

## F-4-3

**Comprehensive Understanding of Electron and Hole Mobility Limited by Surface Roughness Scattering in Pure Oxides and Oxynitrides Based on Correlation Function of Surface Roughness**

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**1. Introduction**

It is well known that oxynitridation of gate insulators causes the change in low field mobility for both electron and hole. It has been reported, in particular, that mobility in high normal field, limited by surface roughness (SR) scattering,  $\mu_{sr}$ , has the different behavior between electrons and holes by oxynitridation [1]. As shown in Fig. 1, electron  $\mu_{sr}$  for NO oxynitrides is larger than that for pure oxides (PO), whereas hole  $\mu_{sr}$  for NO is smaller than that for PO [1]. This behavior has not been understood yet.

SR is characterized not only by  $\Delta$  (roughness r.m.s value) and  $\Lambda$  (correlation length), but also by roughness correlation function  $S(r)$ . Although the gaussian form is often assumed for  $S(r)$ . We have confirmed that the gaussian form of  $S(r)$  cannot explain the different  $E_{eff}$  dependences of electron and hole  $\mu_{sr}$  for PO under same values of  $\Delta$  and  $\Lambda$  between NMOS and PMOS. As shown in Fig. 2, the experimental hole  $\mu_{sr}$  has smaller values and weaker  $E_{eff}$  dependence. It has been reported, on the other hand, that the different  $E_{eff}$  dependence between electron and hole  $\mu_{sr}$  can be explained by an appropriate form of the SR power spectrum, different from the gaussian form [2].

In this study, it is shown, for the first time, that the change in electron and hole  $\mu_{sr}$ , associated with oxynitrides can be reasonably explained by the optimum choice of the form of  $S(r)$ .

**2. Model**

In order to calculate  $\mu_{sr}$ , the roughness power spectrum,  $\tilde{S}(q)$ , which is the Fourier transform of  $S(r)$ , must be determined. Although the functional form of  $S(q)$  in k space is often discussed, we use, in this study, the following roughness correlation function in real space

$$S(r) = \Delta^2 e^{-\left(\frac{r}{\Lambda}\right)^n} \quad (1)$$

where n is a parameter to determine the functional form of  $S(r)$ . The roughness power spectrum  $\tilde{S}(q)$  is obtained by the Fourier transform of Eq. (1).

**3. Results**

Fig. 3 shows  $\tilde{S}(q)$  in k space as a parameter of n and the range of electron and hole  $k_F$ , where  $N_s$  is varied from  $5 \times 10^{12}$  to  $10^{13}$  cm<sup>-2</sup>. Note that scattering rate decreases with a decrease in  $\tilde{S}(q)$ . It is found in Fig. 3 that the change in the function form of  $\tilde{S}(q)$  (n) causes much larger impact on the value of  $\tilde{S}(q)$  for holes than for electrons, because hole  $k_F$  is larger than electron one [2]. This result suggests that hole  $\mu_{sr}$  is much more sensitive to the change of n than electron  $\mu_{sr}$ . This prediction is actually confirmed by Fig. 4. It is also found in Fig. 5 that, by taking n of 0.9, hole  $\mu_{sr}$  for PO can be represented well under the same values of  $\Delta$  and  $\Lambda$  as in Fig. 2, meaning that both electron and hole  $\mu_{sr}$  are consistently explained under the same parameter set. The value of n, obtained here, is consistent with the previous reports [3,4] that the exponential correlation function (n=1) is in better agreement with experiments.

However, when n is taken to be the same as that for PO, the best fitting with experimental  $\mu_{sr}$  for NO provides the different values of  $\Delta$  between electrons (4.6 Å) and holes (6.3 Å), which is not reasonable physically. It is found in Fig. 6, on the other hand, that, when n is taken to be 1.8 and  $\Delta$  is taken to be a smaller value (4.5 Å), electron and hole  $\mu_{sr}$  for NO can be consistently represented again under the common parameter set. The parameters used in the calculations are summarized in Table. 2.

The above results are schematically shown in Fig. 7. It is concluded from the analysis for the correlation function form that the increase in electron  $\mu_{sr}$  for NO and the decrease in hole  $\mu_{sr}$  for NO against  $\mu_{sr}$  for PO are attributable to the decrease in  $\Delta$  and the increase in n, respectively. This suggests that the surface roughness formed by NO oxidation has more enhanced randomness (large n), while the height of roughness decreases, compared with that by thermal oxidation.

**4. Conclusions**

It has been demonstrated that, by choosing the optimum form of  $S(r)$ , both electron and hole  $\mu_{sr}$

for PO and NO can be represented well under the same roughness parameters for both electron and hole. As a result, the opposite change in electron and hole  $\mu_{sr}$  for NO against  $\mu_{sr}$  for PO is reasonably explained by the change in the form of correlation function and the height of roughness.

