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A NEW ANALYTICAL EXPRESSION FOR THE INTERFACE INDEX OF METAL-SCHOTTKY CONTACTS ON SEMICONDUCTORS

J. J. SZE and H. C. CHENG

Department of Electronics Engineering and Institute of Electronics, Engineering Building 4IV, National Chiao Tung University, 1001 Ta Hsueh Road, Hsin Chu 300, Taiwan, R. O. China

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Abstract—By reconsidering the effect of the penetration depth of the interface states, a new analytical expression of the interface index has been achieved to successfully explain the role of the semiconductor ionicity in the behavior of metal-Schottky contacts on semiconductors. The derived interface indices not only fit quite well with the previous experimental data but also exhibit a sharp transition from the Bardeen limit to the Schottky limit for semiconductor ionicity around 0.8, which agrees well with the experiment reports.

1. INTRODUCTION

The dependence of Schottky barrier height ϕ_{bn} on the metal electronegativity χ_m has gained a great deal of attention in study of the characteristics of Schottky contacts[1–8]. Empirically, this correlation is assumed to be linear and the barrier heights of Schottky contacts can then be expressed as $\phi_{bn} = S\chi_m + \phi_s$, where the phenomenological parameter S is called the interface index of the metal/semiconductor interface, and ϕ_s is a constant depending only on the semiconductor properties. Then, the interface index S can be used to identify the behaviors of the metal/semiconductor contacts as being in the Bardeen limit or the Schottky limit, which is corresponding to $S = S_{min}$ or $S = S_{max}$, respectively. From an extensive compilation of the experimental data, Kurtin *et al.*[1] found that S is a function of the semiconductor ionicity $\Delta\chi$. For the covalent semiconductors, S is close to the S_{min}, whereas for the ionic semiconductors, S saturates at S_{max}. Furthermore, the values of S rise sharply at a critical semiconductor ionicity which seems to separate the Bardeen limit for the Schottky limit.

In the classical interfacial-layer model developed by Cowley and Sze[2], the interface index is firstly expressed as an analytical function of the interface state density and the interfacial layer thickness. In that model, the space distribution of the interface states was considered as a delta distribution, and then it was necessary to introduce an insulating layer at the metal/semiconductor interface to build up the interface dipole. The need for this insulating interfacial-layer impacts the accuracy of this interfacial-layer model. In addition, the variation of the interface index against the semiconductor ionicity predicted by this classical interfacial-layer model is too smooth when compared with the experimental results[6]. Instead of the delta distribution approximation, Louie, Chelikowsky and Cohen[3] (later abbreviated to LCC) considered the effect of the penetration of the interface states from the metal into the semiconductor and suggested that a variation of the metal electronegativity will result in a change of the interface dipole originating from the change of the dipole charge $eD_s d\phi_{bn}$, where D_s is the surface density of the interface states and $d\phi_{bn}$ is the change of the Schottky barrier height resulted from the variation of the metal electronegativity. Then, a new analytical form of the interface index was derived from the LCC theory and it provided a successful explanation of the effect of the semiconductor ionicity on the value of the interface index. However, in accordance with the solutions of the Poisson equations in the metal and semiconductor for Schottky contacts[9,10], the top of the energy band profile is usually at a distance away from the metal/semiconductor interface if the space distribution of the interface states is taken into account. Hence, it implies that the derivation of the interface index from the LCC theory was based on an incorrect model. Therefore, it is necessary to more exactly realize the role of the semiconductor ionicity in the behavior of the metal/semiconductor contacts via rederiving the interface index.

