CAPACITANCE AND CONDUCTIVITY OF SPACE CHARGE REGION IN METAL

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The paper contains a theoretical analysis of the electric effect caused by the formation of a space charge in the metal of a metal-insulator-metal structure. The analytic expression for the capacity of the space charge region was derived. The numerical values of this capacity for several metals were calculated, they range from 0.05 to 0.15 $\mathrm{Fm^{-2}}$. The surface conductivity caused by the presence of the space charge region at the surface of the metal was considered. The analytic equation for the relative conductivity change was derived. The numerical value of this conductivity change was determined; it amouted to about 0.2% for high electron density metals and can be greater for low electron density metals.

1. *Introduction*

It has been observed by Mead [1] that the capacitance of metal-insulator-metal sandwiches deviates from the geometric capacitance. Results of measurements indicated that:

1. the capacitance of the metal-insulator-metal (*M-I-M*) structure is a series combination of two parallel-plane capacitances, and

2. the capacitances are practically constant and independent of applied voltage and dielectric thickness.

Mead [1] has attributed this effect to electric-field penetration of the electrodes. As a result of electric-field penetration there is a space-charge region just inside the surface of each electrode and the applied voltage drops somewhat in these regions, so that not all of the applied voltage appears across the dielectric.

Ku and Ullman [2], using degenerate Fermi statistics, studied the electric-field penetration of electrodes theoretically and derived results that are in substantial agreement with Mead's observations. Simmons [3] expressed the equations of Ku and Ullman in analytic form by means of a suitable approximation, and further interpretation of the effect was obtained. Papers [2, 3] dealt with the symmetric *M-I-M* structure, but also the asymmetric structure was considered theoretically by Simmons [4].

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It is object of this paper to express in analytic form the capacitance of *M-I-M* structure with space-charge region in electrodes, and to incorporate electric-field penetration of the metal film in electric conductance calculations.

2. *Voltage drop in the space charge region of the electrodes (symmetric M-I-M structure)*

If there is no electric field penetration into the metal, the potential drop across the dielectric is equal to the applied potential and the capacitance is given simply by geometrical capacitance per unit area (in F/m² units), equal to ε_d/d, where ε_d is the permittivity of the dielectric (in F/m units) and d is the dielectric thickness (in meters).

However, when the electric field penetrates the electrodes, only a part of the contact potential appears across the insulator. The voltage absorbed in the electrodes results in a space charge build-up just inside the surface of the electrodes.

The energy diagram of an *M-I-M* structure is illustrated in Fig. 1. Voltage bias across the electrodes is V_a. Because of the field penetration of the electrodes, the surface of the

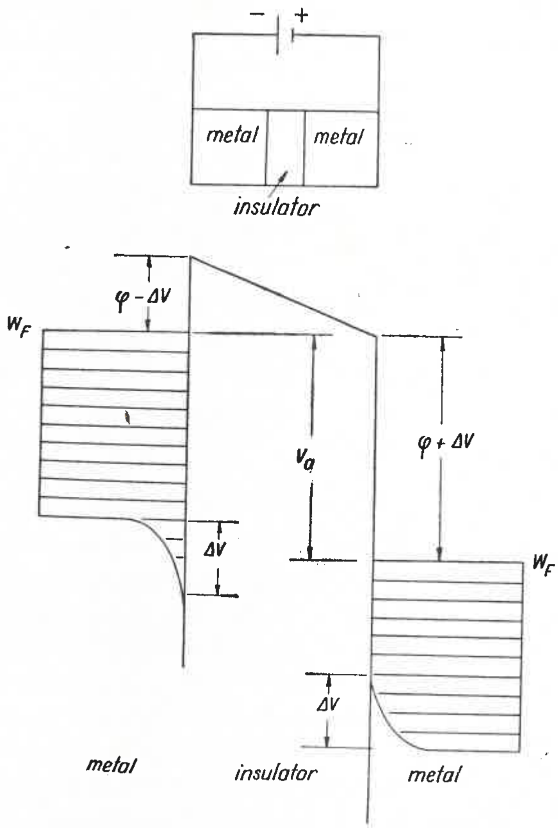

Fig. 1. Energy band model of parallel-plane capacitor with electric-field penetration of the electrodes. ΔV is the voltage drop in the electrodes (Eq. 9). φ is the barrier height if the penetration effect is neglected. V_a is applied voltage. W_F is the Fermi level

negatively biased electrode is at a potential V_1 lower than the interior of the electrode, and that of the positively biased electrode is $(V_a - V_2)$ above the interior.

