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Study on Carrier Transport Limited by Coulomb Scattering due to Charged Centers in HfSiON MISFETs

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1. Introduction

In regard to the electrical characterization of high-*k* dielectrics, it is important to understand the carrier transport properties. Scattering due to interface optical phonons [1], Coulomb scattering associated with charged centers, and remote surface roughness scattering [2] have been known to be the origins of the mobility degradation. However, the carrier transport under high-*k* dielectrics has not yet been fully understood due to the coexistence of these scattering components. In view of this background, we focus on Coulomb scattering at low temperature, where the well separation is achieved between Coulomb and phonon scattering components, and have conducted an extensive study on Coulomb scattering associated with charged centers under high-*k* dielectrics, taking HfSiON dielectric as an example.

2. Coulomb scattering model

Figure 1 compares the calculated μ_{rcs} (Coulomb-scattering-limited mobility) by the conventional scattering model [3] and the experimental μ_{rcs} [4, 5]. Figure 1 clearly shows the discrepancy between the two. This fact indicates that the effect inherent to the charged centers needs to be considered in the scattering model.

Stern [6] addressed the problems associated with the presence of charged centers. It was found [6] that Coulomb potential fluctuation (FL) associated with a random array of charged centers causes the band tailing in density of states (DOS) and the resultant change in the DOS leads to the suppressed screening effect. In order to include these effects in the evaluation of μ_{rcs}, we take the long-range part of Coulomb potential associated with charged centers as the potential fluctuation that causes the band tailing in DOS [7], whereas the short-range part of Coulomb potential is treated as the scattering matrix element in relaxation time approximation of Boltzmann equation. According to the idea proposed in Ref. [8], the long-range part of Coulomb potential is extracted by separating the short-range part.

The experimental results [4, 5] also indicate the coexistence of positively and negatively charged centers ($\sim 1\times10^{12}$ cm^{-2}). Positively and negatively charged centers attract electrons and holes through Coulomb potential, respectively, and lead to bound states. The positively (1.7×10^{12} cm^{-2}) and negatively (2.7×10^{12} cm^{-2}) charged centers located 0.3nm and 1.3nm from the MOS interface are considered in the calculation. The larger concentration of negatively charged centers than that of positively charged centers is chosen based on the experimental finding of the positive shift of flat-band voltage [4]. The binding energy associated with charged centers is calculated according to Ref. [3]. The band tail in DOS and carrier trapping at the deep bound states cause the reduction in the amount of mobile carriers.

3. Calculation procedure

The potential fluctuation is evaluated by the envelope function obtained by solving Poisson and Schrödinger equations self-consistently. The Gaussian broadening approximation is used for the evaluation of DOS [9]. The impurity band (IB) associated with charged centers is also considered. The 2-D sub-band structure is calculated again by considering the modulated DOS. The modulated DOS is also reflected in the evaluation of screening length and the potential fluctuation. Thus, the self-consistent calculation is performed (Fig. 2). Finally, μ_{rcs} is calculated by relaxation time approximation.

4. Results

Figure 3 shows the band tailing in DOS caused by the long-range potential fluctuations. For low N_s regions, Coulomb potential becomes longer range due to the weak screening effect. As a result, the band tailing in DOS is more enhanced. As shown in Fig. 4, the amount of the binding energy also becomes large for low N_s regions due to the weak screening effect. The band tailing in DOS and the deep binding energy lead to the reduction in Fermi energy (Fig. 4). The reduction in Fermi energy leads to the further suppressed screening effect (Fig. 5) because Fermi energy is in the region of the band tailing in DOS for low N_s regions. For high N_s regions, on the other hand, the Fermi energy is sufficient to prevent to form the bound states associated with charged centers, and the conventional screening model holds (Fig. 5).

Since the bound states for low N_s regions are deep enough to trap carriers due to the suppressed screening effect, the amount of mobile carriers decreases as shown in Fig. 6. The existence of the non-mobile carriers raises the problem on the interpretation of the experimental N_s. It is appropriate to interpret the experimental N_s as the total N_s (N_s^{tot}), since the experimental N_s is determined through gate-to-channel capacitance measurement. Therefore, it is reasonable to express μ_{rcs} as a function of the total N_s^{tot} in the comparison with the experimental μ_{rcs}. Actually, Fig. 7 shows that μ_{rcs} as a function of N_s^{tot} corresponds well with the experimental μ_{rcs} compared to μ_{rcs} as a function of N_s^{mobile}. The apparent decrease in the amount of μ_{rcs} as a function of $N_s=N_s^{tot}$ compared to μ_{rcs} as a function of $N_s=N_s^{mobile}$ is a consequence of the decrease in the amount of the mobile carriers, as is schematically shown in Fig. 7.

It is found from Fig. 8 that for both electrons and holes the calculated μ_{rcs} as a function of N_s^{tot} explains well the experimental results. For holes, the consideration of the negatively charged centers is necessary to represent the experimental results. Thus, the consideration of the coexistence of the positively and negatively charged centers is indispensable for the understanding of Coulomb scattering under HfSiON dielectric.

5. Conclusions

Carrier transport properties limited by Coulomb scattering associated with charged centers under HfSiON dielectric has been studied. It was found that the carrier trapping at the deep bound states for low N_s regions decreases the amount of the mobile carriers. The existence of the non-mobile carriers leads to the apparent decrease in the amount of μ_{rcs} when expressed as a function of total carrier concentration. By considering the coexistence of positively and negatively charged centers, the experimental μ_{rcs} for both electrons and holes can be explained well.