In this study, a modified interfacial-layer model of a Schottky contact is proposed to depict the dependence of the Schottky barrier on the contact parameters, including the metal work function,

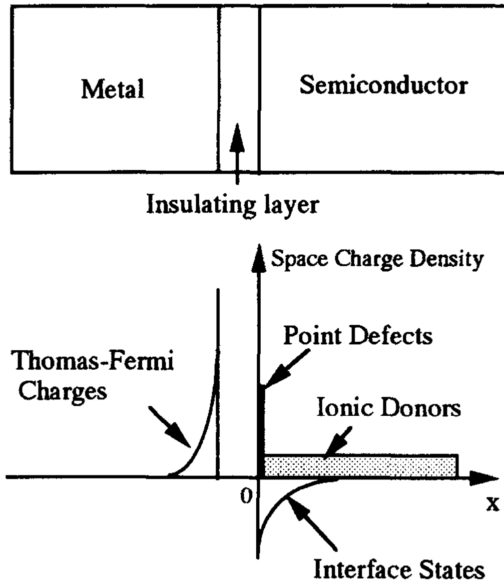

Fig. 1. The schematic space charge distribution of a metal Schottky contact on a semiconductor with an insulating interfacial-layer.

insulating interfacial-layer thickness, surface density of the interface states and the penetration depth of the interface states. From this model, the interface index of the Schottky contact can be obtained as a function of these contact parameters. Finally, the prediction of the theoretical derivation about the dependence of the interface index on the semiconductor ionicity is examined with the previous experimental data to prove the accuracy of this modified model.

2. THE PROPOSED MODIFIED INTERFACIAL-LAYER MODEL OF THE METAL SCHOTTKY CONTACTS ON THE SEMICONDUCTORS

For the conventional fabrication processes of the Schottky diodes, a thin native oxide layer may be present on the surface of the semiconductor before the metal deposition. This oxide layer will decouple the metal film from the semiconductor and act as an insulating interfacial-layer between the metal and the semiconductor. The space charge distribution in this metal-insulating-semiconductor (MIS) structure is schematically shown in Fig. 1. To make the following analysis become tractable, six assumptions for the space charge distribution in the MIS structure are adopted: (1) the space distribution of the interface states can be described by Heine's equation[11]; (2) the dopant distribution in the semiconductor is uniform; (3) the net charges contributing from the point defects, such as the vacancies, are described with a delta distribution at the oxide/semiconductor interface; (4) the space charges in the metal are characterized as Thomas–Fermi charges; (5) there is no charge existing in the oxide layer; and (6) the investigated semiconductors are n-type.

Under the assumptions stated above, the potential distribution $v(x)$ in the metal and semiconductor can be derived by solving the Poisson equations in the metal and semiconductor as:

$$v(x) = v(-\delta)\exp\left(-\frac{x+\delta}{\lambda_{\mathrm{TF}}}\right) \quad \text{for } x \leqslant -\delta, \qquad (1)$$

and

$$v(x) = v(0) + x\sqrt{\frac{2eN_{\mathrm{D}}v_{\mathrm{b}}}{\epsilon_{\mathrm{s}}} - \frac{eN_{\mathrm{D}}x^2}{2\epsilon_{\mathrm{s}}} - \frac{e}{\epsilon_{\mathrm{s}}}D_{\mathrm{seff}}\lambda_{\mathrm{s}}} \times\left[1-\exp\left(-\frac{x}{\lambda_{\mathrm{s}}}\right)\right] \quad \text{for } x \geqslant 0, \qquad (2)$$

where δ is the thickness of the native oxide layer; λ_{TF} is the Thomas–Fermi screening length of the metal; e is the elementary charge; ϵ_{s} is the semiconductor permittivity; N_{D} is the donor concentration in the semiconductor; the magnitude of v_{b} is equal to $\phi_{\mathrm{m}} - \chi - v_{\mathrm{t}}\ln(N_{\mathrm{C}}/N_{\mathrm{D}}) - v(0) + e/\epsilon_{\mathrm{s}}D_{\mathrm{seff}}\lambda_{\mathrm{s}}$, ϕ_{m} is the metal work function, χ is the electron affinity of the semiconductor, v_{t} is the thermal voltage, N_{C} is the effective density of the states in the conduction band of the semiconductor; λ_{s} is the penetration depth of the interface states in the semiconductor; and D_{seff} is given by:

