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Theory of electrical characteristics of a Schottky barrier having exponentially distributed impurity states and metal–insulator–metal structures

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Abstract. The metal–insulator or metal–amorphous semiconductor blocking contact is still not well understood. Here, we discuss the steady state characteristics of a non-intimate metal–insulator Schottky barrier. We consider an exponential distribution (in energy) of impurity states in addition to impurity states at a single energy level within the depletion region. We present analytical expressions for the electrical potential, field, thickness of depletion region, capacitance, and charge accumulated in the depletion region. We also discuss ln I versus V_{ap} data. Finally, we compare the characteristics in three cases:

(i) impurity states at only a single energy level;
(ii) uniform energy distribution of impurity states; and
(iii) exponential energy distribution of impurity states.

In general, the electrical characteristics of Schottky barriers and metal–insulator–metal structures with Schottky barriers depend strongly on the energy distribution of impurity states.

1. Introduction

The metal–insulator contact, particularly that of an amorphous material, is a complicated problem because of the presence of large impurity states at the contact (Henisch 1957, Rhoderick 1978, Cohen and Lang 1982, Lindau and Kendelewicz 1986, Bryant *et al* 1987). These impurity states are due to lattice mismatch or impurities otherwise present in the insulator (Mott 1967, 1980, Rhoderick 1978, Liliental-Weber 1987, Aldao *et al* 1990). Considering these localized impurity states, recently many workers have discussed the metal–amorphous silicon contact because of its technological importance (Abraham and Doherty 1982, Lang *et al* 1982, Shiau and Bube 1986, Yapsir *et al* 1988). Most of the recent work is either on the formation of Schottky barrier and relation of barrier height to impurity distribution at the contact (Chattophadhyay and Daw 1985, Lindau and Kendelewicz 1986, Aldao *et al* 1990) or on the determination of the energy distribution of these impurity states in amorphous materials through the capacitance–voltage relationship (Abraham and Doherty 1982, Lang *et al* 1982).

A large number of classical (Schottky 1939, Bardeen 1947) and quantum mechanical (Louie and Cohen 1976) models have been proposed for the Schottky barrier. The most classical is that proposed by Schottky in 1939, which is based on perfect contact between the metal and the semiconductor, leading to Fermi level alignment and band bending which neutralizes the charge transfer. In this model, donor-type impurity states at a single energy level are considered (Henisch 1957). In crystalline materials, impurities are better controlled and, for doped crystalline semiconductor devices, this model may be sufficient.

The energy distribution of impurity states has been extensively studied in amorphous silicon and other amorphous semiconductors (Le Comber and Spear 1979, Snell *et al* 1979, Mott 1980, Singh and Cohen 1980, Anderson 1982, Cohen and Lang 1982, Lang *et al* 1982, Della Sala *et al* 1990, Drchal and Malek 1990). There is now considerable evidence that interface states are an important factor in amorphous materials and are of central importance to the understanding of the transport and optical properties (Ast and Brodsky 1980, Solomon and Brodsky 1980).

The importance of energetically distributed impurity states in the variations in electrical field and potential within the depletion (space-charge) region and in the electrical characteristics of the Schottky barrier has not been widely discussed. Recently we discussed the influence of energetically distributed impurity states along with impurity states at a single energy level on various electrical characteristics of a metal–insulator Schottky barrier and a metal–insulator–metal structure with blocking contacts (Gupta and Morais 1990). We found that characteristics change remarkably owing to these impurity states. In this work, impurities are considered to be distributed uniformly throughout the prohibited energy band. In general, the energy distribution of impurity states is complex and cannot be represented by an analytical expression. However, it can be better approximated as an exponential distribution (Mathur and Dahiya 1974, Chattophadhyay and Daw 1985) rather than as a uniform distribution. Therefore it is interesting to study a Schottky barrier considering an exponential distribution of interface states to attain a better understanding of amorphous material Schottky barriers.

