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A SIMPLE THEORETICAL ANALYSIS OF THE MAGNETO–GATE CAPACITANCE IN MOS STRUCTURE OF p–CHANNEL INVERSION LAYERS ON TELLURIUM

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An attempt is made to study the gate capacitance of MOS structure of p-channel inversion layers on tellurium in the presence of a quantizing magnetic field by considering all types of anisotropies of the valence bands of tellurium within the framework of $\vec{k} \cdot \vec{p}$ theory. We have derived an analytical expression of the surface electron concentration in low electric field limit in the presence of a quantizing magnetic field. We have then formulated a model expression of the magneto-gate capacitance with the proper use of the electron concentration. For the purpose of relative comparison, we have also derived the same capacitance by including the broadening effects and without any approximations of low or high electric field limits. It has been observed that the gate capacitance of p-channel inversion layers on tellurium exhibits spiky oscillations with changing magnetic field. The corresponding well-known results for p-channel inversion layers on parabolic energy bands have also been obtained under certain limiting conditions from the generalized expressions.

1. Introduction

In recent years, there has been considerable interest in the study of semiconductor inversion layers which are formed at the surfaces of semiconductors in devices under the influence of a sufficiently strong electric field, applied perpendicularly to the surface in the presence of a large gate bias [1]. In such layers, the carriers form a two-dimensional gas and are free to move parallel to the surface while their motion is quantized in a direction perpendicular to it, leading to the formation of electric sub-bands. This quantized motion gives rise to many special features of MOSFET devices. One such important feature is the capacitance of MOS structures, since its dependence on the surface electric field becomes oscillatory in the presence of a quantizing magnetic field. The fact that the gate capacitance can be easily controlled by varying the gate voltage is of much importance from the point of view of technical considerations. Incidentally, it may be stated in this context that, though there has been considerable work on the magneto-transport in inversion layers in MOS structure of tellurium [1], the gate capacitances in these structures have yet to be investigated. It would, therefore, be of much interest to study the effect of magnetic quantization on the gate capacitance of MOS structures of tellurium by using the generalized band model, since the above class of materials is increasingly used for different technical applications [2].

In what follows, we shall first derive the model expressions for gate capacitance of MOS structures of p-type Te under magnetic quantization. This will make our study a generalized one, since we can obtain the corresponding expressions for p-channel inversion layers on parabolic semiconductors under certain limiting conditions. However, we shall consider the low-electric-field limit since the creation of large surface field is experimentally difficult. Besides, we shall also derive the gate capacitance by including the broadening effects. We shall then investigate, theoretically, the effect of a quantizing magnetic field on the gate capacitance.

2. Theoretical background

In MOS structures, the gate capacitance per unit area is given by

$$C_g^{-1} = C_{ins}^{-1} + C_{sc}^{-1}, \tag{1}$$

where $C_{ins} = \epsilon_{ins}/d_{ins}$, ϵ_{ins} and d_{ins} are the permittivity and the thickness of the insulating layer, respectively,

$$C_{sc} = e\frac{\mathrm{d}}{\mathrm{d}V_0}[N_s] = e\frac{\mathrm{d}p_s}{\mathrm{d}V_g}\left(1 - \frac{ed_{ins}}{\epsilon_{ins}}\frac{\mathrm{d}p_s}{\mathrm{d}V_g}\right)^{-1}. \tag{2}$$

e is the magnitude of the carrier charge, p_s is the hole concentration per unit area, $V_0 = V_g - (ep_s d_{ins}/\epsilon_{ins})$ is the surface potential and V_g is the gate voltage. It appears, therefore, that the derivation of the magneto-gate capacitance, with the help of Eq. (1), requires an expression of the total hole concentration under magnetic quantization as a function of the gate voltage which, in turn, is determined by the corresponding two-dimensional hole-energy spectra. Incidentally, it may be noted in this context that the detailed structure of the energy bands near H point of Te was derived by many authors [2]. All of them used a $\vec{k}\cdot\vec{p}$ perturbation considering the coupling of the upper two branches of the valence band. Non–parabolic valence band terms ($\sim k^4$) are given by a second order interaction between the vH4, vH5, vH61, vH62 states.