Poisson's equation was written for the problem by Ku and Ullman [1], and they derived the equations connecting V_1 and V_2 with V_a. Because of their intractability, the equations are inconvenient to use as they stand. It has been shown that these equations can be expressed in an analytic form [3] not only by means of a suitable approximation but can be also derived from Poisson's equation written in the following form for the negatively charged electrode,

$$\frac{d^2V^-}{dx^2} = \frac{3e^2 n_0}{2\varepsilon_m W_F} V^- \tag{1}$$

and for the positively charged electrode in the form,

$$\frac{d^2V^+}{dx^2} = \frac{3e^2 n_0}{2\varepsilon_m W_F} (V^+ - V_a). \tag{2}$$

Here, x is depth in the metal measured from the surface into the interior of the electrodes separately for each electrode (Fig. 1). V^- and V^+ are electrostatic potentials at depth x in the negatively and in the positively charged metal, respectively. ε_m is the permittivity of the metal electrodes (in F/m units), n_0 is the free electron density when no potential is applied, W_F is the Fermi energy, and e is the electron charge.

Solutions of Eqs (1) and (2) are exponential functions derived by Simmons [3]. We will express the solutions in a form which will be more convenient for deriving analytic expressions for the capacitance of the *M-I-M* structure and for the surface conductivity of the thin metal film with the space charge region.

The solutions of Eqs (1) and (2) are

$$V^- = \frac{V_a}{2+K} \exp(-x/x_0) \tag{3}$$

and

$$V^+ = V_a \left[1 - \frac{1}{2+K} \exp(-x/x_0) \right], \tag{4}$$

where

$$K = \varepsilon_m d / \varepsilon_d x_0, \tag{5}$$

and

$$x_0 = \frac{2}{\sqrt{3}} \left(\frac{\varepsilon_m W_F}{2 n_0 e^2} \right)^{\frac{1}{2}} \tag{6}$$

is the characteristic panetration length in the metal.

From Fig. 1, the boundary conditions are: $V = 0$ and $dV/dx = 0$ at $x = \infty$, and $-\varepsilon_m (dV/dx)_{x=0} = \varepsilon_d (V_2 - V_1)$ for the negatively charged electrode. From (3) and (4) we have (see Fig. 1)

$$V_1 = V_a/(2+K) \tag{7}$$

and

$$V_2 = V_a\left(1 - \frac{1}{2+K}\right). \tag{8}$$

Equations (7) and (8) show that the voltage drop in each electrode due to electric field penetration is the same (this is true for electrodes of the same material only). The voltage drop in the negatively charged electrode is

$$\Delta V_1 \equiv V_1 = V_a/(2+K) \tag{9}$$

and in the positively charged electrode

$$\Delta V_2 \equiv V_a - V_2 = \Delta V_1.$$

From Eq. (9) we see that $\Delta V_1 \to V_a/2$ when $d \to 0$ and $\Delta V_1 \to 0$ when $d \to \infty$.

An interesting case is the application of the above results for an M-I-M structure with an extremely thin film of insulator. If $x_0 = 0.5$ Å and $\varepsilon_m = \varepsilon_0 = 8.85 \times 10^{-12}$ F/m (typical values for metals) and $\varepsilon_d = 10\,\varepsilon_0$, we obtain $K = d/5$ and from (9) we obtain $\Delta V_1 = \Delta V_2 = V_a/(2+d/5)$. Using $d = 50$ Å, the potential drop in both electrodes is $2\Delta V_1 = V_a/6$. Therefore, for this case, the applied voltage drops by about 17% in the electrodes. The remaining 83% of the applied voltage drop is in the insulator.

The dielectric displacement in the negatively charged electrode is

$$D = \varepsilon_m \left|\frac{dV}{dx}\right| = \frac{\varepsilon_m V_a}{(2+K)x_0}\, e^{-\frac{x}{x_0}}.$$

This equation shows that D falls with increasing depth in the electrode.

3. *Voltage drop in the space charge region of the electrodes (asymmetric M_1-I-M_2 structure)*

