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Exact Trap Level Estimation of HfSiON Films with Various Atomic Compositions

Masahiro Koike, Tsunehiro Ino, Yuuichi Kamimuta, Yuichiro Mitani, and Akira Nishiyama

Advanced LSI Technology Laboratory, Corporate Research&Development Center, Toshiba Corporation
1 Komukai Toshiba-cho, Saiwai-ku, Kawasaki, Kanagawa 212-8582, Japan

Phone: +81-44-549-2313 *Fax:* +81-44-520-1257 *E-mail:* m-koike@amc.toshiba.co.jp

I. Introduction

Hafnium silicon oxynitride (HfSiON), especially with high nitrogen concentration, is one of the promising gate dielectrics for future generations of LSIs. It is mainly because of the relatively high permittivity (~24), the high thermal stability that can keep noncrystalline phase at high temperatures of over 1000°C, and the high immunity against boron penetration from gate poly-Si into silicon substrate even for ultra-thin films.[1] Therefore, it is extremely important to decide the leakage current mechanism and extract relevant physical parameters of these materials. On the other hand, Hf-based high-k dielectrics such as HfSiON tend to have defect levels in the band gap energy.[2,3] In order to ascertain the origin of the defect for the reduction of leakage current as well as to model the leakage current through the film, the extraction of defect levels has great significance. However, the defect levels in these films have yet to be fully clarified. The difficulty mainly comes from the existence of an interfacial layer (IL) generated between HfSiON and Si substrate.[2] If the equivalent oxide thickness of an HfSiON film is as thin as that of the IL, high voltage is imposed on the IL, leading to the overestimation of electric field inside high-k layer because of the dielectric constant difference between them (Fig.1(a)). Besides, the IL would strongly affect the leakage current in view of the existence of large barrier height. It is therefore difficult to examine the genuine leakage current in HfSiON film. In this study, we fabricated capacitors with thick HfSiON films (~100nm) to precisely evaluate leakage currents and to exactly estimate trap levels. The use of the thick films enables us to avoid the influence of the IL on the leakage currents, and to simply define the electric field ($E_{\text{high-k}}$) in an HfSiON film itself as the gate voltage (V_G) divided by the entire film thickness (T_{phys}) (Fig.1(b)).

II. Experimental

HfSiON films were deposited on HF-last p-Si(100), n+Si(100) and HfSi(~5nm)/n+Si(100) substrates by co-sputtering of Hf and Si targets in O_2/N_2/Ar ambient. The atomic compositions were precisely controlled; the Hf/(Hf+Si) ratio was adjusted by the power imposed on Hf to Si targets. The nitrogen concentrations ([N]) were regulated by changing the flow rates of O_2/N_2/Ar. Hf/(Hf+Si) ratios were 15, 35, 80, and 100%. [N] were varied up to ~50at.%. The compositions were estimated with RBS. The physical thickness was exactly confirmed with both an ellipsometer and an SEM. Various metals, Al, Mo, TiN, and Au, were deposited as the gate electrodes. Different metals enable us to examine the effect of the different work functions on the leakage current through the films. We measured the *JV* characteristics at various temperatures (20~473K) and in a wide range of voltage (-100~100V). High-frequency dielectric constants (ε_{inf}) were obtained by the square of refractive indexes measured by ellipsometry. The band gap energies were measured by Reflection EELS.[1,4]

III. Results and Discussion

We examined the thickness dependence of the leakage current. Figure 2 shows that the leakage currents plotted as a function of electric field (E) are almost the same. This indicates that E defined as V_G/T_{phys} is correctly estimated, and the leakage currents are represented by a function of E. Substrate dependence of *JV* characteristics for HfSiON capacitors shows that the leakage currents are almost the same and symmetrical in terms of the polarity (Fig.3). We would also like to point out here that when [N] exceeds 20at.%, there is an abrupt increase of the leakage current in accordance with Hf-N bond formation.[1] Figure 4 shows the Arrhenius plots for the capacitor that explains the temperature dependence of leakage current in HfSiON films. The leakage currents tend to increase with temperature, whereas they have weak dependence on temperatures under ~100K. This suggests that the conduction is thermally activated at high temperatures and governed by quantum tunneling at low temperatures. It should be noted that the room temperature (~300K) is sorted as 'high temperature' region in this category. Figures 5(a) and 5(b) show the *JV* characteristics at 300K and 473K for MIM capacitors with different four metal electrodes. Interestingly, no gate electrode dependences were observed at these high temperatures. We can say that neither Schottky emission nor F-N tunneling is major conduction because they are electrode-limited currents. We therefore conclude that the major conduction mechanism is bulk-limited current, which should be Poole-Frenkel (P-F) conduction (field-assisted thermal ionization)[5] at high temperatures (Fig.6(a)). We confirmed the possibility of P-F conduction defined as

$$J = CE\exp\left(-\frac{q\Phi_T - \beta\sqrt{E}}{\xi k_B T}\right),$$

where C is a proportionality constant, E is electric field in a film, T is temperature, q is an elementary charge, k_B is Boltzmann constant, Φ_T is trap level from band edge of the material, and β is P-F constant given by