The energy spectra of the holes in valence bands of bulk specimens of Te can be expressed as [2]

$$E = Ak_\perp^2 + Bk_z^2 + \beta k_\perp^4 + \beta' k_\perp^2 k_z^2 - 2|\Delta_1| \pm$$

$$\left[(2|\Delta_1| + \eta k_\perp^2 + \zeta k_\perp^4 + \zeta' k_\perp^2 k_z^2)^2 + S^2 k_z^2\right]^{1/2}, \tag{3a}$$

where E is the total hole energy as measured from the top of the upper valence band in the downward direction in the absence of any quantization, S is the first-order $\vec{k}\cdot\vec{p}$ term, $|\Delta_1|$ is the first-order spin–orbit term, A, B, β, β', η, ζ and ζ' contain different contributions of first- and second-order $\vec{k}\cdot\vec{p}$, first-order spin–orbit and second-order spin–orbit $\vec{k}\cdot\vec{p}$ interaction with $\vec{k}$–independent spin–orbit interaction terms, and $k_\perp^2 = k_x^2 + k_y^2$. Thus, in the presence of a quantizing magnetic field B_0 applied along the crystal axis, the modified hole energy spectra can be written as

$$E_n = a(n) + b(n)k_z^2 \pm \sqrt{\left[c(n) + d(n)k_z^2\right]^2 + e_1 k_z^2}, \tag{3b}$$

where E_n is the total energy in the presence of magnetic field as measured from the top of the upper valence band in the downward direction in the absence of any quantization,

$$a(n) = -\frac{2eB_0 A}{\hbar}\left(n + \frac{1}{2}\right) - 2(|\Delta_1|) + \beta\left[\frac{2eB_0}{\hbar}\left(n + \frac{1}{2}\right)\right]^2.$$

e is the carrier charge, $\hbar = h/2\pi$, h is the Planck's constant, $n(= 0, 1, 2, ...)$ is the magnetic quantum number,

$$b(n) = B - \frac{2eB_0\left(n + \frac{1}{2}\right)\beta'}{\hbar},$$

$$c(n) = 2|\Delta_1| - \frac{2\eta eB_0}{\hbar}\left(n + \frac{1}{2}\right) + \zeta\left[\frac{2eB_0}{\hbar}\left(n + \frac{1}{2}\right)\right]^2,$$

$$e_1 = S^2 \ \text{ and } \ d(n) = -\frac{2eB_0\zeta'}{\hbar}\left(n + \frac{1}{2}\right).$$

Thus, the carrier energy spectra in p–channel inversion layers of the above class of materials in the presence of a uniform DC quantizing magnetic field, B_0, along c–axis can be expressed, in low electric field limit, as

$$\frac{\alpha_1(n)}{3}\left[T_1(n) \pm 2\alpha_2(n)\sqrt{T_1(n)} + \alpha_3(n)\right]^{3/2}$$

$$\pm\frac{\alpha_1(n)\alpha_2(n)}{2}\left[\left(\sqrt{T_1(n)} \pm \alpha_3(n)\right)\left(T_1(n) \pm 2\alpha_2(n)\sqrt{T_1(n)} + \alpha_3(n)\right)^{1/2}\right.$$

$$\left.+\alpha_4(n)^2 \log\left|(\sqrt{T_1(n)} \pm \alpha_2(n)) + \left(T_1(n) \pm 2\alpha_2(n)\sqrt{T_1(n)} + \alpha_3(n)\right)^{1/2}\right|\right]$$

$$-\frac{\alpha_1(n)}{3}\left[T_3(n) \pm 2\alpha_2(n)\sqrt{T_3(n)} + \alpha_3(n)\right]^{3/2}$$

$$\mp\frac{\alpha_1(n)\alpha_2(n)}{2}\left[\left(\sqrt{T_3(n)} \pm \alpha_3(n)\right)\left(T_3(n) + \alpha_3(n) \pm \sqrt{T_3(n)}2\alpha_2(n)\right)^{1/2}\right.$$

$$\left.+\alpha_4(n)^2 \log\left|(\sqrt{T_3(n)} \pm \alpha_2(n)) + \left(T_3(n) \pm 2\alpha_2(n)\sqrt{T_3(n)} + \alpha_3(n)\right)^{1/2}\right|\right]$$