References

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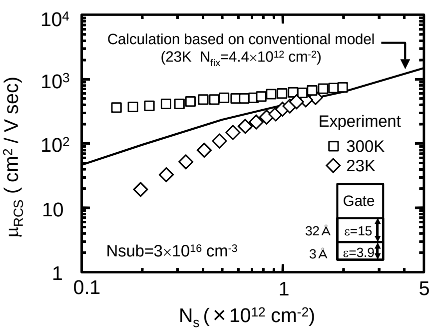

Fig. 1 Comparison of the calculated μ_{rcs} by the conventional Coulomb scattering model with the experimental μ_{rcs} [3,4].

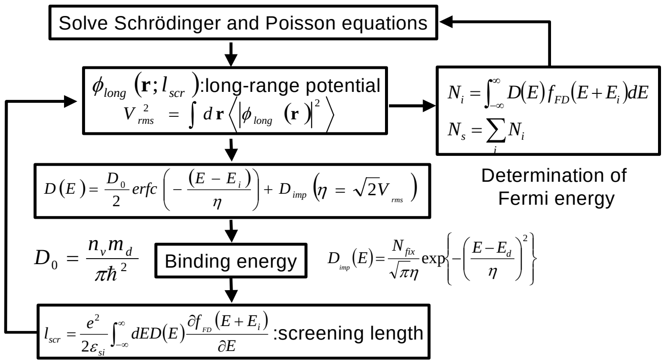

Fig. 2 Schematic diagram explaining the self-consistent calculation procedure to obtain the sub-band structure under impurity band and potential fluctuation associated with charged centers.

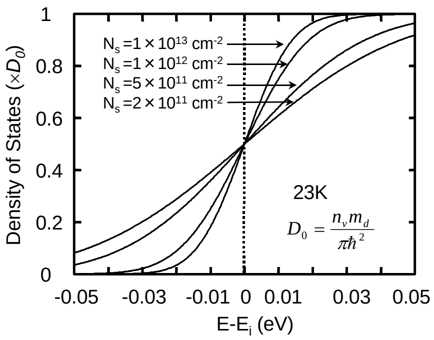

Fig. 3 Band tailing in DOS induced by the long-range potential fluctuations at 23K for electron. E_i represents the sub-band energy for the lowest sub-band.

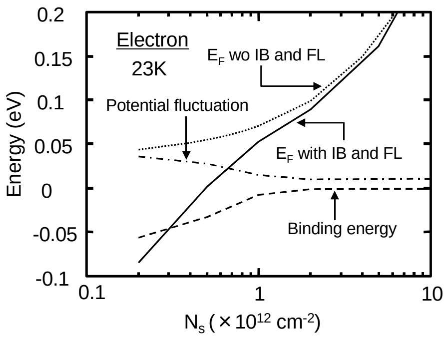

Fig. 4 Binding energy, potential fluctuation, and Fermi energy as a function of N_s at 23K for electron.

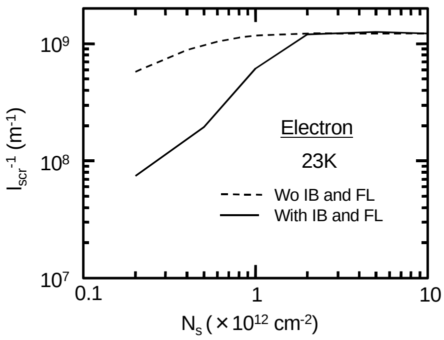

Fig. 5 l_{scr}^{-1} (l_{scr} means screening length) as a function of N_s at 23K for electron.

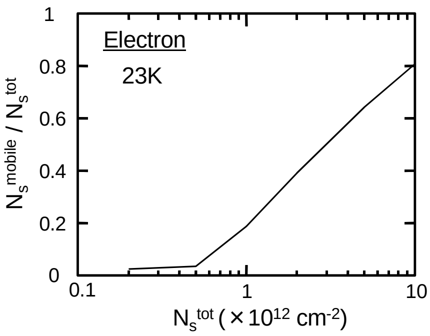

Fig. 6 Rate of the concentration of mobile electrons (N_s^{mobile}) to that of total electrons (N_s^{tot}) at 23K.

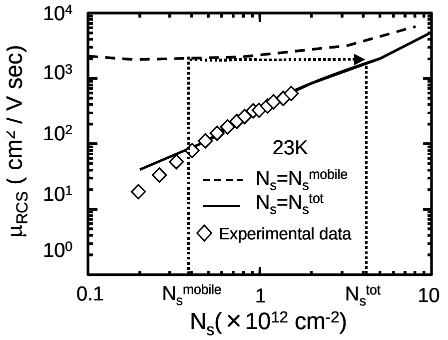

Fig. 7 Comparison of μ_{rcs} as a function of mobile carrier concentration (N_s^{mobile}) with μ_{rcs} as a function of total carrier concentration (N_s^{tot}).

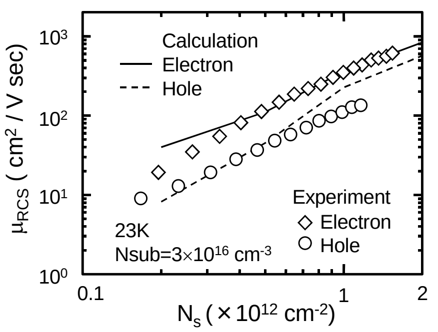

Fig. 8 Comparison of the calculated and the experimental μ_{rcs} as a function of total carrier concentration (N_s=N_s^{tot}) for electron and hole at 23K.