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Effect of surface electric field on the gate capacitance of metal-oxide-semiconductor structures of ternary semiconductors

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An attempt is made to derive a generalized expression for the gate capacitance of metal-oxide-semiconductor structures of ternary semiconductors without any approximations of weak or strong electric field limits. It is found, taking n-channel layers on p-type $Hg_{1-x}Cd_xTe$ as an example, that the same capacitance increases with increasing surface field and the approximated results overestimate the numerical values for both limits. The theoretical formulation is in good agreement with the experimental observation as reported elsewhere, and the corresponding well-known results for n-channel inversion layers on parabolic semiconductors are also obtained from the expressions derived.

INTRODUCTION

In recent years, there has been considerable interest in studying the various electronic properties of inversion layers on small-gap semiconductors under different physical conditions.[1-9] Although both experimental and theoretical investigations have been carried out on the transport phenomena of two-dimensional (2D) electron gases formed on small-gap semiconductors, these still remain as scopes in the investigations made, while the interest for further research on the other different physical aspects of such systems is becoming increasingly important. One such useful parameter is the gate capacitance of metal-oxide-semiconductor (MOS) structures under the application of a large gate bias (hereafter referred to as C_g) which has been studied under different approximations. The interesting point is that the carrier concentration in such layers can be controlled by changing the gate voltage, which changes the surface electric field, and hence C_g becomes surface field dependent. The C_g in n-channel inversion layers on p-type Si has been found to exhibit certain peculiar characteristics due to the 2D nature of the motion of the carriers in quantized layers. Since the density-of-states function for nonparabolic layers depends sharply on energy unlike that for inversion layers on parabolic semiconductors, it would be of interest to derive a generalized expression of C_g of small-gap semiconductors whose energy band structures are defined by the two-band Kane model without any approximations of weak or strong electric field limits. In particular, such studies for ternary semiconductors having nonparabolic energy bands would be very interesting, and we shall take $Hg_{1-x}Cd_xTe$ as an example for the purpose of numerical computations. It may be noted that the compound $Hg_{1-x}Cd_xTe$ is an important optoelectronic material because its band gap can be varied over the entire spectral range from 0.8 μm to over 30 μm by adjusting the alloy composition.[10] Its use as an infrared detector material has spurred $Hg_{1-x}Cd_xTe$ technology for the production of high-mobility single crystals with specially prepared surface layers.[11] The same semiconductor is ideally suited for narrow-gap subband physics, because the relevant physical parameters are within easy experimental reach.[11] In addition, one can obtain the corresponding results for inversion layers on parabolic semiconductors by equating the nonparabolicity parameter with zero in the generalized expression.

In what follows, we shall first derive an expression of the surface electron concentration per unit area in n-channel inversion layers on ternary semiconductors without any approximations of weak or strong electric field limits. We shall then derive the gate capacitance with the proper use of the electron statistics. The dependence of the gate capacitance on surface electric field has also been studied on the basis of the theoretical considerations made in this work.

THEORETICAL BACKGROUND

The gate capacitance of MOS structures of n-channel inversion layers on semiconductors can, in general, be expressed[2] as

$$C_g^{-1} = C_{\rm ins}^{-1} + C_s^{-1}, \quad (1)$$

in which $C_{\rm ins}$ ($= \epsilon_{\rm ins}/d_{\rm ins}$) is the fixed capacitance due to oxide layers, $\epsilon_{\rm ins}$ and $d_{\rm ins}$ are the permittivity and the thickness of the insulating layers, respectively, C_s [$= e(dN_s/dV_0)$] is the surface capacitance due to the space-charge layer, N_s is the surface electron concentration per unit area, V_0 ($= V_g - eN_s d_{\rm ins}\epsilon_{\rm ins}^{-1}$) is the surface potential, V_g is the gate voltage, and e is the electron charge. It appears then that the derivation of C_g using Eq. (1) requires an expression of N_s which in turn is determined by the corresponding density-of-states function. Incidentally, the $E - \mathbf{k}_s$ dispersion relation for 2D electrons in n-channel inversion layers on Kane-type semiconductors can be written[1] as

$$\tfrac{1}{2}\left(w_0\sqrt{1+w_0^2} - \ln|w_0 + \sqrt{1+w_0^2}|\right) = (a+\tfrac{1}{4})^{-1}K(n), \quad (2)$$

where the notations are the same as in Ref. 1.