In the case of an asymmetric M_1-I-M_2 structure (the electrodes are made of different metals 1 and 2), the Poisson's equations (1) and (2) are still valid. Assuming $n_0 = n_{01}$ and $W_F = W_{F1}$ for the negatively charged electrode and $n_0 = n_{02}$ and $W_F = W_{F2}$ for the positively charged electrode we can write after Simmons [4], in a more convenient form in our case, the following expressions:

voltage drop in the negatively charged electrode

$$\Delta V_1 = \lambda_1 V_a; \tag{10}$$

voltage drop in the positively charged electrode

$$\Delta V_2 = \lambda_2 V_a, \tag{11}$$

where $\lambda_1 = K_2/(K_1+K_2+K_1K_2)$ and $\lambda_2 = K_1/(K_1+K_2+K_1K_2)$, with $K_1 = \varepsilon_{m1}d/\varepsilon_d x_{01}$ and $K_2 = \varepsilon_{m2}d/\varepsilon_d x_{02}$;

potential in the space charge region of the negatively charged electrode

$$V^- = \lambda_1 V_a \exp(-x/x_{01}), \tag{12}$$

and in the positively charged electrode

$$V^+ = V_a[1-\lambda_2 \exp(-x/x_{02})], \tag{13}$$

where x_{01} and x_{02} are the characteristic penetration lengths in metals 1 and 2, respectively (Eq. 6).

4. *Capacitance of the space charge region in the metal*

The total capacitance of the *M-I-M* structure is the series combination of the capacitances of the dielectric C_d and the electrodes C_m. It can be shown that the distance l_0 between the electrodes of the capacitor of capacitance C_m is equal x_0. Indeed, the mean distance of the space charges from the surface of the metal is

$$l_0 = \frac{\int\limits_0^\infty \varrho(x) x dx}{\int\limits_0^\infty \varrho(x) dx} \tag{14}$$

where $\varrho(x)$ is the density of the space charge. Poisson's equation can be written in the form

$$\frac{d^2V}{dx^2} = \frac{\varrho(x)}{\varepsilon_m}. \tag{15}$$

From (15) and (1) we obtain:

$$\varrho(x) = \frac{3e^2 n_0}{2W_F} V. \tag{16}$$

Substituting (3) and (7) in (16) yields

$$\int\limits_0^\infty \varrho(x) dx = \frac{3e^2 n_0 V_1 x_0}{2W_F} \tag{17}$$

and

$$\int\limits_0^\infty \varrho(x) x dx = \frac{3e^2 n_0 V_1 x_0^2}{2W_F}. \tag{18}$$

Substituting (17) and (18) in (14) yields $l_0 = x_0$.

The reciprocal capacitance of the space charge region is $1/C_m = x_0/\varepsilon_m + x_0/\varepsilon_m$, and substituting (6) yields

$$C_m = \left(\frac{3\varepsilon_m n_0 e^2}{8W_F}\right)^{\frac{1}{2}}. \tag{19}$$

Equation (19) shows that the electrode capacitance is a constant independent of voltage bias, a result observed experimentally by Mead [1]. C_m depends on the electric properties of the metals. Calculated values of C_m (from Eq. (19)) and x_0 (from Eq. (6)) for a few metals are shown in Table I.

For normal dielectric thicknesses (microns or greater) the contribution of the electrodes to the total capacitance of the *M-I-M* structure is negligible; therefore, it is not necessary to consider this effect, unless measurements concern capacitors with very thin dielectric layers. For instance, if $\varepsilon_d = 10\varepsilon_0$ and $d = 30$ Å, we obtain $C_d = \varepsilon_d/d \approx 0.03$ F/m², but for $\varepsilon_d = 10\varepsilon_0$ and $d = 20$ Å we have $C_d = 0.044$ F/m².

TABLE I

Calculated values of C_m and x_0 for some metals in *M-I-M* structure. $C_m = 7.3\times10^{-16}\, n_0/W_F$

Metal	W_F (eV)	$n_0\times10^{-28}$ (m^{-3})	C_m (Fm^{-2})	x_0 (Å)
Al	4.08	18.2	0.154	0.287
Cu	7.04	8.5	0.080	0.555
Ag	5.51	5.8	0.075	0.59
Au	5.54	5.9	0.075	0.59
Cs	1.53	0.85	0.054	0.815

For asymmetric M_1-I-M_2 structure the capacitance of the space charge of the electrodes is, of course, expressed as $1/C_m = 1/C_{m1}+1/C_{m2}$, where $C_{m1} = \varepsilon_{m1}/x_{01}$ and $C_{m2} = \varepsilon_{m2}/x_{02}$. Table I gives the capacitances concerned with the space charge region of some metals.

5. *Surface conductivity of the metals*

This section incorporates electric-field penetration of thin metal films in the film conductivity calculations. It will be shown that the metal conductivity will change if a space charge region appears, and this change may be measurable in the case when a thin metal film is considered.

