Strain-Induced Leakage Current in High-k Gate Oxides Simulated with First-Principles Calculation

Hiroshi Moriya*, Tomio Iwasaki*, and Hideo Miura**
*Mechanical Engineering Research Laboratory, Hitachi, Ltd.
832-2, Horiguchi, Hitachinaka, Ibaraki, 312-0034, Japan
hiroshi.moriya.fd@hitachi.com
** Fracture and Reliability Research Institute, Tohoku University

***Abstract* - We propose a new leakage mechanism that depends on the mechanical strain in high-k gate oxides, namely "high strain-induced leakage current". To explain this current, we analyzed the strain dependence of the leakage current of gate oxides by performing a first-principles calculation. The analysis showed that the leakage current drastically increases with tensile strain.**

I. INTRODUCTION

High-permittivity (high-k) dielectrics such as HfO_2, ZrO_2, and TiO_2 are candidates for gate oxides of CMOS devices with gate lengths under 90 nm. These materials have higher dielectric constants than the current gate dielectric, SiO_2, but have much smaller bandgaps than SiO_2. Accordingly, the increase in Fowler-Nordheim leakage current through high-k gate oxides is of concern. In addition, it has been found that tensile stress higher than 1 GPa often occurs in new gate-electrode materials such as metal-silicide and tungsten[1]. Since it is known that tensile strain in crystals reduces the bandgap of materials, such high tensile strain may decrease the bandgap of the gate oxide film and, thus, further increase the leakage current[2) 3)], which we call "high strain-induced leakage current".

Given this background, we investigated the mechanical strain-induced leakage current through high-k gate oxides. First, we estimated the strain field in a MOSFET structure by using a finite element method (FEM). Next, we analyzed the change in the bandgap of oxides caused by crystallographic strain by performing a first-principles calculation[4] and estimated the leakage current by applying the Wentzel-Kramers-Brillouin (WKB) approximation[5]. Finally, we quantitatively evaluated the increase in leakage current caused by intrinsic stress of a tungsten gate electrode.

II. FEM ANALYSIS

To estimate the strain in gate oxides, we did an FEM analysis of the material dependence of the strain field in a gate oxide film. In this analysis, gate-electrode formation conditions such as film-deposition temperature and change in shape of the deposited film caused by etching were taken into account by adding FEM elements at each temperature. The intrinsic stress of thin films used for the gate structure was also considered in the analysis[6]. We used the measured intrinsic stresses for the gate electrode (0.7 GPa for poly-Si and 2.5 GPa for tungsten) and for the side wall of the gate electrode (-1.0 GPa for SiN).

Figure 1 shows the distribution of principal strain in the gate oxide on which poly-Si or tungsten was deposited as a gate electrode. Tensile strain concentrates at the bottom edge of the gate electrode. A maximum strain of about 1% develops when poly-Si is deposited on the oxide. The strain reaches about 3.5% for tungsten as the gate material.

Thus, the strain in the gate oxide increases by 3.5 times when the gate electrode is made of tungsten instead of poly-Si. When the stresses of shallow trench isolation, etc., are taken into account, the total strain could easily reach about 10%. Therefore, we conclude that new gate materials easily increase the tensile strain in high-k gate oxide film to several percent.

III. FIRST-PRINCIPLES CALCULATION

The band structures of HfO_2, ZrO_2, TiO_2, and SiO_2 were analyzed by self-consistently solving the Hohenberg-Kohn-Sham equations according to the framework of the local density approximation (LDA) [7]. The structures of HfO_2 and ZrO_2 were assumed to be fluorite. The TiO_2 and SiO_2 structures are assumed as the rutile and β-cristobalite, respectively. For example, Fig. 2 illustrates the positions of atoms in fluorite HfO_2 and ZrO_2.