In the present paper, we consider an exponential distribution of impurity states. The uniform distribution of impurity states turns out to be a special case of the present analysis. We present an analytical approach to various electrical characteristics in the steady state. We found that characteristics depend strongly upon the energy distribution of impurity states in the depletion region and must be taken into account.

2. Formulation

We consider a metal–oxide–insulator contact at a metal–insulator interface. The thickness of the oxide layer is about 50 Å, so that the metal and the insulator states are no longer in intimate contact. As the anode is forward biased and offers very little resistance to current, we continue to consider it as an insulator–metal contact. Thus, the so-called metal–insulator–metal structure turned out to be a metal–oxide–insulator–metal structure as shown in figure 1. The energy band diagram for metal–oxide–insulator contact before and after applying a contact potential is shown in figure 2.

The oxide layer is considered to be free from any kind of electrical charge. This means that the electrical field is constant throughout the oxide layer.

The bulk impurity states are distributed throughout an amorphous insulator. Apart from this we have the interface impurity states at the oxide–insulator interface. The impurity states in question include both kinds of impurity state. We assume that the variation in the density of impurity states with distance from interface is very small in the depletion region and an average value can be used. In general, we can best represent

Figure 1. Metal–oxide–insulator–metal structure.

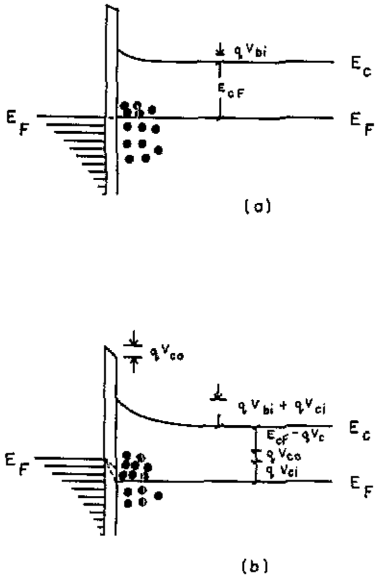


Figure 2. Energy band levels at a blocking metal–oxide–insulator contact (*a*) before applying a potential and (*b*) after applying an external contact potential.

the energy distribution of impurity states as an exponential distribution, which in the space-charge region can be given as

$$N(E) = N_t' \exp[-(E - E_t)]/k_B T_t \tag{1}$$

where $N(E)$ is the impurity density per cubic centimetre per electronvolt at energy E. N_t', E_t and K_t are constants of the distribution of impurity states and depend on the fabrication conditions. N_t' is in reciprocal cubic centimetre electronvolts. The energy level E_t is supposed to lie much below the Fermi level so that only impurities above E_t are effective in forming the depletion region. T_t is a characteristic temperature of the impurity state distribution whose magnitude designates a sharp or diffuse distribution. For a uniform distribution, $T_t \to \infty$.

Let us consider that for an applied potential $-V_{ap}$ the contact potential at any point x inside the depletion region is $V(x)$, where x is the distance inside the insulator from oxide–insulator interface. In a reverse-biased Schottky barrier, $V(x)$ is negative. The total potential on the depletion region is $-V_c$. This means that contact potential is zero at $x = W$ and $-V_c$ at $x = 0$. W is the thickness of the depletion region. The positive charge density due to these impurities at any point x is

$$\int_{E_F+qV(x)}^{E_F} qN_t' \exp\left(\frac{-(E - E_t)}{k_B T_t}\right) dE = qN_t \left[\exp\left(\frac{qV(x)}{k_B T_t}\right) - 1\right] \tag{2}$$

where

$$N_t = k_B T_t N_t' [\exp(E_t - E_F)/k_B T_t]. \tag{3}$$

N_t is in reciprocal cubic centimetres. Apart from these energetically distributed impurity

