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STUDY OF THE DENSITY OF STATES DISTRIBUTION IN THE SiO_2/Si STRUCTURE

Interface properties of Al/SiO_2/Si MOS structures with NAOS oxide layer were analyzed by the construction of the capacitance-voltage model with the interface states. Energy distributions associated with the localized states in silicon band gap were modeled by the Gaussian distribution. Energy levels of localized states and the densities of interface states were determined. The results correspond with the results of the interface states study performed by the acoustic deep-level transient spectroscopy.

1. Introduction

High quality ultrathin SiO_2 layers with unique structural and electrical properties were prepared on n-type silicon substrate by the nitric acid oxidation of silicon method (NAOS) [1–3]. The interfacial properties between silicon and SiO_2 layer severely impact the carrier mobility and influence the electrical properties of the structure. The interface defects need to be well characterized in order to improve the quality of the whole semiconductor device. Chemical impurities or defects in periodical crystal lattice structure of silicon create the perturbations of the lattice. The periodicity of crystal lattice is important for the band structure properties. Many defects cause bound states in the energy band gaps of a given crystal. It is very difficult to calculate the energy levels of these bound states and, therefore, various specific approximations are used. The states in the band gap can be divided into shallow states close to the edges of the band gap and the deep states, which lie near the middle of the band gap. Defect states in the band gap influence the properties of the semiconductor by modifying the mobility of charge carriers and by acting like donors or acceptors.

Typical interface state densities in metal-oxide-semiconductor (MOS) structures can be on the order of 10^{11} – 10^{13} $eV^{-1}cm^{-2}$, depending on materials and processing. A simply way to evaluate the interface trap density includes capacitance-voltage (C–V) measurements at low frequencies. The leakage current in thin dielectric film disturbs these low frequency C–V measurements. In order to model the C–V curve including the interface state behavior, the energy distribution and frequency response of the interface state should be described properly.

In our work we constructed a simple physical model to describe frequency dependent C–V curves of Al/SiO_2/Si MOS structure with NAOS oxide layer and with interface states. The model is based on a superposition of several types of energy distributions describing the density of interface states which enables computation of the frequency response of these interface states.

2. Model of Capacitance curves for MOS Structure with Interface States

The total charge density in the semiconductor ρ is given by equation

$$\rho = q\left(p - n + N_d^+ - N_a^-\right) , \tag{1}$$

where p and n are hole and electron densities, N_d^+ and N_a^- are the densities of the ionized donors and acceptors, relatively. The total space charge density Q_S as a function of the surface potential Φ_S is shown in Fig. 1.

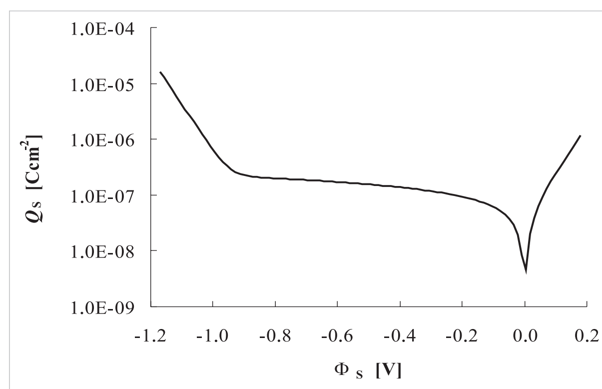

Fig. 1 The total space charge density Q_S in MOS structure

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Solution of the Poisson equation with this charge density leads to the capacitance of MOS structure without the interface states C_c [4]. Important electrical effect of the deep states in the band gap is the emission and capture of charge carriers. The defects play role of recombination and trapping centers, influence the carrier lifetimes and cause various transient processes. In the case of an n-type of semiconductor in deep depletion mode the presence of holes is negligible. Trap states interact only with electrons and define the semiconductor-oxide interface properties. Both neutral and positively charged traps can capture an electron. A negatively charged trap does not capture an electron; it remains negative and behaves as fixed charge in the MOS structure. Charge capture/emission processes connected with the interface states can be modeled by the equivalent effective capacitance C_{ite} associated with the interface states [5]

$$C_{ite} = \frac{dQ_{ite}}{d\Phi_S} = qD_{it} \tag{2}$$

where Q_{ite} is total charge at the effective interface state, Φ_S is a surface potential, q is an unit charge and D_{it} is the interface state density. We compute the D_{it} by superposition of several distributions