**References**

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 [3] S. M. Goodnick *et al.*, Phys. Rev. B32, 8171(1985).  
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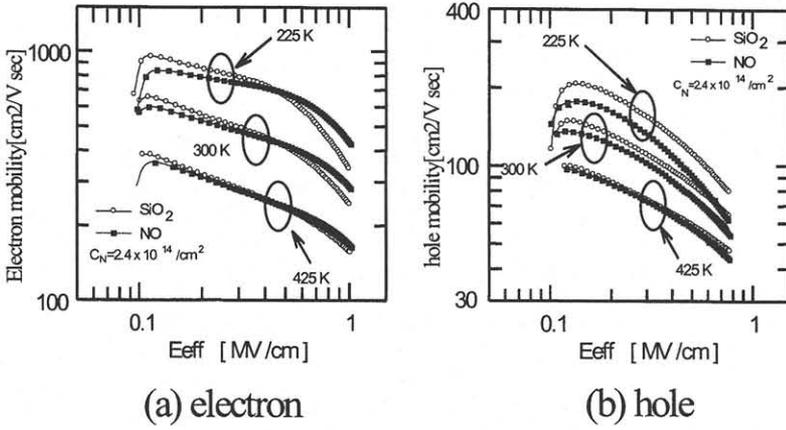


Fig. 1 Dependence of effective mobility on the effective electric field,  $E_{eff}$ , for pure oxides and oxynitrides.

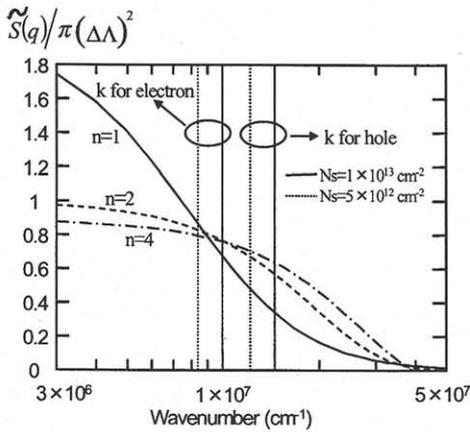


Fig. 3 Power spectral densities obtained by the Fourier transform of Eq. (1) as a parameter of  $n$ . Straight lines show  $k$ -values of electrons and holes estimated from carrier concentration of  $5 \times 10^{12} \text{ cm}^{-2}$  and  $10^{13} \text{ cm}^{-2}$ .  $\Delta$  is taken to be  $10 \text{ \AA}$ .

	Pure oxide	NO
$n$	0.9	1.8
$\Delta$	5.5	4.5

Table. 1 Roughness r.m.s value  $\Delta$  and  $n$  obtained by the fitting.

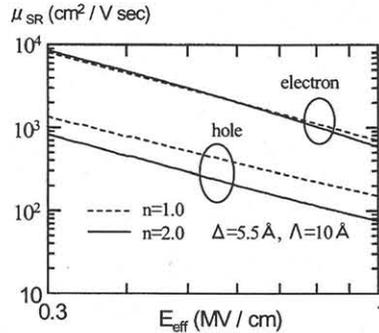


Fig. 4  $E_{eff}$  dependence of electron and hole  $\mu_{sr}$  for  $n$  of 1 and 2.

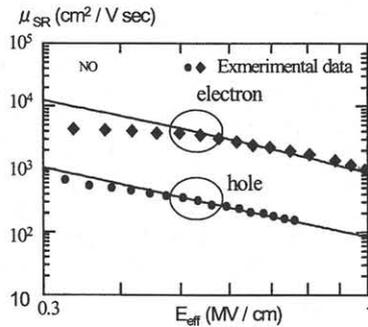


Fig. 6  $E_{eff}$  dependence of  $\mu_{sr}$  for NO oxynitrides. Solid line represents the calculated results using  $n$  of 1.6,  $\Delta$  of  $4.5 \text{ \AA}$  and  $\Lambda$  of  $10 \text{ \AA}$ .

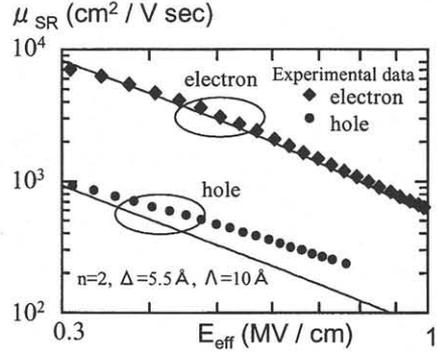


Fig. 2  $E_{eff}$  dependence of electron and hole  $\mu_{sr}$  for pure oxide. Solid line represents the calculated results using  $n$  of 2,  $\Delta$  of  $5.5 \text{ \AA}$  and  $\Lambda$  of  $10 \text{ \AA}$ .

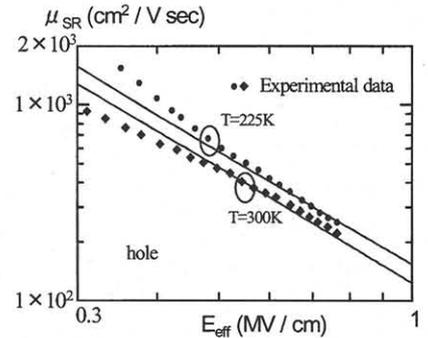


Fig. 5  $E_{eff}$  dependence of hole  $\mu_{sr}$  for pure oxide for  $T$  of 225K and 300K. Solid line represents the calculated results using  $n$  of 0.9,  $\Delta$  of  $5.5 \text{ \AA}$  and  $\Lambda$  of  $10 \text{ \AA}$ .

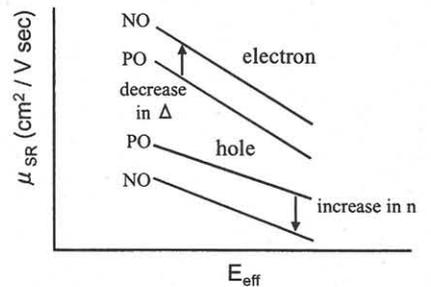


Fig. 7 Schematic diagram of electron and hole  $\mu_{sr}$  for PO and NO and physical origin for the difference.