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Influence of Dielectric Constant Distribution in Stacked Gate Dielectrics on Electron Mobility in Inversion Layers

Mizuki Ono, Takamitsu Ishihara, and Akira Nishiyama
Advanced LSI Technology Laboratory, Corporate R&D Center, Toshiba Corporation
8 Shinsugita-cho, Isogo-ku, Yokohama 235-8522, Japan
Phone: +81-45-770-3693, Fax: +81-45-770-3578, E-mail: m-ono@amc.toshiba.co.jp

Abstract
In this paper it is shown that electron mobility in the inversion layer is strongly affected by the dielectric constant distribution in gate dielectrics. An explanation of this phenomenon based on physical considerations is provided using a simplified model. Preferable dielectric constant distributions for high mobility are discussed.

1. Introduction

The trend toward miniaturization has resulted in gate dielectrics being thinned, and it is estimated that they will soon be 1 nm for 35-nm MOSFETs [1]. In order to avoid the drastic leakage current increase that is inherent in SiO_2 gate dielectrics, high-k materials for gate dielectrics are being intensively investigated [2]. It has been reported that mobility (μ_{eff}) in MISFETs with high-k gate dielectrics is lower than that in MOSFETs with SiO_2 gate dielectrics. This is thought to be because of the fixed charges within gate dielectrics and at interfaces between gate dielectrics and substrates; therefore, the fabrication of interfacial layers (ILs) at high-k film/substrate interfaces has been studied [3-5]. We investigated the influence of the dielectric constant distribution on the electron mobility determined by remote Coulomb scattering by fixed charge (μ_{RCS}) using numerical simulations and a physical model, and found that μ_{RCS} is strongly affected by dielectric constant distributions in gate dielectrics.

2. Simulation and Results

Simulations of μ_{RCS} were carried out for the stacked gate dielectric structure shown in Fig.1. The simulation model uses a pseudo-2 dimensional approximation and takes the screening of electric potential by other electrons into consideration. Only the lowest sub-band is considered. The reported interfacial charge density ranges from the order of 10^{11} to 10^{13} cm^{-2} [4,6,7]. In this study, fixed charges ($1x10^{12}$ cm^{-2}) were located at the high-k layer/IL interface. The results were almost the same whether they were located at the interface or inside the high-k layer provided that the distance from the channel was the same. The dielectric constants of both the high-k layer (ε_h) and the IL (ε_i) were varied from 3.9 to 100. The dependences of μ_{eff} and μ_{RCS} on the inversion carrier density (N_{inv}) with fixed ε_h are shown in Fig. 2 with ε_i as a parameter. Figure 2(a) shows that μ_{eff} at N_{inv} = $5x10^{12}$ cm^{-2} (carrier density around $V_G = V_{DD}$ [8]) is about 10% lower than the corresponding universal curve (UC) value [9] in the case of ε_i = 15. Figure 2(b) shows that μ_{RCS} increases with N_{inv} due to the decrease in the scattering cross section caused by the increase in the average electron energy as well as the increase in the electric field screening effect. Interestingly, it can be seen that as ε_i increases, μ_{eff} and μ_{RCS} first decrease and then increase for the entire N_{inv} region studied. The dependences of μ_{RCS} on ε_i and ε_h are shown in Fig. 3 with N_{inv} as a parameter. Here, μ_{RCS} at N_{inv} = $5x10^{12}$ cm^{-2} is divided by 5. Figure 3(a) shows that μ_{RCS} has a minimum at an ε_i value of about 15. Figure 3(b) shows that μ_{RCS} shows a similar dependence on ε_h. However, the tendency is much weaker and μ_{RCS} increases virtually monotonically with ε_h.

3. Discussion

μ_{RCS} is inversely proportional to scattering probability, which is proportional to the square of the electric potential within the Born approximation. A stacked gate dielectric structure with a fixed charge (Fig. 4) was studied. The electric potential induced by the charge in the substrate can be analytically calculated by Fourier transformation in the plane parallel to the substrate surface, and can be represented as the infinite series of exp(-qTj) (j = 1, 2...), where q is a wave number in the Fourier transformation. The most dominant term in the series reveals that the electric potential is equivalent to that of a charge at the same position with a magnitude given by (1), provided that the dielectric constant of all layers is ε_{Si}.