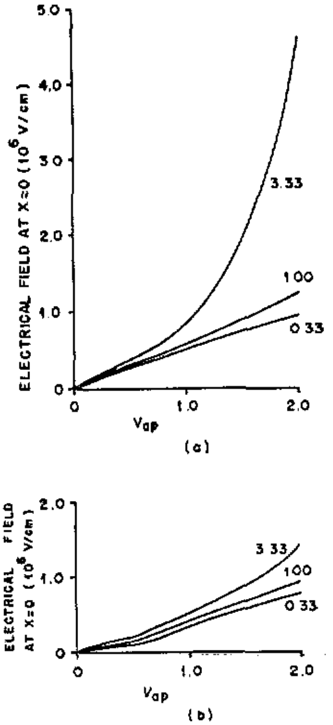


Figure 3. Variation in the electrical field at $x = 0$ with applied potential for several values of $(1/k_B T_t)$: (*a*) $L_{ox} = 0$; (*b*) $L_{ox} = 50$ Å.

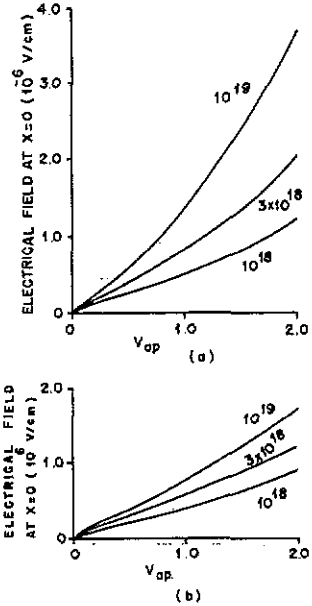


Figure 4. Variation in the electrical field at $X = 0$ with applied potential for several values of $(N_t/k_B T_t)$: (*a*) $L_{ox} = 0$; (*b*) $L_{ox} = 50$ Å.

states, we are considering N_d impurity states per cubic centimetre at an energy level E_d, such that $E_d = E_F$. These impurity states can be due to doped impurities. Thus, the positive charge density at any point x is

$$\rho(x) = q[\![N_d + N_t\{\exp[-qV(x)/k_B T_t] - 1\}]\!]. \tag{4}$$

As the contact is blocked, we consider that, in the reverse-biased steady state, almost the entire applied potential appears across the contact. Thus,

$$V_c = V_{bi} + V_{ap} - V_{ox}$$

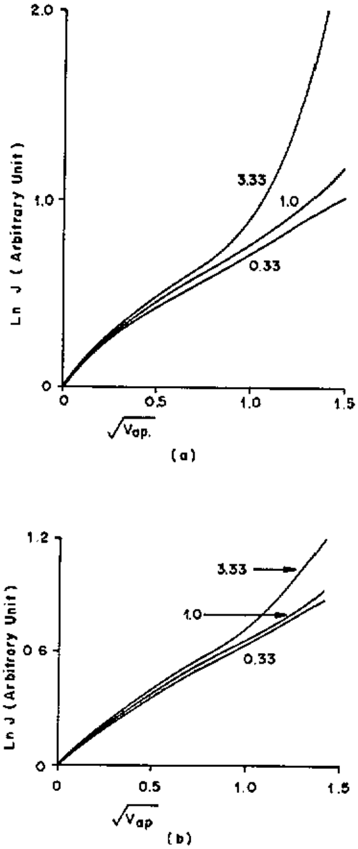
where V_{bi} is the internal built-in potential (Sze 1981). V_{ox} is the potential on the oxide layer and is given by $L_{ox}E_{ox}$, where L_{ox} is the thickness of the oxide layer and E_{ox} is the electrical field in the oxide layer which is equal to the electrical field E_{co} at the oxide–insulator contact. Thus,

$$V_c = V_{ap} + V_{bi} - L_{ox}E_{co}. \tag{5}$$

3. Calculations

The distribution of electrical potentials and fields are obtained from the solution of Poisson's equation, which in the present case is

$$d^2V/dx^2 = -(q/K\varepsilon_0)[\![N_d + N_t\{\exp[-qV(x)/k_B T_t] - 1\}]\!]. \tag{6}$$



