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On the evaluation theory of C - V measurements on narrow gap semiconductor MIS structures

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Résumé. — On a développé et utilisé un modèle théorique pour évaluer les courbes expérimentales capacité-voltage dans des structures MIS réalisées sur des semiconducteurs avec une bande interdite étroite. On a discuté et démontré l'influence de certains facteurs sur le comportement des courbes C - V théoriques et sur la densité des états d'interface, comme l'utilisation de la statistique de Fermi-Dirac, l'ionisation incomplète et la recharge des dopants, le caractère non parabolique de la zone de conduction.

Abstract. — A theoretical model for evaluating experimental capacitance — voltage curves on narrow — gap semiconductor (NGS) MIS structures is developed. The features of NGS are taken into account. Demonstrated and discussed is the effect of utilizing Fermi-Dirac statistics, incomplete ionization and recharging of dopants and conduction band nonparabolicity on the behaviour of theoretical C - V curves and interface state density assessment. The analysis so conducted shows that these features must be accounted in C - V analysis of NGS MIS structures. Otherwise incorrect densities of interface states distributed across the band-gap of the semiconductor are obtained.

1. Introduction.

The preparation of metal-insulator-semiconductor (MIS) structures based on narrow-gap semiconductors (NGS) has considerably succeeded recently. This is stimulated by the efforts for producing basic elements of various infrared imaging devices [1, 2]. From a fundamental point of view MIS structures appear as a tool for investigating the quasi-two-dimensional systems in the potential well at NGS-insulator interface [3, 4] and the interface itself [5-7] whose nature is far from common satisfactory explanation yet [8].

The performance of MIS devices relies strongly on the electrical properties of the insulator-semiconductor interface. Commonly as an interface characteristics is utilized the density distribution of the localized states across the band-gap of the semiconductor. The interface state spectra are obtained from the comparison of a measured C - V curve with a theoretical one. The computation of the theoretical C - V curve requires a model of an ideal structure to be developed assuming

all basic semiconductor features and differing from the real one through the absence of interface states only.

Thus in the case of NGS must be considered the nonparabolicity of the conduction band, the recharging of the dopants at low temperatures, degenerate statistics, tunnelling and surface quantization [6, 9, 10]. Hence, the development of a model for the analysis of the space-charge region in an ideal NGS MIS structure considers effects that in the theory of conventional silicon MOS devices need not be taken into account.

In this paper we propose a theoretical model of NGS MIS structure which is applied to evaluate C - V data obtained on InSb MIS structures. Both low frequency (LF) and high frequency (HF) occasions are considered. A convenient algorithm and computer program were elaborated to calculate the ideal MIS C - V curves and to evaluate the measured data. Discussed and demonstrated is the effect of the NGS features taken into account. The analysis so conducted shows that these features must be accounted in C - V analysis of NGS MIS structures. Otherwise incorrect densities of interface

states distributed across the band-gap of the semiconductor are obtained.

2. Basic considerations.

For the calculation of the theoretical C-V curve it is necessary to know the dependence of the total charge density Q_{sc} in the semiconductor space-charge region on the surface potential ψ_s . The dependence $Q_{sc}(\psi_s)$ is determined from the numerical solution of the one-dimensional Poisson's equation [11]

$$\frac{d^2\psi}{dx^2} = -\frac{q}{\epsilon_s kT} \rho(x), \quad (1)$$

where $\rho(x)$ is the charge density in the semiconductor space-charge region, ϵ_s is the semiconductor permittivity, $\psi(x)$ is the normalized electrostatic potential in kT units,

$$\psi(x) = \frac{E_i(x) - E_{ib}}{kT}$$

(E_{ib} is the bulk intrinsic Fermi-level).

The boundary conditions for the solution of equation (1) of zero electric field in the substrate and a specified potential at the insulator-semiconductor interface are

$$\left. \frac{d\psi}{dx} \right|_{x \rightarrow \infty} = 0, \quad \psi_s = \psi(x)|_{x=0}. \quad (2)$$

The charge density in the semiconductor space-charge region that enters Poisson's equation (1) is

$$\rho = q[p - n + N_D^+ - N_A^-], \quad (3)$$

where p and n represent the free hole and electron concentrations, respectively. N_D^+ and N_A^- are the ionized donor and acceptor impurities concentrations, respectively.

Due to the specific conduction-band structure of NGS these materials become degenerate at moderate bulk or surface electron concentrations so that Fermi-Dirac statistics should be used when calculating n . Furthermore, the concentration of electrons is calculated taking into account the nonparabolicity of NGS conduction-band in the Kane approximation [12]

$$n = 2 \int_{E_c} N(E) f(E) dE, \quad (4)$$

where

$$N(E) = \frac{1}{2\pi^2} \left(\frac{2m_n}{\hbar^2} \right)^{3/2} \left(E + \frac{E}{E_g} \right)^{1/2} \left(E + \frac{2E}{E_g} \right)^{1/2} \quad (5)$$

and $f(E) = \frac{1}{1 + \exp\left(\frac{E - E_F}{kT} - \psi\right)}$ is Fermi distribution function.

m_n is the electron effective mass at the conduction-band edge and E_g is the band-gap. So, we obtain from equations (4) and (5)

$$n(\mu(\psi)) = \frac{(2m_n kT)^{3/2}}{3\pi^2 \hbar^3} J_n(\mu, \beta), \quad (6)$$

where $\mu(\psi) = \frac{E_F}{kT} + \psi$ is the normalized Fermi-level in the space charge region, $\beta = \frac{kT}{E_g}$ is the nonparabolicity parameter and $J_n(\mu, \beta)$ is generalized Fermi-integral of order $n = \frac{3}{2}$ [13].