$$D_{\mathrm{seff}} = \int_{E_{\mathrm{V}}}^{E_{\mathrm{C}}} \rho(E) f(E)\,\mathrm{d}E, \qquad (3)$$

where $\rho(E)$ is the extra density of the states per unit energy of the interface states in the band gap of the semiconductor; $f(E)$ is the occupation function of the interface states and E_{C} and E_{V} are the conduction band minimum and valence band maximum of the semiconductor, respectively. Because there is no charge existing in the native oxide, the electric field is a constant through this layer. The potential distribution in the oxide layer, therefore, can be expressed as:

$$v(x) = v(-\delta) - (x+\delta)F_i \quad \text{for } -\delta < x < 0, \qquad (4)$$

where F_i is the electric field in the native oxide layer.

Then, the solutions of the Poisson equations in the MIS structure, i.e. the eqns (1), (2) and (4), must satisfy the boundary conditions:

$$-\epsilon_{\mathrm{M}}\left.\frac{\mathrm{d}v}{\mathrm{d}x}\right|_{x=-\delta} = \epsilon_i F_i, \quad \text{and} \qquad (5)$$

$$-\epsilon_{\mathrm{s}}\left.\frac{\mathrm{d}v}{\mathrm{d}x}\right|_{x=0+} = \epsilon_i F_i + e\sigma_{\mathrm{eff}}, \qquad (6)$$

where ϵ_{M} is the metal permittivity; ϵ_i is the oxide permittivity; $e\sigma_{\mathrm{eff}}$ is the net charge contributed from the point defects, the value of σ_{eff} is equal to the product of the surface density σ of the point defects and their occupation function $g[v(0)]$. In accordance with the eqns (1)–(6), the determination of the potential distribution can be completed by solving the following equation:

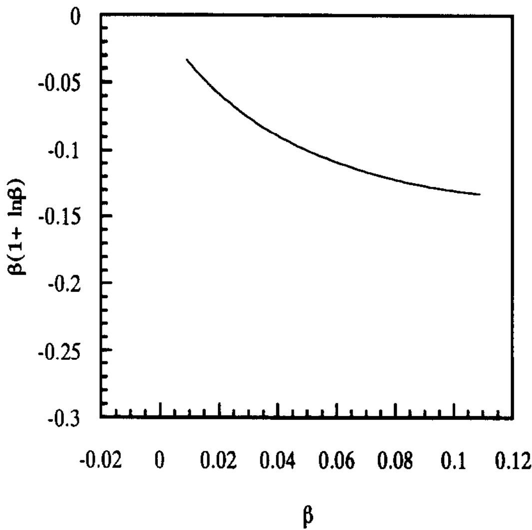

Fig. 2. The plot of the value of $\beta(1+\ln\beta)$ vs β.

$$v(0)=\left(\frac{\lambda_{TF}}{\epsilon_M}+\frac{\delta}{\epsilon_i}\right)(\sqrt{2e\epsilon_s N_D v_b}+e\sigma_{eff}-eD_{seff}). \quad (7)$$

As can be seen in eqn (7), the correlation of D_{seff} with $v(0)$ must be realized to solve the value of $v(0)$. According to the previous reports[3–4,7–8], the value of $\rho(E)$ is nearly a constant in the midgap of the semiconductor. Therefore, the integration of the eqn (3) can be approximately replaced by:

$$D_{seff}=D_s(E_g-\phi_m+\chi+ev(0)-\phi_0), \quad (8)$$

where D_s is the surface density per electron volt of the interface states in the midgap of the semiconductor; E_g is the band gap of the semiconductor; and ϕ_0 is the "neutral level" of the interface states defined by Cowley and Sze[2]. Then, the value of $v(0)$ can be attained by substituting eqn (8) into eqn (7).