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Using Eq. (2), the density-of-states function can be expressed[6] as

$$D(\epsilon) = l_0 \sum_{n=0}^{n_{\max}} [(1+2\alpha\epsilon)(1+\delta)^{-1}] H(\epsilon - \epsilon_n), \quad (3)$$

where

$$l_0 \equiv m_0^* / \pi\hbar^2,$$

$$\alpha \equiv 1/E_g,$$

$$\delta \equiv w_0^2 - 2[w_0(a+\tfrac{1}{4})^{-1}] K(n) \sqrt{1+w_0^2},$$

where H is the Heaviside step function and ϵ_n is obtained by setting $a=0$ and $\epsilon = \epsilon_n$ in Eq. (2). Combining Eq. (3) with the Fermi–Dirac occupation probability factor, the surface electron concentration of MOS structures of Kane-type semiconductors can be expressed,[6] without any approximation of weak and strong electric field limits, as

$$N_s = l_0 k_B T \sum_{n=0}^{n_{\max}} [\phi(n)]^{-1} [(1+2\alpha\epsilon_n) F_0(\eta_n) + 2\alpha k_B T F_1(\eta_n)], \quad (4)$$

where k_B is the Boltzman constant, T is the temperature,

$$\varphi(n) \equiv (1+G_{0n}^2)^{-1/2} G_{0n}^{-1} (\ln|G_{0n}^2 + \sqrt{1+G_{0n}^2}|),$$

$$G_{0n}^2 \equiv 4\alpha\epsilon_n(1+\alpha\epsilon_n),$$

where $F_j(\eta_n)$ is the one-parameter Fermi-Dirac integral of order j as defined by Blakemore,[12]

$$\eta_n \equiv (k_B T)^{-1} [E_F - \epsilon_n],$$

$$E_F = eV_g - N_s e^2 d_{\text{ins}} \epsilon_{\text{ins}}^{-1} - E_{fb}$$

is the Fermi energy as measured from the edge of the conduction band at the surface, and E_{fb} is the energy separation between the Fermi level and the conduction-band edge of the bulk of the substrate material.

Thus, using Eqs. (4) and (1), the generalized expression for the gate capacitance can be written as

$$C_g = l_0 \Delta e^2 \left(\sum_{n=0}^{n_{\max}} \{\varphi(n)\}^{-1} \times [(1+2\alpha\epsilon_n) F_{-1}(\eta_n) + 2\alpha k_B T F_0(\eta_n)] \right), \quad (5)$$

where

$$\Delta \equiv \left(1 + l_0 k_B T \sum_{n=0}^{n_{\max}} \{\Omega(n)\} \{\varphi(n)\}^{-2} [(1+2\alpha\epsilon_n) F_0(\eta_n) + 2\alpha k_B T F_1(\eta_n)] + w(n)(k_B T)^{-1} \{\varphi(n)\}^{-1} \{[(1+2\alpha\epsilon_n) F_{-1}(\eta_n) + 2\alpha k_B T F_0(\eta_n)] - 2\alpha F_0(\eta_n) P(n)\} \right)^{-1},$$

$$\Omega(n) \equiv P(n) Q(n),$$

$$P(n) \equiv [\alpha G_n N_s (1+2\alpha\epsilon_n)]^{-1} [2A(n)\sqrt{1+G_n^2}],$$

$$Q(n) \equiv 2\alpha G_n^{-2} (1+2\alpha\epsilon_n)(1 - G_n^{-1} \ln|G_n + \sqrt{1+G_n^2}|),$$

and

$$G(n) \equiv [P(n) + e^2 d_{\text{ins}} \epsilon_{\text{ins}}^{-1}].$$

From Eqs. (4) and (5) the expressions for the electron statistics and the gate capacitance in MOS structures of Kane-type semiconductors under weak and strong electric field limits assume, respectively, the following forms:

$$N_s = l_0 k_B T \sum_{n=0}^{n_{\max}} [(1+\tfrac{2}{3}\alpha\epsilon_n) F_0(\eta_n) + 2\alpha k_B T F_1(\eta_n)], \quad (6a)$$

$$N_s = l_0 k_B T \sum_{n=0}^{n_{\max}} [(1+2\alpha\epsilon_n) F_0(\eta_n) + 2\alpha k_B T F_1(\eta_n)], \quad (6b)$$

$$C_g = e^2 l_0 (\Delta_1) \sum_{n=0}^{n_{\max}} [(1+\tfrac{2}{3}\alpha\epsilon_n) F_{-1}(\eta_n) + 2\alpha k_B T F_0(\eta_n)], \quad (7a)$$

and

$$C_g = e^2 l_0 (\Delta_2) \sum_{n=0}^{n_{\max}} [(1+2\alpha\epsilon_n) F_{-1}(\eta_n) + 2\alpha k_B T F_0(\eta_n)], \quad (7b)$$