$$D_{it} = D_{itu} + D_{it\,exp} + \sum_i D_{it} G_i \tag{3}$$

Distribution D_{itu} describes the uniform distribution of interface states across the band gap of semiconductor

$$D_{itu} = D_u, \tag{4}$$

where D_u is constant. Distribution $D_{it\,exp}$ describes an exponential change of interface state density as the energy level becomes shallower to the band edge

$$D_{it\,exp} = D_{mid} \exp\left(\frac{E_t - E_i}{\alpha}\right), \tag{5}$$

where D_{mid} is the density of interface states at the midgap, α is constant, E_t and E_i are energy level and intrinsic Fermi level, respective. Distributions D_{itG} are used for the description of interface states localized in its energy levels. The Gaussian distribution is used in this work

$$D_{itG} = D_{G0} \exp\left(-\left(\frac{E_t - E_{t0}}{2\sigma}\right)^2\right). \tag{6}$$

Here, D_{G0} is the maximum energy of localized interface state, E_{t0} is the central energy of localized state, and σ is the standard deviation. We use superposition of several Gaussian distributions localized in different central energies E_{t0_i} with different maxima D_{G0_i} and standard deviations σ_i.

The capture/emission times of interface states affects the frequency response of the capacitance. The effective equivalent capacitance and interface state density determined experimentally change with energy level and frequency. We measured capacitance of MOS structure at various frequencies and we fitted experimental capacitances by theoretical models of capacitance curves with the interface states. These theoretical capacitances were computed by considering the equivalent circuit of actual MOS structure as shown in Fig. 2. The equivalent effective capacitance associated with the interface states C_{ite} and C_c is connected in parallel.

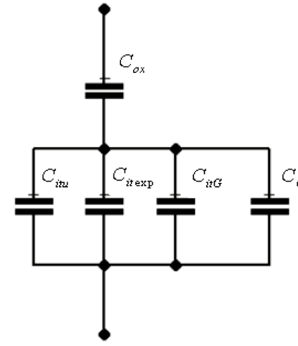

Fig. 2 Equivalent circuit for the MOS structure with interface states. C_{ox} is capacitance of NAOS oxide layer, C_{itu}, $C_{it\,exp}$ and C_{itG} are capacitances associated with D_{itu}, $D_{it\,exp}$ and D_{itG}, respectively

3. Experiment

Silicon MOS structure was prepared at n-type (10 Ωcm) Si(100) substrate. The substrate was cleaned by the RCA method and etched in diluted hydrofluoric acid. Ultrathin SiO_2 layer with ~2.5 nm thickness was then prepared by the NAOS method and finally the Al layer was formed. Electrical measurement of MOS capacitance was performed using FLUKE programmable automatic RCL meter at frequencies 1, 10, 100 and 1000 kHz.

4. Results and Discussion

The details of experimental C-V curves for given MOS structures are shown in Fig. 3. The influence of the interface states

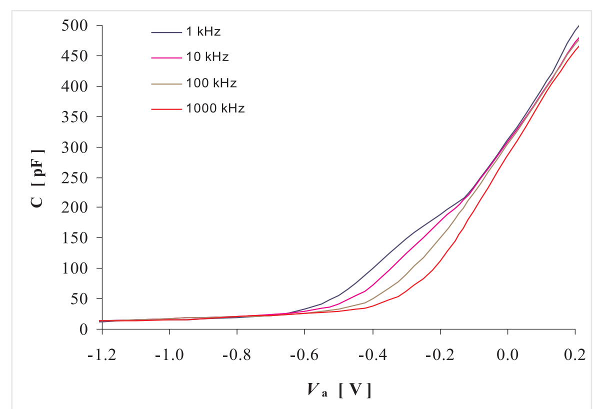

Fig. 3 C-V curves measured at Al/SiO_2/Si MOS structure with NAOS SiO_2 layer prepared at n-type silicon substrate

occurring at the semiconductor/oxide boundary can be observed in the depletion region of C-V curves. Experimentally determined MOS capacitance and theoretical model of MOS capacitance with the interface states at frequency $f = 1$ kHz are compared in Fig. 4.

Mean value of energy of localized states modeled by D_{itG_1} is in this case $E_{itg10} - E_i = -0.39$ eV, value of density of states associated with this energy level is $D_{itG_{10}} = 1{,}11.10^{13}$ eV^{-1}cm^{-2}.