The potential distribution derived above can be thus used to determine the barrier heights of the metal/semiconductor contacts, leading to the expressions:

$$\phi_{bn}=\phi_m-\chi-ev(0) \quad \text{if } v(0)>0, \text{ and} \quad (9a)$$

$$=\phi_m-\chi-ev(x_m) \quad \text{if } v(0)<0, \quad (9b)$$

where ϕ_{bn} is the barrier height of the Schottky contact and $v(x_m)$ is the local minimum of the electric potential in the semiconductor. Since $v(x_m)$ occurs at the abscissa x_m where the electric field is vanished, i.e. $dv/dx|_{x=x_m}=0$, the value of x_m must satisfy:

$$N_D\left(x_m-\sqrt{\frac{2\epsilon_s v_b}{eN_D}}\right)+D_{seff}\exp\left(-\frac{x_m}{\lambda_s}\right)=0. \quad (10)$$

Because $x_m \ll \sqrt{2\epsilon_s v_b/eN_D}$, the value of x_m can be approximately written as:

$$x_m=\lambda_s\ln\left(\frac{D_{seff}}{\sqrt{\frac{2\epsilon_s N_D v_b}{e}}}\right). \quad (11)$$

In accordance with the eqns (2) and (11), the value of $v(x_m)$ is derived as:

$$v(x_m)=v(0)-\frac{e}{\epsilon_s}D_{seff}\lambda_s[1-\beta(1+\ln\beta)], \quad (12)$$

where $\beta=\sqrt{(2\epsilon_s N_D v_b/e)}/D_{seff}$. Here, the second order term of the x variable in eqn (2) is omitted. The curve of $\beta(1+\ln\beta)$ vs β is shown in Fig. 2. For most Schottky contacts, the values of β range from 0.01 to 0.1. In this regime, the product of $\beta(1+\ln\beta)$ and $(e/\epsilon_s)D_{seff}\lambda_s$ is negligible in determining the value of $v(x_m)$. Hence, $v(x_m)$ can be approximated by $v(0)-(e/\epsilon_s)D_{seff}\lambda_s$. Then, eqn (9b) can be rewritten as:

$$\phi_{bn}=\phi_m-\chi-ev(0)+\frac{e^2}{\epsilon_s}D_{seff}\lambda_s, \quad \text{if } v(0)<0. \quad (13)$$

From the eqns (9a) and (13), the general expression of the barrier heights of the metal/semiconductor contacts can be expressed as:

$$\phi_{bn}=\phi_m-\chi-ev(0)+u[-v(0)]\left(\frac{e^2}{\epsilon_s}D_{seff}\lambda_s\right), \quad (14)$$

where $u(x)$ is the unit step function.

3. THE INTERFACE INDEX OF THE METAL/SEMICONDUCTOR INTERFACE IN THE MODIFIED MODEL

The dependence of the barrier height on the electronegativity χ_m of the metal is discussed in this section. Moreover, the influence of the semiconductor ionicity Δ_χ on the value of interface index is also examined. Using the modified interfacial-layer model

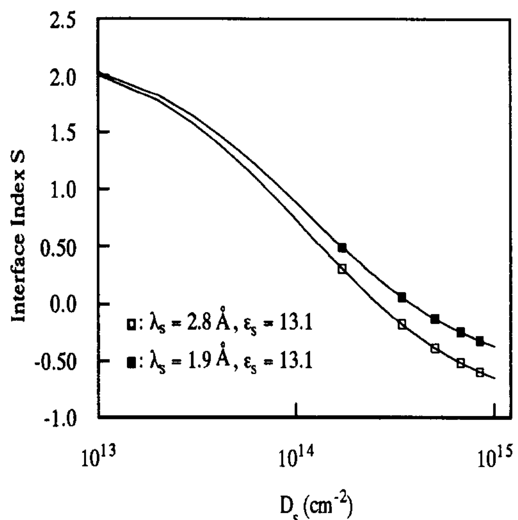

Fig. 3. The curves of the interface index S vs D_s with λ_s as a parameter.