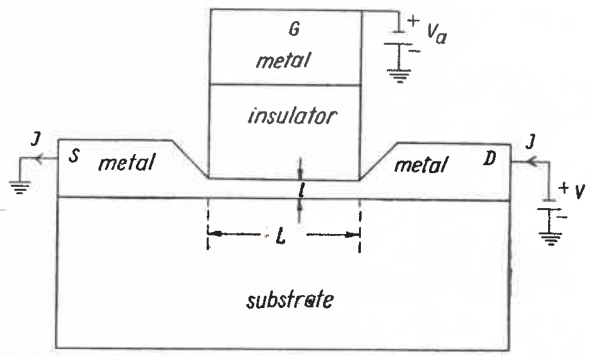

Fig. 2. Cross-section of the metal-insulator-metal structure which can be used in conductivity changes measurements. The structure is similar to that of thin-film transistor (S — source, D — drain, G — gate)

Let us consider a rectangular surface of length L and width b (Fig. 2). The space charge is given by $e\Delta nLb$, where $e\Delta n$ is the space charge per unit area. The application of voltage V will shift the charge $e\Delta nLb$ after a time τ over a distance L if $\tau v = L$. The rate of drift of the charge carriers is given by $v = \mu E = \mu V/L$. The current intensity is given by

$$I = \frac{e\Delta nLb}{\tau} = \frac{e\Delta n\mu bV}{L}.$$

The surface conductivity is given by

$$\Delta G = \frac{I}{V} = \frac{b}{L} e\mu\Delta n.$$

If $b = L$, ΔG is independent of the size of the square and

$$\Delta G = e\mu\Delta n \tag{20}$$

ΔG is conductivity "per square". Equation (20) gives the surface conductivity as a function of the space charge.

Conductivity of the metal film is given by $G = \frac{bl}{L}\mu e n_0$, where l is the thickness of the film. If $b = L$, G is independent of the size of the square and the conductivity "per square" is given by

$$G = e\mu n_0 l. \tag{21}$$

From (20) and (21) we obtain the relative conductivity change in the following form:

$$\frac{\Delta G}{G} = \frac{\Delta n}{n_0 l}. \tag{22}$$

Δn can be found from

$$\Delta n = \int_0^\infty (n - n_0)\, dx = \frac{1}{e} \int_0^\infty \varrho(x) dx. \tag{23}$$

Substituting (17) and (7) into (23) gives

$$|\Delta n| = \frac{3en_0 x_0 V_a}{2W_F(2+K)}. \tag{24}$$

Substituting (24) into (22) yields

$$\left|\frac{\Delta G}{G}\right| = \frac{3ex_0 V_a}{2(2+K)W_F l}. \tag{25}$$

This is relative conductivity change of the metal film of thickness l (Fig. 2). The change in conductivity is influenced by the space charge that is induced in the metal film.

The following question arises: can $\Delta G/G$ be made so high experimentally, that would be measurable? For bulk metals it would not be measurable, of course. But what about thin metal films? For an assumed x_0 and W_F of gold, (25) becomes

$$\frac{\Delta G}{G} \approx 2.6 \times 10^{-11} \frac{V_a}{(2+K)l} \tag{26}$$

where V_a is in volts and l in meters. If $l = 10^{-8} m = 100$ Å, $V_a = 100$ V: $\Delta G/G = 0.26/(2+K)$. If the thickness of the insulator (Fig. 2) is $d = 1000$ Å, $\varepsilon_m = \varepsilon_0 = 0.85 \times 10^{-12}$ F/m, $\varepsilon_d = 10\varepsilon_0$ and $x_0 = 0.6$ Å, K can be calculated from (5). We get about a 0.2% change of conductivity, and this is measurable quantity.

6. *Discussion*

When the electric field penetrates the electrodes in *M-I-M* structure, a potential drop across the space charge region appears. This effect causes both deviation of the capacitance of the *M-I-M* structure from the true geometric capacitance and the appearance of surface conductivity of the metal electrodes. An analytic expression for electrode capacitance was derived, Eq. (19). Some calculated values of this capacitance are given in Table I. It is shown by comparison that when measurements on capacitors with very thin dielectric films are being made it is necessary to consider the electric field penetration effect.

It is shown that the metal conductivity will change if an electric field normal to the surface of the metal is applied. This is due to the thin layer of space charge near the surface of the metal. The problem is solved in analytic form and the relative change of the conductivity is obtained, Eq. (25). It can be shown from Eq. (25) that for normal metal film thicknesses (tenths of microns or greater) the contribution of the space charge to the total conductance is negligible; it is necessary to consider this effect, however, if conductivity measurements with very thin metalic films are being performed. For lower electron density metals, such as Bi, the depth of penetration of the space charge is greater than for metals such as gold. Thus it can be expected that the conductivity of lower electron density metals will undergo larger changes than that of the higher electron density metals.

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