The pseudopotentials were generated with a method developed by Troullier and Martins[8]. Moreover, the exchange-correlation potential of Ceperley and Adler[9] parameterized by Perdew and Zunger[10] was applied. The wave functions were expanded in a plane-wave basis set with an energy cutoff of 60 Ry. we calculated the unstrained band structure by using the measured lattice constant. The unstrained lattice constants were 0.512 nm and 0.507 nm for HfO_2 and ZrO_2, respectively. To analyze the effect of strain on the bandgap, HfO_2, ZrO_2, TiO_2 and SiO_2 were hydrostatically deformed and the change in the

bandgap was calculated.

Figure 3 and 4 show the band structures for unstrained and +10% strained crystals for HfO_2 and ZrO_2. Positive strain represents tensile strain and negative strain represents compressive strain. The conduction band and valence band are shown clearly. The valence-band maximum was set as 0 eV.

The calculated bandgaps are 3.45 eV for unstrained HfO_2 and 3.36 eV for unstrained ZrO_2. It is known that the energy bandgap calculated using LDA will be smaller than the measured value. The measured bandgaps are 5.63 eV and 5.40 eV for unstrained HfO_2 and ZrO_2, respectively. As expected, the calculated bandgaps are 37-38% smaller than the measured values, with calculation errors of 2.18 eV for HfO_2 and 2.04 eV for ZrO_2.

The band structure changed and the bandgap drastically decreases under the tensile strain field. The bandgap, E_g, is approximately given by using the ionization potential, I, the electronegativity, A, and the madelung potential, V_M, as follows,

$$E_g = I - A + 2eV_M \quad \cdots(1)$$

where e is the electron charge magnitude. It can be said that the V_M is inversely proportional to atomic distance, so that V_M decreases with increasing tensile strain. Consequently, E_g decreases with increasing tensile strain.

Figure 5 shows the calculated strain dependence of the bandgaps of HfO_2, ZrO_2, TiO_2, and SiO_2. Note that the values of the bandgaps shown in Fig. 3 and 4 are modified from the original calculated value to compensate for the calculation error. The bandgaps drastically decrease as tensile strain increases. The bandgaps of high-k materials and SiO_2 at 10% strain were about 1 and 2 eV smaller than at zero strain.

IV. STRAIN DEPENDENCE OF THE LEAKAGE CURRENT

We calculated the strain dependence of the leakage current by using the WKB approximation[7]. The leakage current can be represented by

$$J(\Phi_B, T_{ox}, E_{ox}) = \frac{n_v m_d k_B T}{2\pi^2 \hbar} \int_0^\infty T_{WKB}(\Phi_B - E + E_F, T_{ox}, E_{ox}) \times \ln\left(1 + \exp\left(\frac{E_F - E}{k_B T}\right)\right) dE. \quad \cdots(2)$$

using the Esaki-Tsu formula. Here, Φ_B is the barrier height between the electrode and the gate dielectric measured from the Fermi level in the electrode, E_F. T_{ox} is the thickness of the gate dielectric, and E_{ox} is the electric field in the gate dielectric. n_v and m_d are the valley degeneracy and the density-of-state mass in the electrode, respectively. The tunneling probability, T_{WKB} is given by

$$T_{WKB}(E, T_{ox}, E_{ox}) = \begin{cases} \exp\left[-\frac{4\sqrt{2m_{ins}}}{3\hbar q E_{ox}}\left\{E^{3/2} - \left(E - qE_{ox}T_{ox}\right)^{3/2}\right\}\right] \\ \qquad (E > qE_{ox}T_{ox} : \text{direct tunneling}) \\ \exp\left[-\frac{4\sqrt{2m_{ins}}}{3\hbar q E_{ox}} E^{3/2}\right] \\ \qquad (E < qE_{ox}T_{ox} : \text{FN tunneling}) \end{cases} \quad \cdots(3)$$

Here, m_{ins} is the tunneling mass in the gate dielectric. We used the m_{ins} of SiO_2 for calculating the leakage current through HfO_2, ZrO_2, and TiO_2. We assumed that the bandgap change caused by the strain field in the gate dielectric changes the barrier height between the electrode and the gate dielectric. