Effect of Remote-Surface-Roughness Scattering on Electron Mobility in MOSFETs with High-k Dielectrics

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A model for remote surface roughness scattering (RSR)-limited electron mobility in the inversion layer of nMOSFETs with high-k dielectrics has been developed in this work. A numerical method is applied to calculate RSR-limited electron mobility. It has been demonstrated that the RSR-limited electron mobility is highly degraded in the high electric field region.

Introduction

Although a great deal of progress has been made for metal-oxide-semiconductor field-effect transistors (MOSFETs) with high-k gate dielectrics, it has been experimentally observed that the effective mobility strongly degrades (1-3). The mechanism of the mobility degradation is not clearly understood so far. In order to explain the mobility degradation mechanism, there are several models proposed for ultrathin MOSFETs with high-k gate stacks (4-10). For the ultrathin MOSFETs with high-k dielectrics, it has been suggested that the mobility degradation might be caused by some phenomena that are specific to the high-k dielectrics, such as remote Coulomb scattering, remote surface roughness (RSR) scattering, and phonon scattering.

Over the past few years, several models have been developed in order to account for RSR induced mobility degradation. A pioneering work was proposed by Li and T. -P. Ma to establish a theoretical model for describing how the electrons inside a MOSFET channel get scattered by the roughness of metal/oxide interface (4). They evaluated scattering potential change due to the fluctuation of the oxide thickness, and calculated perturbation Hamiltonian for the lowest subband at a very low temperature (4.2 K). It was suggested that RSR should be carefully considered as the gate oxide thickness decreases to less than 10 nm. Nowadays, the equivalent oxide thickness (EOT) of the scaled MOSFETs is already around 1 nm. Hence, for such an ultrathin oxide MOSFETs, RSR is strongly effecting on carrier mobility in the channel. Saito *et al*. extended the theory proposed by Li and T.-P. Ma for the ultrathin poly-Si/Al_2O_3 gated MOSFETs (5). They were taken disturbance of surface potential and distribution of the charge centers into account to calculate RSR-limited carrier mobility. In fact, in the high electric field region, the calculated RSR-limited hole mobility is nearly fitted with the experimental result. Furthermore, their result shows that RSR-limited mobility decreases in the high electric field region. Gamiz and Roldan investigated the RSR-limited electron mobility by Monte Carlo method for MOSFETs with Poly-Si/SiO_2 gate (6). They took screening of the perturbation potential, finite thickness of the gate oxide, and higher energy subbands into account evaluated the RSR-limited electron mobility at the room temperature. However, the RSR-limited electron mobility behaves in a similar way as Coulomb scattering, i.e., it increases as the inversion charge increases. This contradiction is not clearly understood yet. Hence, further investigating is required to fully understand the mechanism of the RSR.

In this work, we investigated the effect of RSR scattering on the electron mobility for MOSFETs with ultrathin high-k gate dielectrics at low temperature. We take screening effect, and quantum fluctuation into account, and also applied an experimentally estimated power spectrum of roughness to evaluate RSR-limited electron mobility in the inversion layer of the MOSFETs. Our calculation result shows that the RSR scattering limited electron mobility is highly degraded in the strong electric field region.

Remote Surface Roughness Scattering Model

The lowest energy subband along the < 100 > direction of Si-substrate is considered. We further assumed that the interface of high-k dielectric layer/Si-substrate is an ideal surface without any surface roughness, and the remote surface, i.e., the interface of gate/high-k dielectric layer is not perfectly smooth. The RSR is considered to be originated from the fluctuation of the high-k dielectric oxide thickness from its average value. We also assumed that the two interfaces, gate/high-k dielectric layer and high-k dielectric layer/Si-substrate are not correlated with each other.