$$\beta = \sqrt{q^3/(\pi\varepsilon_0\varepsilon_{\text{inf}})}.$$

Although ξ is usually taken as unity, it was originally two.[5] Besides, there are reports that ξ can take values ranging from 1 to 2 depending on the position of the Fermi level.[6-9] In this study, we took this parameter as an unknown one, and determined this from experimental data. Figures 7(a) and 7(b) show the typical examples of P-F plots [log (J/E) vs. $E^{1/2}$]. These plots exhibit good linearity over the wide range of E, and clearly show the saturation of P-F effect at which a field-induced barrier lowering $\beta E^{1/2}$ is equal to a trap level $q\Phi_T$ (Fig.6(b)).[8,9] The exact trap levels are evaluated from this electric field of saturation together with β calculated using ε_{inf} (Fig.8(a)). The slopes of these P-F plots reveal the value ξ ranging from 1 to 2 (Fig.9). Figure 10 shows the relationship between the trap levels and the atomic compositions. As a result of exact trap level estimation of HfSiON films with various atomic compositions, we found that the trap levels become smaller as Hf/(Hf+Si) and [N] increase, which seems to have correlation with the band gap energy (Fig.8(b)).

IV. Conclusions

We investigated the leakage current mechanism and extracted exact trap levels of HfSiON films with various atomic compositions, especially in high [N] region. Thick films (~100nm) were used to avoid the effect of an interfacial layer between the film and Si substrate on leakage current, and to simply determine electric field in high-k layer alone. It was revealed that the leakage currents were represented as a function of electric field, and independent of the substrates and electrode materials. From these results, we concluded that the leakage current was bulk-limited current, P-F conduction at high temperatures. The P-F plots showed good linearity and the saturation of P-F effect. The trap levels were precisely estimated using the saturation field of P-F effect, and showed the tendency to decrease as Hf and N concentrations increase.

References

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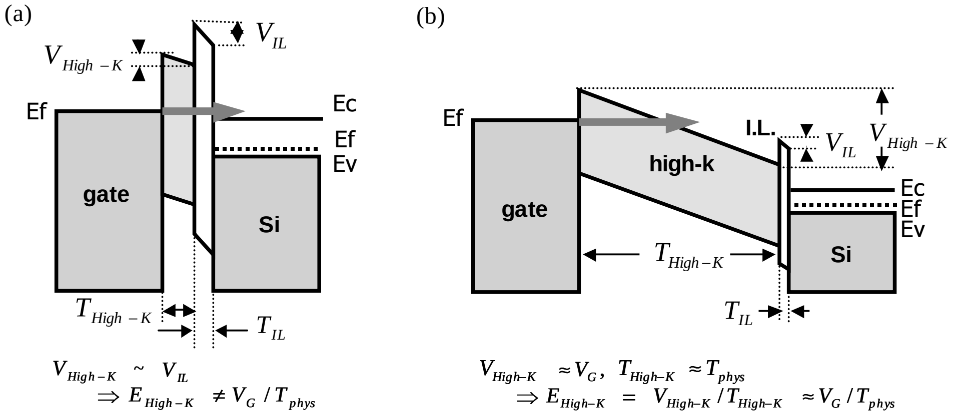

Fig. 1: The concept of leakage current measurement using thick high-k dielectrics.

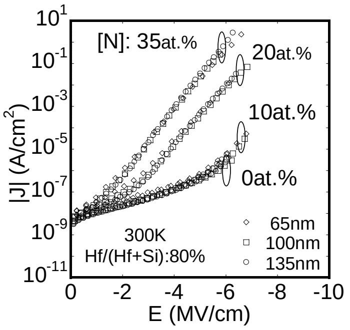

Fig. 2: Thickness dependence of leakage current in HfSiON in unit of electric field E. The film thicknesses were 65, 100, and 135nm. Hf/(Hf+Si) were 80%.

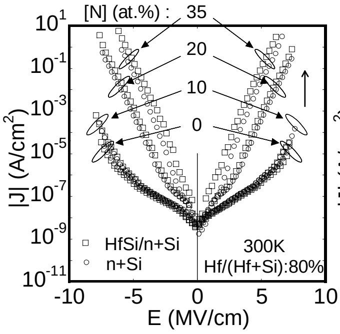

Fig. 3: Substrate dependence of leakage current. n+Si(100) and HfSi(5nm)/ n+Si(100) were used. The film thicknesses were 100nm.

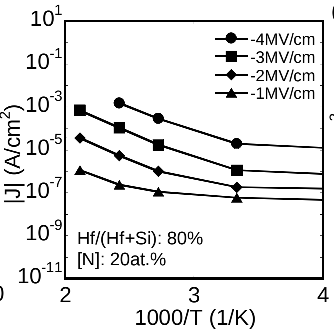

Fig. 4: Temperature dependence of leakage current in HfSiON films (100nm).