where the energy corresponding to the bottom of the nth electric subband as measured from the edge of the conduction band at the surface for both the limits can, respectively, be expressed through the equations

$$\alpha\epsilon_n(1+\alpha\epsilon_n) - [3k(n)(\alpha\epsilon_n + \tfrac{1}{2})]^{2/3} = 0 \quad (8a)$$

and

$$\alpha\epsilon_n(1+\alpha\epsilon_n) - 2k(n) = 0, \quad (8b)$$

$$\Delta_1 \equiv \left(1 + l_0 \sum_{n=0}^{n_{\max}} \{[(1+\tfrac{2}{3}\alpha\epsilon_n) F_{-1}(\eta_n) + 2\alpha k_B T F_1(\eta_n)][(t_1 + e^2 d_{\text{ins}} \epsilon_{\text{ins}}^{-1}) - \tfrac{2}{3}\alpha k_B T F_0(\eta_n) t_1]\} \right)^{-1},$$

$$t_1 \equiv 2N_s^{-1} 3^{-1/3}\{k(n)\}^{2/3} \times (\alpha\epsilon_n + \tfrac{1}{2})^{2/3}[\alpha(1+2\alpha\epsilon_n) - \tfrac{2}{3}\alpha(1+\alpha\epsilon_n)^{-1/3}\{3k(n)\}^{2/3}]^{-1},$$

$$\Delta_2 \equiv \left(1 + l_0 \sum_{n=0}^{n_{\max}} \{[(1+2\alpha\epsilon_n)F_{-1}(\eta_n) + 2\alpha k_B T F_1(\eta_n)][(t_2 + e^2 d_{\rm ins}\epsilon_{\rm ins}^{-1}) - 2\alpha k_B T F_0(\eta_n) t_2]\}\right)^{-1},$$

and

$$t_2 \equiv 2k_n[\alpha N_s(1+2\alpha\epsilon_n)]^{-1}.$$

It may be mentioned in this context that Eqs. (6a) and (6b) were derived for the first time by Chakravarti *et al.*[13(a)] Besides, the expressions of C_g for both weak and strong electric field limits were derived by Choudhury *et al.*[5] in different forms together with various approximations. For $\alpha \to 0$, as for inversion layers on parabolic semiconductors, the above equations are further simplified to[13(b)]

$$N_s = l_0 k_B T \sum_{n=0}^{n_{\max}} [F_0(\eta_n)] \tag{9}$$

and

$$C_s = l_0 e^2 \left(\sum_{n=0}^{n_{\max}} F_{-1}(\eta_n)\right)\left[1 + \sum_{n=0}^{n_{\max}} F_{-1}(\eta_n) \times \left(\frac{e^2 d_{\rm ins}}{\epsilon_{\rm ins}} + \frac{2}{3}\frac{g_0(n)}{N_s}\right)\right]^{-1}, \tag{10}$$

where

$$g_0(n) \equiv (\tfrac{3}{2}\pi e^2 N_s \hbar/\epsilon_{\rm sc}\sqrt{2m_0^*})^{2/3} n',$$

$\epsilon_{\rm sc}$ is the semiconductors permittivity $n' \equiv (n + \frac{3}{4})^{2/3}$, and $\eta_n \equiv (k_B T)^{-1}[E_F - g_0(n)]$.

RESULTS AND DISCUSSION

Using Eqs. (4) and (5) and taking the parameters[14,15]

$$E_g(x) = [-0.304 + 5\times 10^{-4}T + (1.914 - 10^3 T)x]eV,$$

$$m_0^*(x) = [3\hbar^3 E_g(x)/4P^2(x)],$$

$$P(x) = [\hbar^2(18+3x)/2m_0]^{1/2},$$

and

$$\epsilon_{\rm sc}(x) = (20.262 - 14.812x + 5.2795x^2)\epsilon_0,$$

as appropriate for $Hg_{1-x}Cd_xTe$, we have plotted the gate capacitance of n-channel inversion layers on $Hg_{1-x}Cd_xTe$ for $x = 0.21$ as a function of surface electric field at 4.2 K taking $\epsilon_{\rm ins} = 2.8\epsilon_0$ (Ref. 16) (the permittivity of Mylar, for example, which is commonly used as the equivalent of the oxide material in MOS structures of small-gap semiconductors) for $d_{\rm ins} = 15\,\mu$m as shown in Fig. 1 under weak electric Eqs. (6a) and (7a) for the purpose of comparison. In Fig. 2,