We numerically calculated the RSR-limited electron mobility by the relaxation time approximation. First we determined the relaxation time by integrating the following integral

$$\tau_{\mathrm{RSR}}^{-1}(\varepsilon) = (2\pi m^{*}/\hbar^{3})\int_{0}^{2\pi} \frac{d\theta}{4\pi^{2}} \left|M_{\mathrm{RSR}}(q)\right|^{2}(1-\cos\theta) \ , \qquad [1]$$

where m^{*} is the effective mass of the electron, M_{RSR} is the matrix element of the RSR potential. The matrix element of the RSR potential was estimated using the following expression:

$$\left|M_{\mathrm{RSR}}(q)\right|^{2} = \tilde{S}(q)\Gamma^{2}(q)/\varepsilon^{2}(q) \ , \qquad [2]$$

where $\tilde{S}(q)$ is the roughness power spectrum, i.e., a Fourier transform of the roughness correlation function. In order to include roughness spectrum, the following expression was used (11)

$$\tilde{S}(q) = \pi(\Delta\Lambda)^{2}(1+q^{2}\Lambda^{2}/2)^{-3/2} \ . \qquad [3]$$

Where Δ is the root mean square (rms) deviation of the roughness, and Λ is the correlation length. In Eq. [2], $\Gamma(q)$ is the averaged RSR potential as determined by T.

Ando (12). By considering the screening effect, the dielectric constant $\varepsilon(q)$ was determined as

$$\varepsilon(q)=\varepsilon_{\mathrm{Si}}(1+\tilde{q}_{\mathrm{s}}(q)/q) \ , \qquad [4]$$

where $\tilde{q}_s(q)$ was determined by screening effect, and wave vector.

$$\tilde{q}_{\mathrm{s}}(q)=q_{\mathrm{s}}[P_{\mathrm{av}}+((\varepsilon_{\mathrm{Si}}-\varepsilon_{\mathrm{ox}})/(\varepsilon_{\mathrm{Si}}+\varepsilon_{\mathrm{ox}}))P_0^2], \qquad [5]$$

where $\varepsilon_{\mathrm{Si}}$, $\varepsilon_{\mathrm{ox}}$ are dielectric constants of the Si substrate and oxide layer respectively. The screening effect factor can be found by considering the quantum fluctuation as derived by Pirovano (13) *et al.* using the following relations:

$$P_0=b^3(b+q)^{-3} \quad , \qquad [6]$$

$$P_{\mathrm{av}}=(8b^3+9b^2q+3bq^2)(b+q)^{-3}/8 \quad , \qquad [7]$$

Indeed, both the parameters P_0 and P_{av} are related to the wave vector and the inversion layer charge density. Here, b corresponds to the average distance of the electron charge density penetrating into the semiconductor.

Results

We considered electron transport in an n-type inversion layer formed at a (100) surface of an MOSFET at low temperature. We evaluated the scattering potential and RSR-limited mobility of the electrons in the inversion layer of MOSFETs with La_2O_3 dielectrics as a function of the electron concentration. We used the effective mass of the electron as $m_l/m_0=0.2$, $m_t/m_0=0.9$, and the dielectric constants of the high-k oxide layer and Si substrate as $\varepsilon_{\mathrm{La_2O_3}}=27$, $\varepsilon_{\mathrm{Si}}=11.7$ respectively.

Figure 1 shows calculated the RSR-limited electron mobility as a function of inversion charge density. The RSR-limited electron mobility is calculated for the roughness Δ as a variable parameter. For the specific value of the roughness, the calculated electron mobility has a peak value while the inversion charge density is increasing, i.e., the RSR-limited electron mobility first increases, and then decreases. However, the peak value of the RSR-limited electron mobility decreases while roughness value increases. The RSR-limited electron mobility for inversion-charge densities less than $\mathrm{N_{inv}}=7\times10^{20}/cm^2$ behaves like the Coulomb scattering limited electron mobility. When the inversion charge density is larger than $\mathrm{N_{inv}}=7\times10^{20}/cm^2$, the electron mobility value is largely degraded compare to in the case of the low inversion charge density.

Figure 2 shows the calculated RSR-limited electron mobility for the roughness correlation length as a variable. The RSR-limited electron mobility decreases rapidly as the correlation length increases in the region of higher inversion charge densities such as higher than $\mathrm{N_{inv}} = 7\times10^{20}/cm^2$. Meanwhile, when the inversion-charge densities are less than $\mathrm{N_{inv}} = 5\times10^{20}/cm^2$, in spite of the correlation lengths are different ($\Gamma = 2nm, 3nm, 4nm$), the RSR-limited electron mobility values are overlapped with each other.