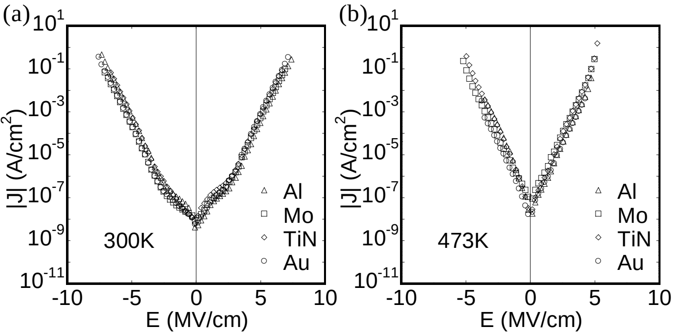

Fig. 5: Electrode dependence of leakage current. Al, Mo, TiN, and Au were used as the gate electrodes. The temperatures were (a)300K and (b)473K, respectively. Hf/(Hf+Si) were 80%, and [N] were 20at.%. The film thicknesses were 100nm.

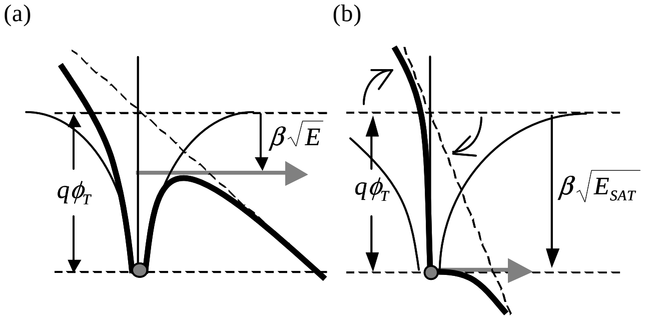

Fig. 6: (a) Poole-Frenkel (P-F) effect and (b) the saturation of P-F effect. In this study, P-F conduction was defined as $J = CE \exp[-(q\Phi_T - \beta E^{1/2})/(\xi k_B T)]$, where $\beta = [q^3/(\pi\varepsilon_0\varepsilon_{\mathrm{inf}})]^{1/2}$. At saturation, i.e. $q\Phi_T - \beta E_{SAT}^{1/2} = 0$, the leakage current has no temperature dependence.

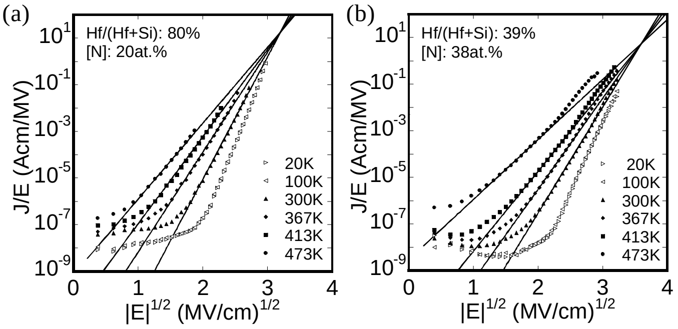

Fig. 7: P-F plots of leakage currents at different temperatures. The thicknesses were 100nm. The saturations of P-F effect (Fig.6(b)) at which fitted lines of P-F plots converge are clearly observed. The trap levels can be precisely estimated by the saturation fields.

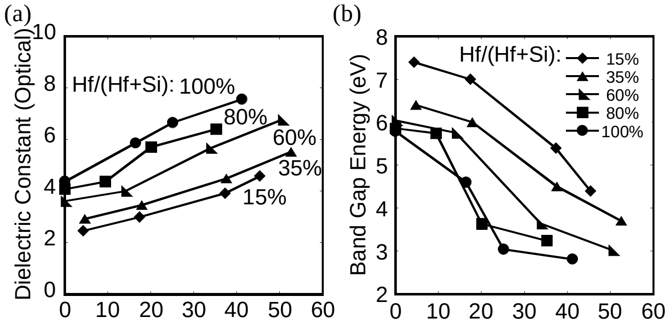

Fig. 8: Effect of atomic composition on (a) high-frequency dielectric constant $\varepsilon_{\mathrm{inf}}$ and (b) band gap energy.

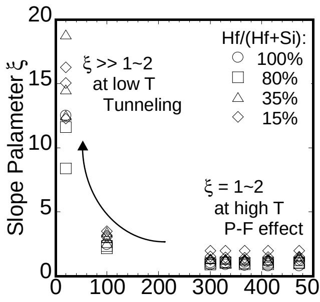

Fig. 9: Temperature dependence of slope parameter ξ.

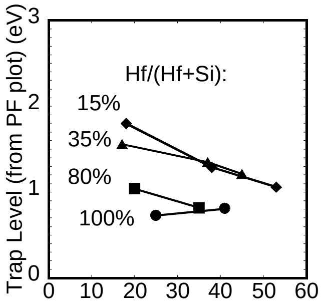

Fig. 10: The relationship between atomic composition and trap level of HfSiON.