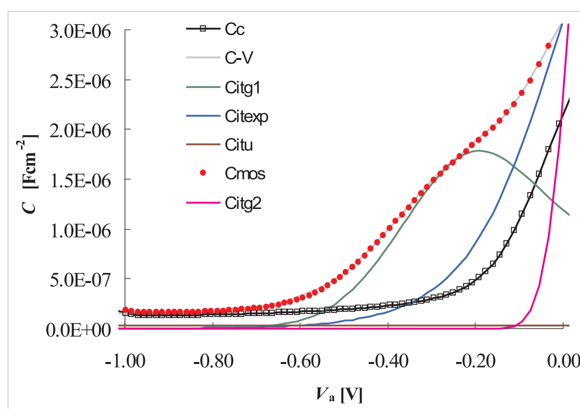

Fig. 4 Theoretical model of the capacitance of real MOS structure at frequency 1 kHz. C_{mos} is capacitance with the interface states, C_c is capacitance without D_{it}, C-V is experimental capacitance curve, C_{itg1}, $C_{it\ exp}$, C_{itu} are capacitances associated with D_{itG1}, $D_{it\ exp}$, D_{itu} respectively

Identical modeling procedure was used for the determination of energy levels and densities of interface states associated with these energies from the capacitance curves measured at a set of different frequencies. Frequency behavior of localized interface

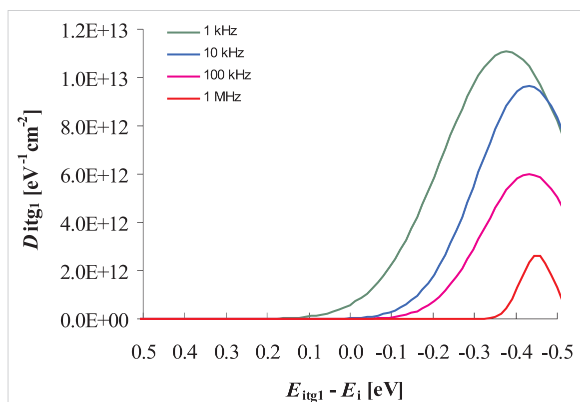

Fig. 5 Theoretical models of the densities of localized states modelled by the Gaussian distribution D_{itG1} at frequencies 1, 10, 100 and 1000 kHz

states described by the distribution extracted from the capacitance curves is shown in Fig. 5.

The frequency shift of the D_{itG1} distribution depends on the emission time of the interface states. The distribution of the interface state density is asymmetric; the density above midgap is lower. At lower frequencies the distributions are higher due to the effective excitation of recombination and trapping centers. The energy levels and corresponding densities of localized interface states in the energy gap of silicon substrate are shown in Table 1.

Results of the density of localized interface state analysis. Table 1

frequency	$E_{itg10} - E_i$	D_{itg10}
kHz	eV	eV^{-1}cm^{-2}
1	− 0.39	$1.11 \,.\, 10^{13}$
10	− 0.43	$9.67 \,.\, 10^{12}$
100	− 0.45	$6.01 \,.\, 10^{12}$
1000	− 0.46	$2.62 \,.\, 10^{12}$

Localized states described by the D_{itG2} distribution do not fall into the energy gap of Si and are not shown in Table 1. Densities of deep interface states in silicon energy gap are extremely reduced in MOS structure with NAOS SiO_2 oxide layer. This result corresponds very well with the results of the interface states study in the MOS structures by the acoustic deep-level transient spectroscopy [6].

5. Conclusions

Density of interface states in MOS structure with ultrathin NAOS SiO_2 layer was determined by the capacitance-voltage measurements at various frequencies. Different frequency responses of C-V curves were experimentally observed and theoretical model for explaining of these experimental results was constructed. Theoretical model of C-V curves is based on computation of equivalent capacitance of MOS structure corresponding to the density of interface states. This approach is motivated by simple physical assumptions and enables modeling of the frequency response of the charge trapping processes. Densities of states in MOS structure were modeled by the superposition of several distributions. Localized interface states modeled by Gaussian distribution provide good description of frequency behavior of C-V curves. Energy levels of interface states determined by extraction of Gaussian distribution from theoretical capacitance model are localized close to the valence band. The densities of deep interface states in silicon band gap are extremely reduced in MOS structure with NAOS oxide layer.

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