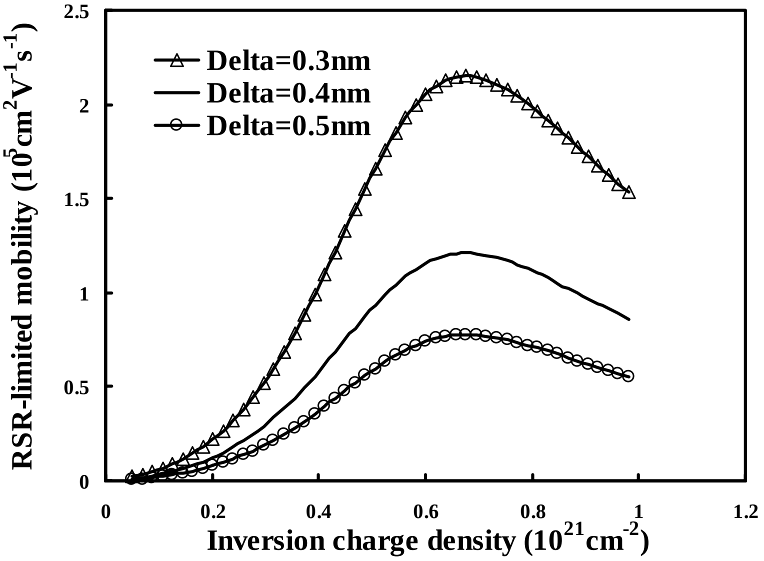

Figure 1. Calculated RSR-limited electron mobility vs. inversion charge density (T=35K, $\Lambda = 4nm$, $\mathrm{T_{ox}}$=3nm).

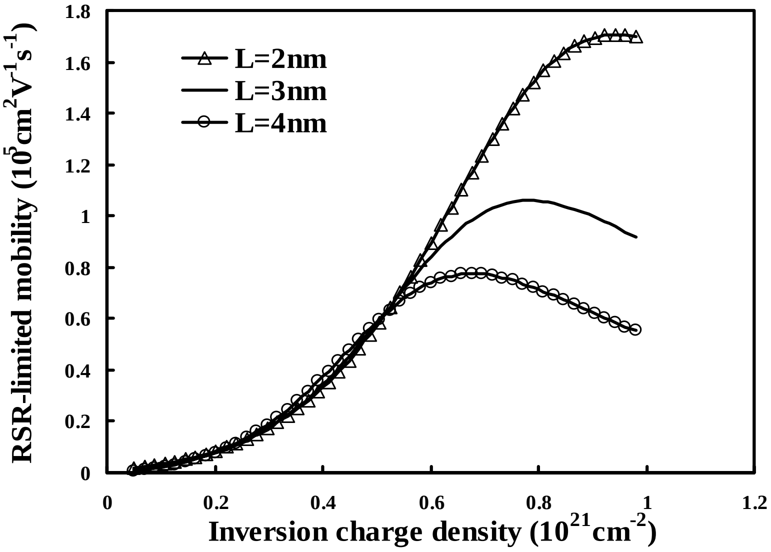

Figure 2. Calculated RSR-limited electron mobility vs. inversion charge density (T=35K, $\Delta = 0.5nm$, $\mathrm{T_{ox}}$=3nm). In legend, the character L corresponds to correlation length Γ.

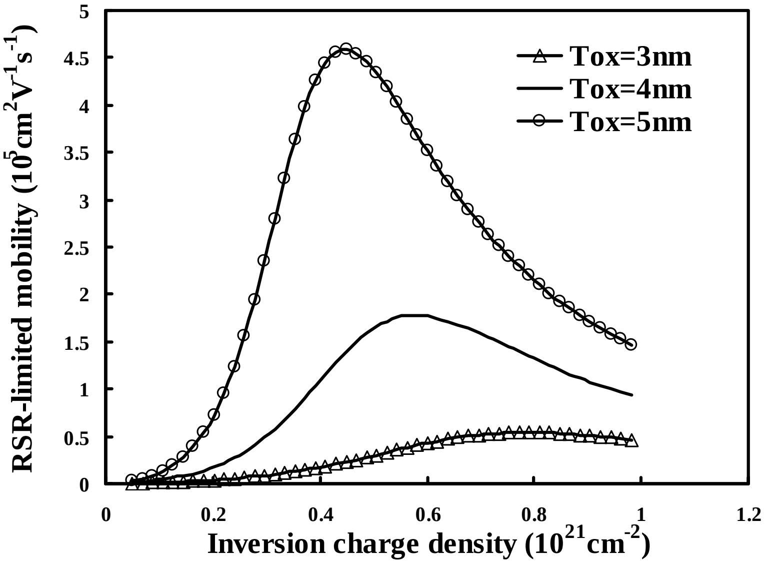

Figure 3. Calculated RSR-limited electron mobility vs. inversion charge density ($\mathrm{T} = 35\mathrm{K}$, $\Delta = 0.5nm$, $\Lambda = 3nm$).