$$\frac{2\varepsilon_{Si}}{\varepsilon_{Si}+\varepsilon_1}\frac{2\varepsilon_1}{\varepsilon_1+\varepsilon_2}\cdots\frac{2\varepsilon_{n-2}}{\varepsilon_{n-2}+\varepsilon_{n-1}}\frac{2\varepsilon_{n-1}}{\varepsilon_{n-1}+\varepsilon_n}Q\ . \qquad (1)$$

In the case of gate stacks as in Fig. 1, μ_{RCS} is expected to be proportional to $[\varepsilon_i/((\varepsilon_{Si}+\varepsilon_i)(\varepsilon_i+\varepsilon_h))]^{-2}$, whose dependence on ε_i when ε_h is fixed is shown in Fig. 5(a) together with the dependence of μ_{RCS} on ε_i. The dependence qualitatively agrees: $[\varepsilon_i/((\varepsilon_{Si}+\varepsilon_i)(\varepsilon_i+\varepsilon_h))]^{-2}$ has minimum at $\varepsilon_i = (\varepsilon_{Si} \text{ x } \varepsilon_h)^{1/2}$ = 15.2... When ε_i is fixed, μ_{RCS} is expected to be proportional to $(\varepsilon_i+\varepsilon_h)^2$, whose dependence on ε_h is shown in Fig. 5(b) together with the dependence of μ_{RCS} on ε_h. The dependences qualitatively agree, except that $(\varepsilon_i+\varepsilon_h)^2$ has no minimum. The reason for this disagreement is that the terms other than the most dominant one and the electric potential screening by other electrons were neglected.

4. Preferable Dielectric Constant Distribution

In the stacked gate dielectric structure in Fig.1, lower and higher ε_i than $(\varepsilon_{Si} \text{ x } \varepsilon_h)^{1/2}$ is preferable from the viewpoint of scattering probability by fixed charges in the high-k layer and/or at the interface between the 2 layers. When HfO_2 (ε_h = 19.5) high-k layer is used, $[\varepsilon_i/((\varepsilon_{Si}+\varepsilon_i)(\varepsilon_i+\varepsilon_h))]^{-2}$ is about 8990 for an SiO_2 (ε_i = 3.9) IL and 4750 for an Si_3N_4 (ε_i = 7.8) IL. Hence the μ_{RCS} for SiO_2 ILs is expected to be almost double that for Si_3N_4 ILs. Note that this has nothing to do with the amount of fixed charge in the film. This is the pure influence of the dielectric constant of the IL. Metal silicate layers, e.g. $(HfO_2)_x(SiO_2)_{1-x}$, at the interface between substrates and metal oxides, e.g. HfO_2, may degrade μ_{eff} because they can have a higher dielectric constant than Si_3N_4 layers. Figure 6 shows the dependence of the available ε_i range on fixed charge density when μ_{eff} values higher than certain specified values are to be achieved with N_{inv} = $5x10^{12}$ cm^{-2} and a fixed ε_h of 19.5 in the case of gate stacks as that shown in Fig. 1. In the case of SiO_2 ILs (ε_i = 3.9), fixed charge density should be lower than $1.7x10^{12}$ cm^{-2} or $8.1x10^{11}$ cm^{-2} in order to realize μ_{eff} higher than 90 or 95% of UC, respectively. It is

known from (1) that upper bound for allowable fixed charge density decreases as ε_i increases, provided that ε_i is lower than $(\varepsilon_{Si} \times \varepsilon_h)^{1/2}$. Considering that ε_i is lower than ε_h in most cases, it is indispensable to suppress fixed charge density in order to realize high μ_{eff} and thin equivalent oxide thickness at the same time.
As for ε_h, higher values are preferable since μ_{RCS} increases almost monotonically with ε_h. It is known from (1) that the available range of ε_i widens/shrinks when ε_h is higher/lower than 19.5.

5. Summary and Conclusion

Our study showed that electron mobility in stacked gate dielectric structures is strongly affected by the dielectric constant distribution in the gate dielectrics, that mobility is minimum when $\varepsilon_i = (\varepsilon_h \times \varepsilon_{Si})^{1/2}$, and that mobility increases almost monotonically with ε_h. Therefore, control of the dielectric constant distribution in gate dielectrics is indispensable.

Acknowledgements

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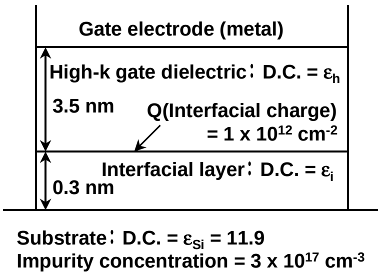

Fig.1 Stacked gate dielectric structure used in the simulations.