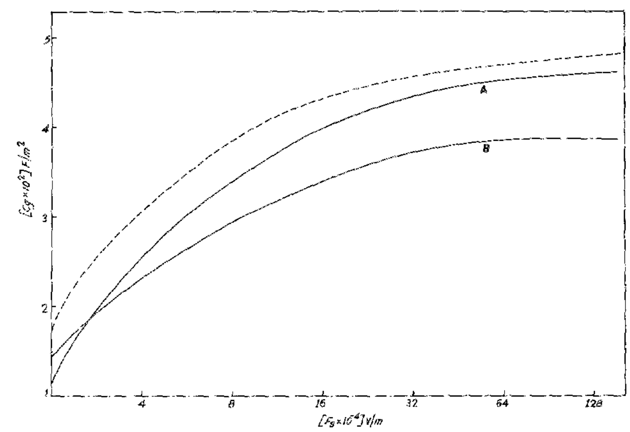

FIG. 1. Curve A is the plot of gate capacitance as a function of surface electric field under weak electric field limit in n-channel inversion layers on $Hg_{1-x}Cd_xTe$ using Eqs. (7a) and (6a), respectively. Curve B exhibits the same capacitance according to the generalized equations. The dotted curve corresponds to inversion layers on parabolic semiconductors.

data similar to that shown in Fig. 1 for low electric field limits have been plotted for the high electric field limit by using Eqs. (4), (5), (6b), and (7b), respectively. In both the figures the dotted curves correspond to the same dependence in inversion layers on parabolic semiconductors. It may be stated in this context that since most of the electrons occupy the lowest electric subband at low temperatures where the quantum effects become prominent, it is sufficiently accurate at such temperatures[17] to consider occupation of only the lowest electric subband, and we have taken the index $n = 0$ for the subsequent numerical computations. It appears from both the figures that the gate capacitance increases with increasing surface field, showing a tendency of saturation at relatively high values of the surface field. Besides, the approximated results overestimate the value of the gate capacitance for both the limits. It may also be noted that the variations shown in the figures are in good qualitative agreement with the experimental observation as reported

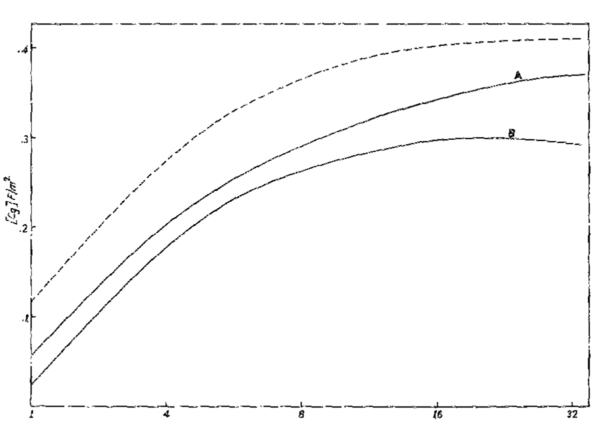

FIG. 2. Curve A is the plot of the gate capacitance as a function of surface electric field under strong electric field limit in n-channel inversion layers on $Hg_{1-x}Cd_xTe$ by using Eqs. (7b) and (6b), respectively. Curve B exhibits the same capacitance according to the generalized equations. The dotted curve corresponds to the same dependence in inversion layers on parabolic semiconductors.

elsewhere.[18] However, the present numerical calculation is valid for $x > 0.17$, since for $x < 0.17$ the band gap becomes negative in $Hg_{1-x}Cd_xTe$, leading to a semimetallic state, although the theoretical results can be used for n-channel inversion layers on small-gap semiconductors whose energy band structures are defined by the two-band Kane model.

It may also be stated that, as far as the determination of the effective mass under degenerate electron distribution at the surface is concerned, measurement of the gate capacitance as compared to that of conductivity experiment would not be more advantageous, considering the experimental facilities required or accuracies achieved. Nevertheless, it is felt that the theoretical investigation presented here would be of much significance, as the interest on gate capacitance has been growing very much in recent years from the point of view of technical applications and of exploration of other fundamental aspects of semiconductor surfaces in MOS structures. Although in a more rigorous treatment the method of achieving the self-consistent solution, the many-body effects, the hot-electron effects, effects of surface states and charges, and the formation of band tails in degenerate semiconductors should properly be considered, this simplified triangular potential-well approximation exhibits the basic features of gate capacitance of MOS structures. It may finally be noted that the basic purpose of the present work is not solely to demonstrate the effect of surface electric field on the gate capacitance, but also to formulate the electron statistics in its most generalized form for n-channel inversion layers on small-gap semiconductors having Kane-type energy bands, since the various transport phenomena and the derivation of the expressions for many important electronic properties of 2D semiconductors devices are based on the electron statistics in such materials.

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