With the use of Fermi-Dirac statistics the concentration of free holes is given by

$$p(\mu(\psi)) = \frac{(2m_p kT)^{3/2}}{2\pi^2 \hbar^3} F_{1/2}(\mu) \quad (7)$$

where m_p is the hole effective mass at the valence-band edge, $F_{1/2}(\mu)$ is Fermi-integral of order 1/2.

As the temperature decreases impurity freeze out can occur when band bending at the semiconductor surface forces the donor or acceptor impurity levels near to the Fermi-level. So, the incomplete ionization and recharging of dopants with the Fermi-level movement should be considered through the use of Fermi-Dirac statistics in the calculation of the ionized dopant concentrations in the space charge region, i.e.

$$N_A^- = N_A / \left[1 + \frac{1}{g} \exp(\epsilon_A - \mu) \right], \quad (8a)$$

$$N_D^+ = N_D / [1 + g \exp(\mu - \epsilon_D)], \quad (8b)$$

where ϵ_A and ϵ_D are the normalized acceptor and donor level energy positions and g is the spin degeneracy factor. All energy positions are counted from the band-gap middle, positive towards conduction-band.

So, including equations (6)-(8) in equation (1) results in more complicated solution of Poisson's equation. The first integration of Poisson's equation gives $Q_{sc}(\psi_s)$

$$Q_{sc}(\psi_s) = -\text{sign}(\psi_s) [2\epsilon_0 \epsilon_s kT \Phi(\psi_s)]^{1/2} \quad (9)$$

where

$$\begin{aligned} \Phi(\psi_s) = & \frac{(2m_n kT)^{3/2}}{3\pi^2 \hbar^3} [J_n^*(\mu_s) - J_n^*(\mu_b)] + \\ & + \frac{(2m_p kT)^{3/2}}{2\pi^2 \hbar^3} [F_{3/2}(\mu_s) - F_{3/2}(\mu_b)] \\ & - \psi_s(N_D - N_A) - N_D \ln \left[\frac{1 + g \exp(\mu_b - \epsilon_D)}{1 + g \exp(\mu_s - \epsilon_D)} \right] \\ & + N_A \ln \left[\frac{1 + \frac{1}{g} \exp(\epsilon_A - \mu_s)}{1 + \frac{1}{g} \exp(\epsilon_A - \mu_b)} \right], \end{aligned} \quad (10)$$

$$J_n^*(\mu) = \int_{\psi} n(\mu) d\psi \quad \text{and} \quad F_{3/2}(\mu) = \int_{\psi} p(\mu) d\psi.$$

μ_b is the bulk Fermi-level and μ_s is Fermi-level at the semi-conductor surface.

The simulation of the capacitance of MIS structure is obtained from the dependence $Q_{sc}(\psi_s)$ using the well-known relations between capacitance, surface potential and gate voltage in low frequency and high frequency approaches [11].

The LF C-V curves were computed under the assumption that minority carriers contribute fully to the capacity. Thus the LF semiconductor capacitance is

$$C_{sc} = -\frac{q}{kT} \frac{\partial Q_{sc}}{\partial \psi_s}. \quad (11)$$

The most commonly accepted approach for accurate HF case calculations is used, i.e. the depletion-charge approximation. In this approach the semiconductor depletion charge calculated from a solution of Poisson's equation is treated as a step-function. Once strong inversion is reached the charge per unit area due to the depletion of minority carriers saturates and the HF capacitance approaches a minimum value asymptotically [11].

Calculation of the surface potential ψ_s and its dependence on the applied voltage V_g is an essential step in the analysis. The LF Berglund's graphical integration [14] method is based on

$$\psi(V_g) = \int_{V_{acc.}}^{V_g} \left(1 - \frac{C_{LF}}{C_{ox}}\right) dv + \Delta, \quad (12)$$

where C_{LF} is the LF capacitance and C_{ox} is the insulator capacitance. The additive constant Δ may be evaluated by calculating the flat-band voltage and by alignment of the surface potentials corresponding to flat-bands in the experimental and theoretical curves.

The HF method for obtaining $\psi_s(V_g)$ is based on numerical inversion of the theoretical formula

$$C_{HF}(\psi_s) = f(\psi_s, E_g, T, C_{ox}, N_D). \quad (13)$$

In both LF and HF methods every deviation of the measured data from the ideal theoretical values is attributed to interface states distributed across the band-gap. The evaluation of interface state density distribution follows the well-known differentiation and integration methods in the AF and LF cases, respectively [11].