Figure 3 shows the calculated RSR-limited electron mobility for different oxide thickness. It can be noticed that as the thickness of the oxide layer increases ($\mathrm{T}_{\mathrm{ox}} = 3nm, 4\mathrm{nm}, 5nm$), the RSR-limited electron mobility also rises. In the region of low inversion charge density ($< \mathrm{N}_{\mathrm{inv}} = 5 \times 10^{20} / cm^2$), the RSR-limited electron mobility is rapidly decreasing than in the case of high inversion charge concentration ($> \mathrm{N}_{\mathrm{inv}} = 7 \times 10^{20} / cm^2$). However, the peak value of the RSR-limited electron mobility shifts toward left as the high-k dielectric oxide thickness increases.

Discussion

In Figure 1, the calculated electron mobility has a peak value at a particular inversion charge depending of on oxide thickness. In the region of low inversion charge concentration, the screening effect is less affected. Therefore the effect of RSR on the electron mobility is increased as the inversion charge density increases. While the inversion charge concentration increases and reaches around a value of $\mathrm{N}_{\mathrm{inv}} = 7 \times 10^{20} / cm^2$, the screening effect start to shield the electrons from scattering by the RSR potential. This leads to electrons feel less scattering potential, and therefore the RSR-limited electron mobility starts to decrease.

In Figure 2, for the parameter of roughness correlation length, as the correlation length increases, the RSR-limited electron mobility decreases. This can be understood from the fact that too small correlation length tends to smooth out perturbation potential, while a large correlation length tends to affect strongly on perturbation potential. The RSR-limited electron mobility is strongly degraded in the region ($> \mathrm{N}_{\mathrm{inv}} = 7 \times 10^{20} / cm^2$)

of high inversion charge concentration, and overlapped in the region of low inversion charge concentration. This is the fact that due to the roughness correlation spectrum the perturbation potential is enhanced. This enhancement of the perturbation potential leads to degrade RSR-limited electron mobility sharply in the region of high inversion charge concentration. This is the common characteristic of roughness scattering.

Meanwhile, as the EOT increases, the distance between the remote interface and the electrons in the inversion layer increases. As a result, the RSR scattering potential decreases. Decreasing of the scattering potential leads to an increase in the RSR scattering-limited electron mobility (Fig. 3). This can be explained by the scattering from the roughness of the gate/high-k dielectric interface, which has a smaller effect on the channel electrons when EOT becomes larger. Nevertheless, in both cases (Fig. 2 and Fig. 3), the peak value of the RSR-limited electron mobility shifts towards left as the roughness correlation length and the oxide thickness increases. This phenomenon turns out to be due to the fact that for a larger value of the roughness correlation length and for a larger value of the oxide thickness, the remote Coulomb scattering play dominant role than RSR scattering. Therefore, in both cases the RSR-limited electron mobility behaves similar to that of Coulomb scattering. This might be the source of the scattering potential in the Coulomb charge distributed on the remote interface.

Conclusion

We have numerically calculated the effect of the remote roughness at the W/high-k interface on the electron mobility (RSR-limited mobility). By using an exponential power spectrum of the roughness correlation, we evaluated electron mobility in the inversion layer of MOSFETs. Our result showed that the calculated electron mobility is strongly affected by RSR in the high electric field region. This is suggests that the RSR scattering is not negligible to the electron mobility in the inversion layer of MOSFETs with high-k dielectrics. Therefore, for the fabrication of the MOSFETs with high-k dielectrics one has to minimize the remote surface roughness.

Acknowledgments

This work was supported by NEDO. One of the authors (M.M) would like to acknowledge for partially supports from G-COE PICE of TIT, and NEC C&C foundation of Japan. He is also grateful to Prof. T. -P. Ma, and Dr. Jia Li for their helpful comments.

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