of the Schottky contacts proposed in the Section 2, the interface index can be determined by the following procedures. At first, the dependence of the barrier height of the Schottky contact on the contact parameters, incouding the metal work function, the native-oxide layer thickness, the surface density of the interface states in the semiconductor midgap, and the penetration depth of the interface states in the semiconductor, is derived from eqns (7), (8) and (14). Secondly, a correlation between the ϕ_m and the χ_m is then used to find the interface index, such as $S \equiv \partial\phi_{bn}/\partial\chi_m = \partial\phi_{bn}/\partial\phi_m \times \partial\phi_m/\partial\chi_m$. Since the occupation function of the point defects is a complex function of the $v(0)$, a numerical method is generally required to determine the value of the interface index. Nevertheless, for most Schottky contacts, it is reasonable to suggest that the surface densities of the point defects are lower than $10^{13}\,\text{cm}^{-2}$. Then, $e\sigma_{eff}$ and $\sqrt{2e\epsilon_s N_D v_b}$ are negligible as compared with eD_{seff}, and the value of $v(0)$ can be solved analytically by eqns (7) and (8) and expressed as:

$$v(0) \approx \frac{-eD_s\alpha}{1+e^2D_s\alpha}(\phi_{crit}-\phi_m), \quad (15)$$

where $\alpha = \lambda_{TF}/\epsilon_M + \delta/\epsilon_i$; $\phi_{crit} = E_g + \chi - \phi_0$. In accordance with the eqn (15), the value of $v(0)$ is positive for $\phi_m > \phi_{crit}$. On the other hand, the value of $v(0)$ becomes negative as $\phi_m < \phi_{crit}$. By substituting eqn (15) into eqn (14), the barrier height of the Schottky contact can be expressed as:

$$\phi_{bn} = \gamma(\phi_m - \chi) + (1-\gamma)(E_g - \phi_0), \quad (16)$$

where the parameter γ, which characterizes the sensitivity of the Schottky barrier height to the metal work function, is given by:

$$\gamma = \frac{1}{1+e^2D_s\alpha} - u(\phi_{crit}-\phi_m)\frac{e^2D_s\lambda_s}{\epsilon_s(1+e^2D_s\alpha)}. \quad (17)$$

Furthermore, a linear relationship of the form $\phi_m = 2.27\chi_m + 0.34$ is empirically used to identify the correlation between the metal work function ϕ_m and the metal electronegativity χ_m. If the dependence of D_s on ϕ_m is ignored, the interface index S is then approximately written as:

$$S = 2.27\gamma. \quad (18)$$

The new expression of the interface index derived above indicates that the result proposed by Cowley and Sze needs modifications at some conditions. The main cause comes from the penetration depth of the interface states. For the case of $\phi_m > \phi_{crit}$, the sign of the charges contributing from the interface states is the same as the ionized dopants and then the top of the energy band profile is at the insulating-interfacial-layer/semiconductor interface. Hence, the expression of the S is analogous to the result proposed by Cowley and Sze except that the parameter α is modified by including the effect of the Thomas–Fermi charge distribution in the metal. Whereas for the case of $\phi_m < \phi_{crit}$, the type of the charges donated by the interface states is negative. At this time, just like introducing a p^+ layer on the n-type substrate, the energy band profile will reach a maximum at some distance inside the semiconductor due to the influence of the penetration depth of the interface states on the Schottky barrier. Consequently, the expression for S proposed by Cowley and Sze is no longer applicable and a correction term must be added to consider the effect of the penetration depth of the interface states.

Previous reports generally suggested that the interface index was a constant depending only on the semiconductor properties and could be deduced from the slope of the plot of ϕ_{bn} vs χ_m by a least-squares fitting method. However, the modified model in this study shows that a piece-wise linear dependence will exist between the barrier height and the metal electronegativity. Hence, the previous fitting on the experimental data become questionable. In practical, this discrepancy seems unimportant due to the following reason. For most of the interesting semiconductors, the values of the associated ϕ_{crit} are either close to 4.0 eV for very small band gap semiconductors, e.g. InAs, or close to 5.0 eV for the semiconductors with larger energy gaps, e.g. GaAs. Since the work functions of the common-used metals for the Schottky contacts range from 4.0 eV to 5.0 eV, the linear relationship between the barrier height and the metal electronegativity is still appropriate.