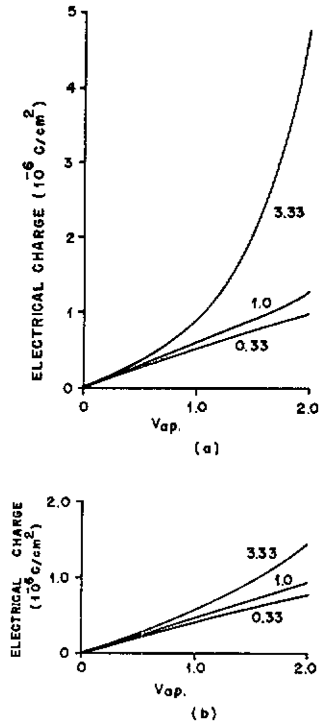


Figure 5. Variation in ln J with applied potential for several values of $(1/k_BT_t$: (*a*) $L_{ox} = 0$; (*b*) $L_{ox} = 50$ Å.

Figure 6. Variation in the charge Q in the depletion region with the applied potential for several values of $(1/k_BT_t)$: (*a*) $L_{ox} = 0$; (*b*) $L_{ox} = 50$ Å.

Integrating with the boundary condition $\mathrm{d}V/\mathrm{d}x = 0$ for $V = 0$, we obtain

$$\mathrm{d}V/\mathrm{d}x = [\![A\{\exp[-qV(x)/k_B T_t] - 1\} - BV(x)]\!]^{1/2} \tag{7}$$

where

$$A = (2/K\varepsilon_0)N_t k_B T_t \qquad B = (2q/K\varepsilon_0)(N_d - N_t). \tag{8}$$

If $V_s(x) = -V(x)$, i.e. V_s gives the magnitude of the potential at x, for a reversed-biased Schottky barrier we obtain

$$-\mathrm{d}V_s/\mathrm{d}x = [\![A\{\exp[-qV_s(x)/k_B T_t] - 1\} + BV_s(x)]\!]^{1/2}. \tag{9}$$

Integrating, we arrive at

$$W = \int_0^{V_c} \mathrm{d}V \left\{A\left[\exp\left(\frac{qV_s(x)}{k_B T_t}\right) - 1\right] + BV_s\right\}^{-1/2}. \tag{10}$$

This cannot be resolved analytically. However, W can easily be calculated through numerical integration. As at the contact $V_s(x)$ is V_c, so the electrical field at $x = 0$ is

$$E_{co} = \{A[\exp(qV_c/k_B T_t) - 1] + BV_c\}^{1/2}. \tag{11}$$

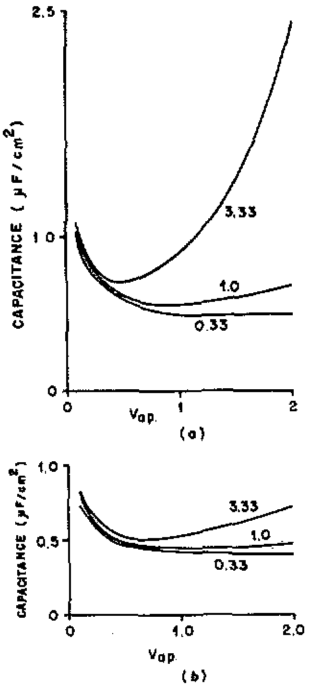


Figure 7. Variation in the capacitance with applied potential for several values of $(1/k_BT_t)$: (*a*) $L_{ox} = 0$; (*b*) $L_{ox} = 50$ Å.

The charge Q inside the depletion region is

$$Q = K\varepsilon_0 E_{c0} = K\varepsilon_0\{A[\exp(qV_c/k_BT_t) - 1] + BV_c\}^{1/2}. \tag{12}$$

When the distribution is very sharp, we have $k_BT_t \ll qV_c$ and

$$Q = K\varepsilon_0 A^{1/2} \exp(qV_c/2k_BT_t). \tag{13}$$

The capacitance in this case is

$$C = (K\varepsilon_0 A^{1/2}/V_c) \exp(qV_c/2k_BT_t) \tag{14}$$

i.e. the capacitance increases with increase in the applied potential. This is the opposite to the case of impurities at a single energy level.