Some basic semiconductor parameters are needed for the computations. These are the semiconductor dielectric permittivity and the permittivity of the insulator, the semiconductor band-gap E_g , the Fermi-level in the bulk of the semiconductor, the effective masses of electrons and holes and acceptor and donor energy level position.

Bulk Fermi-level position in any particular case of fixed doping level N_D and N_A and temperature in the range 4.2-77 K is calculated from the solution of electroneutrality equation in the semiconductor bulk.

Moreover, Fermi-Dirac statistics, conduction-band nonparabolicity and incomplete ionization and recharging of dopants are considered. The intrinsic Fermi-level position for each temperature considered is calculated too. The computation used includes iterative techniques for numerical solution.

The temperature dependences of E_g , m_n and m_p must also be considered. We have utilized the graphical presentation of $E_g(T)$ from reference [15] and temperature dependences of the effective masses values from references [16, 17] in the range of 4.2-77 K. The intrinsic carrier density n_i is utilized in the calculations and its temperature dependence is taken into account. A numerical problem arises as temperature is reduced. The quantities n , p and n_i are all upon terms of the form $\exp(E/kT)$. At $T = 30$ K, $kT = 0.002585$ eV and the normalized gap is approximately $E_g = 93.46 kT$ placing $\exp\left(\frac{E_g}{2}\right)$ outside the range of most computer arithmetic. The use of logarithms and proper ordering of multiplications and divisions has allowed our programme to operate down to 4 K.

3. Results and discussion.

There are many factors that may introduce error into determination of interface characteristics. One of these is an incorrect ideal $C_{sc}(\psi_s)$ curve for evaluating C-V analysis. We have studied what sort of error can introduce an ideal C-V curve when NGS features here discussed are not taken into account.

An illustration of the result of applying degenerate statistics on the C-V behaviour is given in figure 1. The figure presents the capacitance in accumulation for n-type InSb MIS structure calculated using both Fermi-

Fig. 1. — Capacitance in accumulation versus surface potential for different statistics — curve 1 — — Fermi-Dirac statistics ; curve 2 — x — Maxwell-Boltzmann statistics.

Dirac and Maxwell-Boltzmann statistics for comparison. The particular parameters for the calculations are temperature of 77 K, acceptor concentration $N_A = 5.3 \times 10^{14} \text{ cm}^{-3}$ and oxide thickness $d_{ox} = 1400 \text{ Å}$. The surface charge concentration in the Maxwell-Boltzmann approximation grows exponentially towards infinity with ψ_s when in the Fermi-Dirac case the surface charge concentration saturates. The corresponding width of the space-charge region in the Maxwell-Boltzmann approximation is larger, the capacitance of the layer is smaller and the C-V curve in accumulation saturates slower. Analogous is the behaviour of the C-V curve in inversion in p-type substrate in the low frequency regime.

The effect of conduction-band nonparabolicity on the C-V behaviour is shown in figure 2. P-type material is considered in the LF regime. The two curves in the figure are calculated using parabolic and nonparabolic dispersion laws $E(k)$. The nonparabolicity of the conduction-band makes the increase of the capacitance in inversion up to the oxide capacitance to begin earlier in respect to ψ_s comparing with the C-V curve calculated for parabolic conduction band.

The results displayed in figure 1 and figure 2 show that the use of Fermi-Dirac statistics and conduction-band nonparabolicity leads to pronounced differences in the theoretical $C_{sc}(\psi_s)$ dependences as compared to the corresponding curves when NGS features are not accounted. It follows to be expected that this is going to have an effect upon the interface spectra evaluated with

Fig. 2. — Theoretical C-V curves for different dispersion laws — curve 1: parabolic conduction band; curve 2: nonparabolic conduction band.

Fig. 3. — Interface states distributions — curve 1 — . — with Fermi-Dirac statistics and nonparabolic conduction band; curve 2 — x — with Maxwell-Boltzmann statistics and parabolic conduction band.

the use of such theoretical curves. This is actually seen from figure 3. The figure presents two interface spectra calculated following two different approaches. A measured curve at 1 MHz and 77 K on the same n-type InSb sample as in figure 1 is utilized. Curve 1 is obtained using Maxwell-Boltzmann statistics and parabolic conduction-band dispersion law. Curve 2 is obtained using Fermi-Dirac statistics and nonparabolic conduction band. From the comparison of the two curves it is evident that degenerate statistics and conduction band nonparabolicity if no accounted (curve 1) would lead to a larger apparent interface state density.

4. Conclusion.

A theoretical model for evaluating experimental capacitance-voltage curves on narrow-gap semiconductor MIS structure is developed.

Theoretical capacitance-voltage curves of MIS structures on NGS considering Fermi-Dirac statistics, incomplete ionization and recharging of dopants and nonparabolic conduction band are calculated in the temperature range of 4.2 to 77 K and employed to evaluate interface state density distribution. The computed results are concerned to InSb MIS structures. Discussed

and demonstrated is the application of the developed model at 77 K. NGS features if no considered lead to apparent interface state density distribution higher than the real one. This is evidence of the worth of our model.

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