$$= \frac{2S_i^{3/2}}{3}, \tag{4}$$

where

$$\alpha_1(n) = \frac{p_2(n)}{T_2(n)^{3/2} eF_s}.$$

F_s is the surface electric field, $p_2(n) = b(n)[-b^2(n) + d^2(n)]^{-1}$, $T_2(n) = t_2(n)[-4b^2(n) + 4d^2(n)]^{-1}$, $t_2(n) = 2e_1 b(n) - 4b(n)c(n)d(n) + 4d^2(n)a(n) - 4d^2(n)E_{ni}$, E_{ni} is the hole energy under magnetic quantization as measured from the edge of the valence band at the surface in the absence of any quantization,

$$\alpha_2(n) = \frac{T_2(n)}{2p_2(n)}, \quad T_1(n) = \frac{t_1(n)}{4b^2(n) - 4d^2(n)},$$

$$t_1(n) = [e_1^2 + 4a(n)b(n)e_1 - 8a(n)b(n)c(n)d(n) - 4e_1c(n)d(n)$$

$$+4b^2(n)E_{ni}a(n) - 2e_1E_{ni}b(n) + 4b(n)c(n)d(n)E_{ni} + 4E_{ni}2d^2(n)$$

$$+4a^2(n)d^2(n) - 8d^2(n)a(n)E_{ni} + 4b^2(n)c^2(n)],$$

$$\alpha_3(n) = \frac{p_1(n)T_2(n) - p_2(n)T_1(n)}{p_2(n)},$$

$$p_1(n) = \frac{a(n)b(n) + (e_1/2) - c(n)d(n) - b(n)E_{ni}}{b^2(n) - d^2(n)},$$

$$\alpha_4^2(n) = \alpha_3(n) - 4\alpha_2^2(n),$$

$$T_3(n) = \frac{p_1^2(n)T_2(n) - 2p_1(n)p_2(n)T_1(n)}{T_2(n) - 2p_1(n)p_2(n)}.$$

$i = 0, 1, 2, ...$ is the electric sub–band index and s_i are the zeros of Airy function.

Under the conditions $A = B = \hbar/2m^*$ (m^* is the effective mass at the band edge), $\beta = 0$, $\beta' = 0$, $|\Delta_1| = 0$, $\eta = 0$, $\zeta = 0$, $\zeta' = 0$ and $s = 0$, Eq. (4) assumes the form

$$E_{ni} = \left(n + \frac{1}{2}\right)\hbar\omega_0 + S_i\left(\frac{\hbar e F_s}{\sqrt{2m^*}}\right)^{2/3} \tag{5}$$

where $\omega_0 = eB_0/m^*$. We wish to note that Eq. (5) is the well–known relation for the carrier energy in inversion layers on parabolic semiconductors under magnetic quantization [1].

Therefore, the density–of–states function can be written as

$$D(E) = \frac{eB_0 g_s g_v}{h}\sum_{n,i}\delta'(\epsilon - E_{ni}), \tag{6}$$

where g_s is the spin degenerancy, g_v is the valley degenerancy and δ' is the Dirac's delta function. Combining Eq. (6) with the Fermi–Dirac occupation probability factor and using the property of delta function, the surface hole concentration per unit area can be expressed as

$$p_s = \frac{eB_0 g_s g_v}{h}\sum_{n,i}\left[1 + \exp\left(\frac{E_{ni} - E'_{FBO}}{k_B T}\right)\right]^{-1}, \tag{7}$$

where k_B is the Boltzmann constant, T is the temperature, E'_{FBO} is the Fermi energy under magnetic quantization as measured from the edge of the valence bands at the surface in the absence of any quantization and is given by

$$E'_{FBO} = eV_g - p_s e^2\frac{d_{ins}}{\epsilon_{ins}} - E_{fbB_0}, \tag{8}$$

in which E_{fbB_0} represents the energy separation between the Fermi level at the edge of the valence band in the bulk of the n–type substrate material in the presence of a quantizing magnetic field. Equation (7) can be written as

$$p_s = \frac{eB_0 g_s g_v}{h} \sum_{n,i} F_{-1}(\overline{\eta}), \tag{9}$$

where $\overline{\eta} = (E'_{FB_0} - E_{ni})/k_B T$ and $F_j(\overline{\eta})$ is the one–parameter Fermi–Dirac integral of order j [3].

