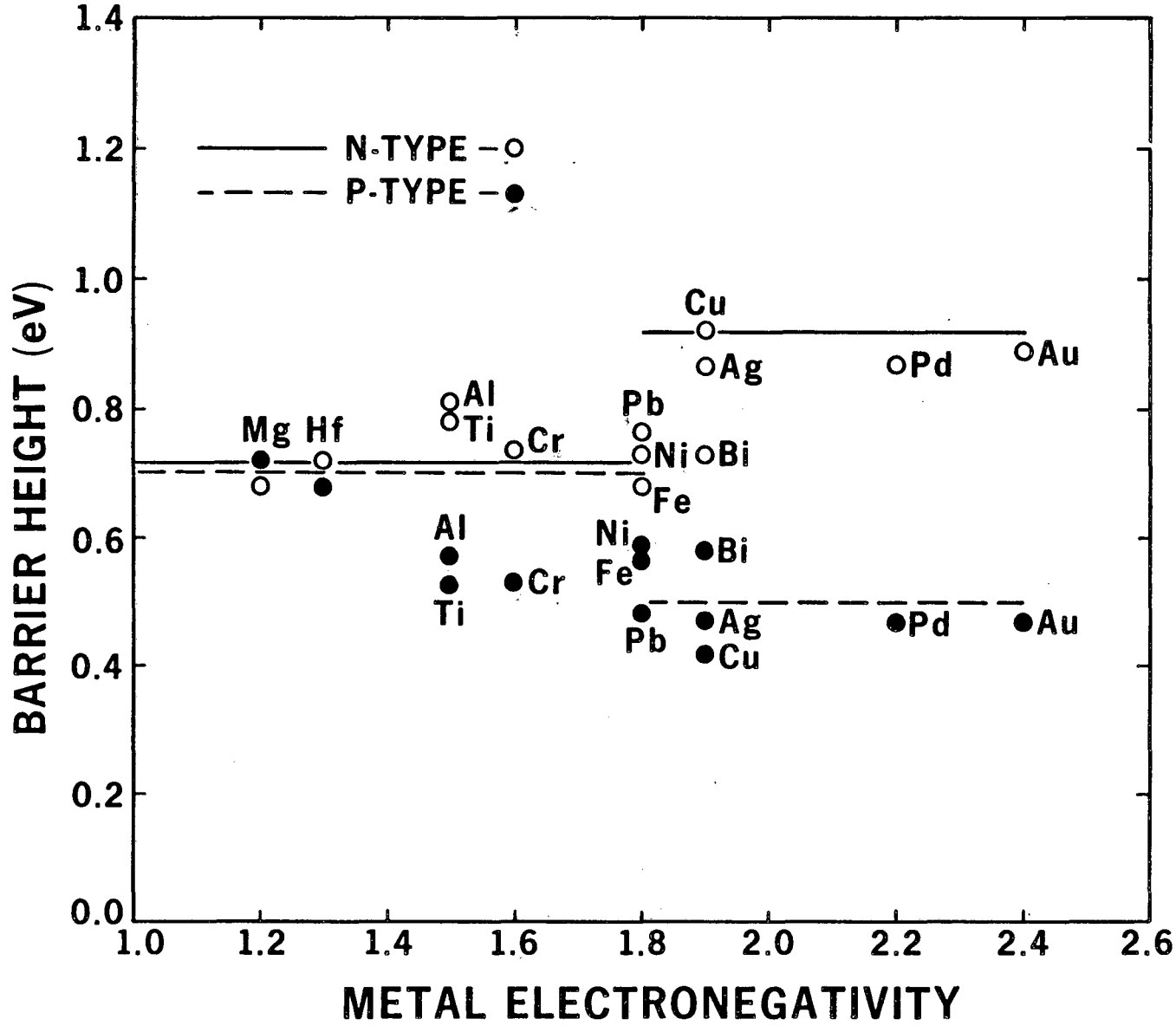

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Figure 2.

Figure 2.

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