4. Discussion

The cases of uniform impurity distribution and impurities at a single energy level have been discussed in our earlier paper (Gupta and Morais 1990). In the present paper we discuss the case of an exponential distribution of impurity states in addition to impurity states at a single level. It is not possible to obtain analytically the variation in potential inside the depletion region. However, experimentally observable characteristics such as current density versus V_{ap}, and capacitance versus V_{ap} can be discussed.

If we consider that the current is contact limited and the Schottky effect is the most important charge injection mechanism in a metal–insulator–metal structure, $\ln J$ is

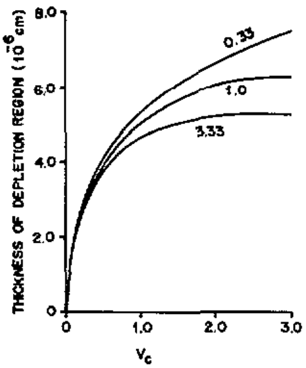


Figure 8. Variation in the thickness of the depletion region with contact potential on the depletion region for several values of $(1/k_BT_t)$.

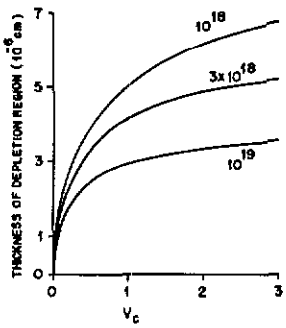


Figure 9. Variation in the thickness of the depletion region with contact potential on the depletion region for several values of (N_t/k_BT_t).

Table 1. Comparison of the electrical characteristics of the Schottky barrier.

		Expressions obtained for the following		
Sample no.	Characteristics	Impurity states at a single energy level	Uniform distribution	Exponential distribution
1	W versus V	$W \propto V_c^{1/2}$	$W \propto \ln(2qN_0V_c/N_d)$	Tends to be constant
2	Q versus V	$Q \propto V_c^{1/2} - V_{bi}^{1/2}$	$Q \propto V_c$	$Q \propto \exp(qV_c/2k_BT_t)$
3	C versus V	$C \propto V_c^{-1/2}$	C is constant	$C \propto (1/V_c)\exp(qV_c/2k_BT_t)$
4	E_{co} versus V	$E_{co} \propto V_c^{1/2}$	$E_{co} \propto V_c$	$E_{co} \propto \exp(qV_c/2k_BT_t)$
5	$\ln I$ versus V	$\ln I \propto V_c^{1/4}$	$\ln I \propto V_c^{1/2}$	$\ln I \propto \exp(qV_c/4k_BT_t)$

proportional to the square root of E_{co}, where J is the current density. Through (5) and (11), E_{co} is given as

$$E_{co} = [\![A\{\exp[(q/k_BT_t)(V_{ap} + V_{bi} - E_{co}L_{ox})] - 1\} + B(V_{ap} + V_{bi} - E_{co}L_{ox})]\!]^{1/2}.$$

Expanding the exponential and considering that $V_{ap} \gg V_{bi}$ or $E_{co}L_{ox}$, we obtain

$$E_{co} = (2q/K\varepsilon_0)^{1/2}[N_dV_{ap} + (qN_t/2k_BT_t)V_{ap}^2 + (q^2N_t/6k_B^2T_t^2)V_{ap}^3 + \dots]^{1/2}.$$

In the case where the only important impurities are those of a single energy level, we have $N_t = 0$. Thus, E_{co} is proportional to $V_{ap}^{1/2}$ and $\ln J$ is proportional to $V_{ap}^{1/4}$.