Thus, combining Eqs. (1) and (9), the generalized expression for the gate of MOS structures of p–type Te under magnetic quantization can be written as

$$c_g(B_0) = \frac{e^2 \overline{\zeta}_0 \sum_{n,i} F_{-2}(\overline{\eta})}{1 + \overline{\zeta}_0 \sum_{n,i} p(n) F_{-2}(\overline{\eta})}, \tag{10}$$

where

$$\overline{\zeta}_0 = \frac{eB_0 g_s g_v}{hk_B T},$$

$$p_n = \rho(n) + e^2 \frac{d_{ins}}{\epsilon_{ins}}$$

and

$$\rho(n) = \frac{\partial}{\partial p_s}(E_{ni}),$$

which can be obtained by using Eq. (4).

It may be noted that under the conditions $A = B = \hbar^2/2m^*$, $\beta = 0$, $\beta' = 0$, $|\Delta_1| = 0$, $\eta = 0$, $\zeta = 0$, $\zeta' = 0$ and $S = 0$, the form of the magneto-gate capacitance for p–channel inversion layers of parabolic semiconductors is expressed by the same Eq. (10), where

$$\rho(n) = \frac{2}{3} p_s^{-1/3} \left(\frac{\hbar e^2}{\epsilon_{sc}\sqrt{2m^*}} \right)^{2/3} S_i.$$

Incidentally, in the presence of broadening effects the density-of-states function of the carriers in 2D inversion layers on semiconductors can, in general, be expressed [1]

$$D(\epsilon) = \frac{eB_0 g_s g_v}{h} \sqrt{\frac{2}{\pi}} \sum_{n,i} \Gamma_n^{-1} \exp\left(\frac{-2(\epsilon - \epsilon')^2}{\Gamma_n^2} \right), \tag{11}$$

where Γ_n is the line width of the broadened Landau levels and ϵ' is the unperturbed energy eigenvalue which in the present case can be determined from the equation

$$\epsilon' = a(n) \pm c(n). \tag{12}$$

Thus, combining Eq. (11) with the Fermi–Dirac occupation probability factor, the surface hole concentration can be expressed as

$$p_s = K_0 \sum_{ni} \frac{X_0}{\Gamma_n}, \tag{13}$$

where

$$K_0 = \frac{eB_0 g_s g_v}{h} \sqrt{\frac{2}{\pi}} k_B T,$$

$$X_0 = \sum_{t=0}^{\infty} Y_+(t) + \sum_{t=1}^{\infty} Y_-(t) - \frac{\gamma\sqrt{\pi}}{2} \left(1 - \mathrm{erf}(U)\right),$$

$$Y_\pm(t) = \sqrt{2\pi} \frac{\gamma}{2} \exp(\overline{Y}_{\prime\pm}) L \left(1 \mp \mathrm{erf}(\overline{Y}^2_{\prime\pm})\right),$$

$$L = (-1)^t \exp(-U^2), \;\; U = \frac{\eta'}{\gamma}, \;\; \gamma = \frac{\Gamma_n}{k_B T \sqrt{2}},$$

$$\eta' = \frac{E'_{FBO} - \epsilon'}{k_B T}, \overline{Y}_{\prime\pm} = \frac{\gamma}{2}(2U\gamma^{-1} \pm t)$$

and erf denotes the error function [4]. Thus, using the appropriate equation, the magneto-gate capacitance for p–channel inversion layers on Te can be expressed including broadening effects as

$$c_g(B_0) = \frac{\alpha_0 \sum_{n,i} \beta_0 (\Gamma_n)^{-1}}{1 + (e\alpha_0 d_{ins}/\epsilon_{ins}) \sum_{n,i} \beta_0 (\Gamma_n)^{-1}}, \tag{14}$$

where

$$\alpha_0 = \frac{eK_0}{k_B T}, \;\; \beta_0 = \exp(-U^2) + \sum_{t=0}^{\infty} Q_{1,+} + \sum_{t=1}^{\infty} Q_{1,-}$$

and

$$Q_{1,\pm} = L\gamma^2 \sqrt{\pi} (1 \mp \mathrm{erf}(\overline{Y}_{\prime\pm})) \overline{Y}_\pm \mp L\gamma^2 - UL \exp(\overline{Y}^2_{\prime\pm})(1 \mp \mathrm{erf}(\overline{Y}_{\prime\pm})).$$