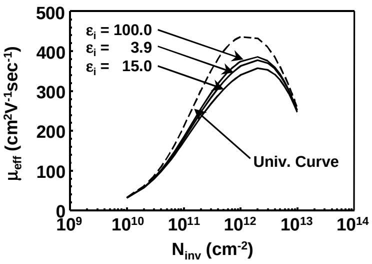

Fig.2(a) Dependences of simulated μ_{eff} on the inversion carrier density with ε_i as a parameter. ε_h is set to 19.5.

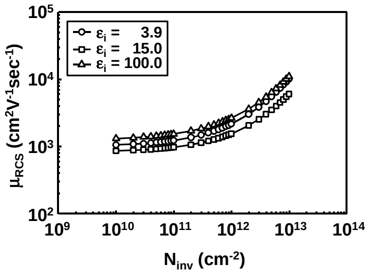

Fig.2(b) Dependences of simulated μ_{RCS} on the inversion carrier density with ε_i as a parameter. ε_h is set to 19.5.

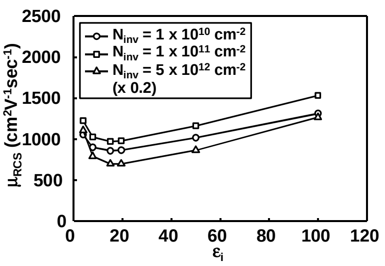

Fig.3(a) Dependences of μ_{RCS} on ε_i with N_{inv} as a parameter. Here, μ_{RCS} at $N_{inv} = 5 \times 10^{12}$ cm^{-2} is divided by 5. ε_h is set to 19.5.

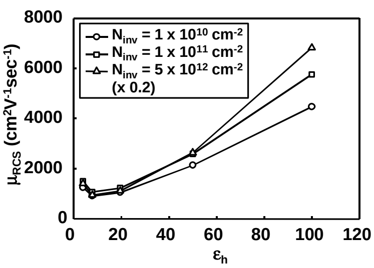

Fig.3(b) Dependences of μ_{RCS} on ε_h with N_{inv} as a parameter. Here, μ_{RCS} at $N_{inv} = 5 \times 10^{12}$ cm^{-2} is divided by 5. ε_i is set to 3.9.

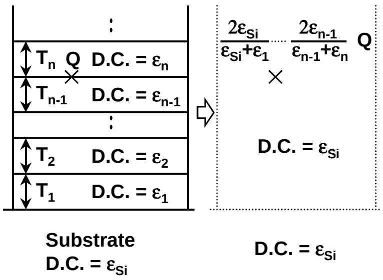

Fig.4 Stacked gate dielectric structure with a fixed charge.

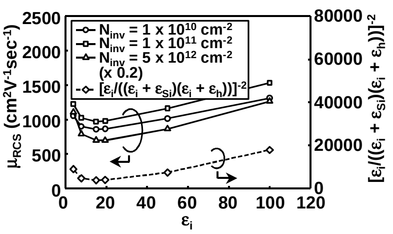

Fig.5(a) Dependences of $[\varepsilon_i/((\varepsilon_{Si}+\varepsilon_i)(\varepsilon_i+\varepsilon_h))]^{-2}$ and μ_{RCS} on ε_i with N_{inv} as a parameter. ε_h is set to 19.5.

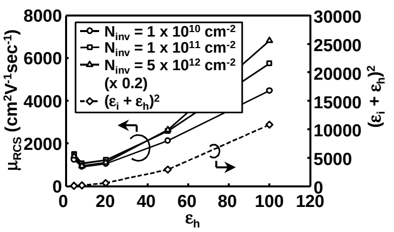

Fig.5(b) Dependences of $(\varepsilon_i+\varepsilon_h)^2$ and μ_{RCS} on ε_h with N_{inv} as a parameter. ε_i is set to 3.9.

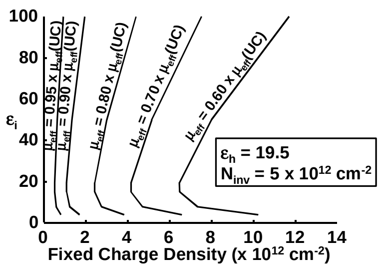

Fig.6 Dependence of available range of ε_i in gate stacks such as that shown in Fig. 1.