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 distorts 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 $\rho$ is given by equation

$$\rho = q\left(p - n + N^+_d - N^-_a\right).$$  \hspace{1cm} (1)

where $p$ and $n$ are hole and electron densities, $N^+_d$ and $N^-_a$ are the densities of the ionized donors and acceptors, respectively. The total space charge density $Q_S$ as a function of the surface potential $\Phi_S$ is shown in Fig. 1.

![Fig. 1 The total space charge density $Q_S$ in MOS structure](image-url)

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*STUDY OF THE DENSITY OF STATES DISTRIBUTION IN THE SiO$_2$/Si STRUCTURE*
Solution of the Poisson equation with this charge density leads to the capacitance of MOS structure without the interface states $C_t$ [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]

$$C_{ite} = \frac{dQ_{ite}}{d\Phi_t} = qD_{n}$$

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

$$D_n = D_n + D_{n,exp} + \sum D_{i,G}$$

Distribution $D_{n,exp}$ describes the uniform distribution of interface states across the band gap of semiconductor

$$D_{n,exp} = D_{n} \exp \left( \frac{E - E_t}{\alpha} \right),$$

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

$$D_{i,exp} = D_{i0} \exp \left( \frac{E - E_t}{\alpha} \right),$$

where $D_{i0}$ is the density of interface states at the midgap, $\alpha$ is constant, $E_t$ and $E_i$ are energy level and intrinsic Fermi level, respective. Distributions $D_{i,exp}$ are used for the description of interface states localized in its energy levels. The Gaussian distribution is used in this work

$$D_{i,G} = D_{i0} \exp \left( - \frac{(E - E_{i0})^2}{2\sigma^2} \right).$$

Here, $D_{i0}$ is the maximum energy of localized interface state, $E_{i0}$ is the central energy of localized state, and $\sigma$ is the standard deviation. We use superposition of several Gaussian distributions localized in different central energies $E_{i0}$ with different maxima $D_{i0}$ and standard deviations $\sigma$.

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 $C_t$ is connected in parallel.

$$Fig. 2 \text{ Equivalent circuit for the MOS structure with interface states.}$$

$C_{ite}$ is capacitance of NAOS oxide layer, $C_{n,exp}$, $C_{ite}$ and $C_{ite}$ are capacitances associated with $D_{n,exp}$, $D_{n,exp}$ and $D_{n,exp}$, 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 $\sim 2.5$ 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 \text{ C–V curves measured at Al/SiO}_2$/Si MOS structure with NAOS SiO$_2$ layer prepared at n-type silicon substrate.}$

$V_0$ [V]
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 \( f = 1 \text{ kHz} \) are compared in Fig. 4.

Mean value of energy of localized states modeled by \( D_{itG_1} \) is in this case \( E_{itG_1} = -0.39 \text{ eV} \), value of density of states associated with this energy level is \( D_{itG_1} = 1.11 \times 10^{13} \text{ eV}^{-1}\text{cm}^{-2} \).

Mean value of energy of localized states modeled by \( D_{itG_2} \) is in this case \( E_{itG_2} = -0.43 \text{ eV} \), value of density of states associated with this energy level is \( D_{itG_2} = 9.67 \times 10^{12} \text{ eV}^{-1}\text{cm}^{-2} \).

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

The frequency shift of the \( D_{itG_1} \) 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 | \( E_{itG_1} - E_i \) | \( D_{itG_1} \) |
|-----------|-----------------|----------------|
| kHz       | eV              | eV^{-1}\text{cm}^{-2} |
| 1         | -0.39           | 1.11 \times 10^{13} |
| 10        | -0.43           | 9.67 \times 10^{12} |
| 100       | -0.45           | 6.01 \times 10^{12} |
| 1000      | -0.46           | 2.62 \times 10^{12} |

Localized states described by the \( D_{itG_2} \) 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 SiO₂ 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 SiO₂ 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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