It may also be noted that the general expression for the carrier statistics and the gate capacitance in inversion layers on parabolic semiconductors under magnetic quantization, including broadening effects, will be given by Eqs. (13) and (14), where

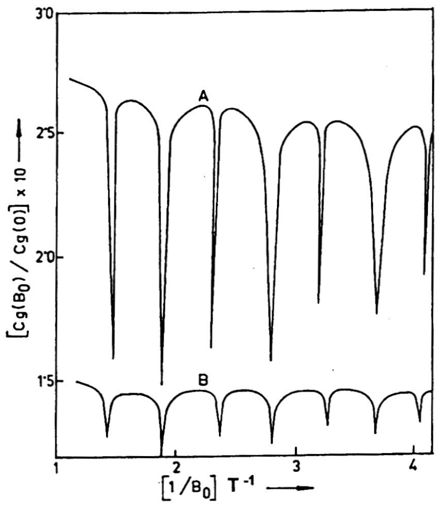
$$\epsilon' = \left(n + \frac{1}{2}\right) \hbar\omega_0. \tag{15}$$

3. *Results and discussion*

Using Eqs. (9) and (10) and taking the parameters [2] $A = -2.57 \times 10^{19}$ eVm^2, $B = -4.09 \times 10^{-19}$ eVm^2, $\beta' = 0$, $g_s = 2$, $g_v = 2$, $\beta = 1.1 \times 10^{-37}$ eVm^4, $2|\Delta_{|}| = 6.315 \times 10^{-2}$ eV, $\eta = -1.18 \times 10^{-19}$ eVm^2, $\zeta = 4 \times 10^{-32}$ eVm, $\zeta' = 0$, $|S| = 2.62 \times 10^{-10}$ eVm, $\epsilon_{sc} = 30\ \epsilon_0$, $d_{ins} = 15$ μm as appropriate for p-Te together with $F_s = 5.6 \times 10^4$ V/m and $\epsilon_{ins} = 2.8\ \epsilon_0$ (the permittivity of Mylar, for example, which is commonly used as the equivalent of the oxide layer in non-parabolic MOS structures), we have plotted -$C_g(B_0)/C_g(0)$ versus $1/B_0$ at 4.2 K as shown in plot A of Fig. 1. Plot B shows the same dependence in accordance with the parabolic band model.

Using the same parameters as used in obtaining Fig. 1 together with $\Gamma_n = 10^{-3}\sqrt{B_0(\mathrm{T})}$ [1], and using Eqs. (13) and (14), we have plotted $C_g(B_0)/C_g(0)$ by including broadening effects, shown in plot A of Fig. 2. The plot B in Fig. 2 exhibits the same dependence for the parabolic model. The depths of the spikes increase with increasing magnetic field. With varying magnetic field, each time a Landau level crosses the Fermi level, a change occurs in the capacitance through redistribution of the carriers among the Landau levels. It may be noted that the 3D quantization, in the absence of broadening of Landau levels, leads to the discrete energy levels, somewhat like atomic energy levels in steps produce very sharp changes. This follows from the inherent feature of the 3D quantization of the 2D hole gas delt with here. Under such quantization, there remains no free hole state in between any two successive Landau levels, unlike that found for 3D hole gases of semiconductors under 2D quantization in the $\vec{k}$ space in the presence of a quantizing magnetic field. Consequently, the crossing of the Fermi level by the Landau level under 3D quantization would have much greater impact on the redistribution of the holes amongst the available states, as compared to that found for 2D quantization. It is basically this impact which results in the increased sharpness of the oscillatory spikes for both models of Te. Incidentally, the collision broadening effects which have been neglected in the theoretical formulation shown in Fig. 1, would, really, reduce the sharpness of the oscillatory spikes. Thus, to assess the influence of broadening, we have plotted the same dependence in Fig. 2. In the presence of broadening, the basic physics behind 3D quantization is not applicable. Hole motion becomes possible in broadened sub-bands and thus the broadening parameter changes the analytical expressions of the hole statistics and magneto-gate capacitance, respectively.