According to the eqns (17) and (18), the interface index S can be exhibited as a function of the D_s by using the λ_s as a parameter, as shown in Fig. 3. As can be seen in Fig. 3, the value of the interface index increases with decrease of either D_s or λ_s. Ihm *et al.*[4] reported that D_s was inversely proportional to the

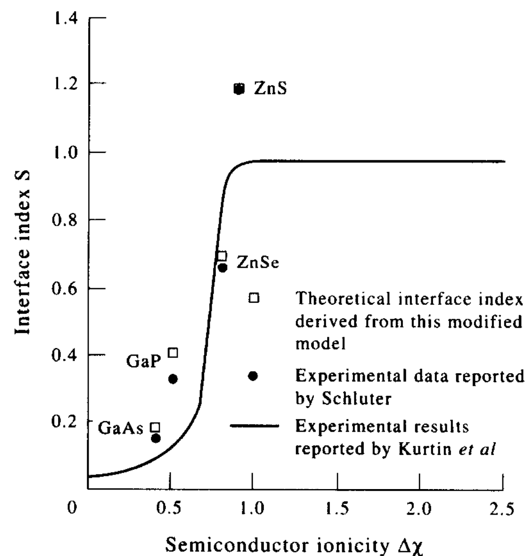

Fig. 4. The theoretical interface indices (□) derived from the modified model for GaAs, GaP, ZnSe and ZnS. The experimental data by Schluter (•) and the experimentally fitting curve by Kurtin *et al.* (——) are also indicated for comparison.

Table 1. The values of D_s, λ_s and the semiconductor ionicity $\Delta\chi$ for GaAs, GaP, ZnSe and ZnS

	GaAs	GaP	ZnSe	ZnS
$D_s(\times 10^{14}\ cm^{-2})$	2.0	1.38	1.0	0.69
$\lambda_s(\times 10^{-8}\ cm)$	2.8	†2.60	1.9	0.90
$\Delta\chi$	0.4	0.50	0.8	0.90

†Estimated according to the WKB approximation method reported in Ref. [4].

minimum energy gap of the semiconductor and λ_s was inversely proportional to the square root of the Phillips' average gap of the semiconductor. Since the semiconductors with high ionicity usually possess both large minimum energy gaps and Phillips' average gaps[12], D_s and λ_s will therefore decrease as the semiconductor ionicity increases. Consequently, the increase of the semiconductor ionicity will result in an increase of the interface index. The theoretical values of the interface index derived from this modified model for GaAs, GaP, ZnSe and ZnS are plotted in Fig. 4. The utilized values of the D_s and λ_s for these four semiconductors are listed in Table 1[3,6]. For comparison, the experimental results reported by Schluter[5] are also shown in Fig. 4. It can be found that the theoretical values derived from the modified model fit quite well with the experimental data. In addition, the theoretical results show that the values of the interface indices exhibit a large variation as $\Delta\chi$ changes from 0.8 to 0.9. This is also consistent with the previous experimental result, which showed that an abrupt transition from the Bardeen limit to the Schottky limit occurred at around $\Delta\chi = 0.8$.

4. CONCLUSIONS

A modified interfacial-layer model based on reconsidering the influence of the penetration depth of the interface states on the Schottky barriers is proposed and a new analytical expression of the interface index is then derived. Furthermore, the correlation between the interface index and the semiconductor ionicity $\Delta\chi$ is investigated. Consequently, the achieved interface indices according to this modified model fit quite well with the previous experimental data. Meanwhile, a sharp transiton from the Bardeen limit to the Schottky limit occurring at around $\Delta\chi = 0.8$, observed in the experimental report, can also be predicted by this model.

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