In the case where uniformly distributed impurity states are the most important, i.e. $qN_t/k_BT_t \gg N_d$ and $k_BT_t/q \to \infty$, we get $E_{co} \propto V_{ap}$ and correspondingly $\ln J$ is proportional to $V_{ap}^{1/2}$. These results are in agreement with our earlier work (Gupta and Morais 1990). If exponentially distributed impurities are the most relevant, $\exp(qV_c/k_BT_t \gg 1$ or qV_c/k_BT_t, we have as an approximation,

$$E_{co} = A^{1/2}\exp(q/2k_BT_t)(V_{ap} + V_{bi} - E_{co}L_{ox}).$$

Thus, $\ln J$ is proportional to $\exp(qV_c/4k_BT_t)$ or $\exp(qV_{ap}/4k_BT_t)$ if $L_{ox}E_{co}$ and V_{bi} are very small compared with V_{ap}. In the same way, charge Q in the depletion region is proportional to $\exp(qV_c/2k_BT_t)$ and the capacitance is proportional to $(1/V_c)\exp(qV_c/2k_BT_t)$.

For the purpose of illustrating the variation in electrical characteristics with the sharpness of the distribution of impurity states, we consider the dielectric constant $K = 11.7$, $V_{bi} = 0$, $N_d = 3 \times 10^{17}\,cm^{-3}$ and $N_t/k_BT_t = 10^{18}\,cm^{-3}\,eV^{-1}$. In figures 3(*a*), 4(*a*), 5(*a*), 6(*a*) and 7(*a*) we consider $L_{ox} = 0$ and in figures 3(*b*), 4(*b*), 5(*b*), 6(*b*) and 7(*b*) we consider $L_{ox} = 50$ Å. In the upper, middle and lower curves we consider that k_BT_t equals 0.3, 1.0 and 3.0 eV, respectively.

In figures 3 and 4 we plot the variation in electrical field at $x = 0$ with potential for various values of $1/k_BT_t$ and for various values of N_t/k_BT_t respectively. E_{co} changes more rapidly with potential when the distribution is very sharp, i.e. $qN_t \gg k_BT_t$. In figure 5, we plot $\ln J$ versus V_{ap}. For the sharply distributed impurities, $\ln J$ tends to vary as $\exp(CV_{ap})$, where C is a constant. This is visible in $L_{ox} = 0$, because in this case $V_{ap} \gg V_{ox}$. In figure 6, we plot the charge Q in the depletion region versus V_{ap}. Q varies more rapidly with V_{ap} for a sharp distribution of impurities. In figure 7, we plot the variation in capacitance with applied potential. In the case of exponentially distributed impurities, the capacitance may increase with increasing applied potential and the increase is faster if the distribution is sharper. In figures 8 and 9, we plot the variation in the thickness W of depletion region with contact potential V_c in the depletion region for various values of $1/k_BT_t$ and for various values of N_t/k_BT_t, respectively. For a sharp distribution, the thickness tends to be constant for higher contact potentials.

In table 1, we compare the electrical characteristics of a Schottky barrier and a metal–insulator–metal structure with blocking contacts in three cases:

(i) impurity states at a single energy level;
(ii) uniformly distributed impurity states in energy;
(iii) exponentially distributed impurities in energy.

Experimental results on *C–V* characteristics of amorphous silicon Schottky barriers (Snell *et al* 1979, Lang *et al* 1982) are in agreement with the present theory for high value of k_BT_t ($\simeq 3$ or more), i.e. when the distribution is not very sharp. The results for a sharp distribution may be important for some other Schottky barriers prepared under different conditions and/or with different materials.

5. Conclusions

Energetically distributed impurities in the depletion region significantly change the electrical characteristics of a Schottky barrier and a metal–insulator–metal structure with blocking contacts. With increase in the sharpness of exponentially distributed impurities, $\ln J$ varies more rapidly with applied potential, while the thickness of depletion region tends to be constant. The capacitance of the depletion region tends to increase instead of decreasing, and thus the charge inside the depletion region increases significantly for the same contact potential. In the present paper, we presented the expected characteristics for various sharpnesses of exponentially distributed impurities. This is useful for interpreting the electrical characteristics of metal–insulator–metal structures and in particular those of amorphous materials and for obtaining a better understanding of Schottky barriers and corresponding devices.

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