It may be noted that Eqs. (8), (9), (13) and (14) are the generalized expressions for the hole statistics and the magneto-gate capacitance, both in the presence and absence of broadening effects, respectively, in p-channel inversion layers on Te under magnetic quantization. For inversion layers on parabolic semiconductors, the general forms of the above equations will be unaltered. The above facts are true only for 2D hole gases in inversion layers under magnetic quantization. Since the basic physics behind the broadening of Landau levels in inversion layers under magnetic quantization is radically different as compared to 3D quantization, we can not obtain the results valid for 3D quantization from the corresponding expressions for broadening under the condition $\Gamma_n \to 0$. That the above conclusion is not true for bulk semiconductors under magnetic quantization has been shown in Ref. 5. Thus, the results which are valid for $\Gamma_n \neq 0$ are not valid for $\Gamma_n = 0$, and are true only for 2D carrier gases in inversion layers under magnetic quantization. It appears from Fig. 2 that even in the presence of broadening, the numerical magnitude of the magneto-gate capacitance in p-channel inversion layers of Te are larger as compared to parabolic model, and the nature of oscillations is found to be somewhat similar to that observed experimentally in Te MOS structures having p-channel inversion layers [2].



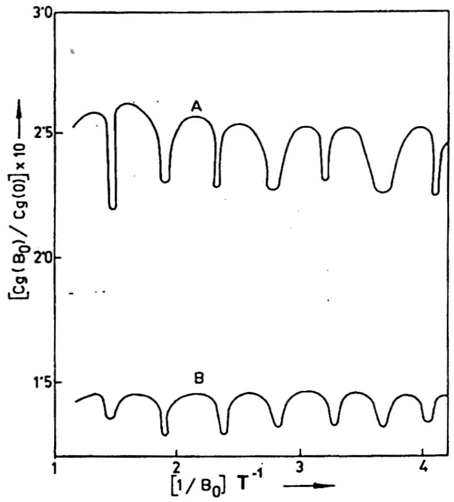


Fig. 1. Plot A shows the magnetic-field dependence of the normalized gate capacitance of MOS structures having p-channel inversion layers under magnetic quantization in the absence of broadening. The plot B corresponds to the parabolic model.

Fig. 2. Plot A shows the magnetic field dependence of the normalized gate capacitance of MOS structures of Te *having p-channel inversion layers under magnetic quantization in the presence of broadening effects. The plot B corresponds to parabolic energy bands (right).*

It may also be noted that, as far as the determination of the effective mass under degenerate carrier distribution at the surface is concerned, the measurement of magneto-gate capacitance, as compared to that of the conductivity or cyclotron resonance, would not be more advantageous regarding 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 fundamental aspects of semiconductor surfaces in MOS structures. It may be noted that since the many-body effects, the carrier-spin, the arbitrary orientation of the quantizing magnetic field, the formation of band-tails, the hot-electron effects and the dependence of Γ_n on other various physical parameters have not been considered in obtaining both plots, therefore, the essential meaning of comparison of the gate-capacitance between the two models would not be meaningless, and this simplified analysis exhibits the basic qualitative features of the oscillatory magneto-gate capacitance in p-channel MOS structures of Te. For a more accurate derivation, the modifications as mentioned above should be taken into account, which present formidable problems due to the lack of analytical techniques. Finally, it may be noted that the basic purpose of the present work is not solely to demonstrate the effects of magnetic quantization on the gate capacitance, but also to formulate the carrier statistics for p-channel inversion layers of Te, since the various transport phenomena and the derivation of the expressions for many important physical parameters of 2D semiconductors devices are based on the carrier statistics in such materials.

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JEDNOSTAVNA TEORIJSKA ANALIZA KAPACITANCIJE MAGNETSKIH VRATA U MOS STRUKTURI p-KANALNOG INVERZIJSKOG SLOJA NA TELURU

Proučavaju se kapacitancija vrata MOS strukture p–kanalnih inverzijskih slojeva na teluru u magnetskom polju na osnovi $\vec{k} \cdot \vec{p}$ teorije. Pokazuje se da kapacitancija vrata mijenja periodički s rastućim magnetskim poljem. Dobiveni rezultati svode se u modelu paraboličkih vrpci, uz određene uvjete, na poznate izraze.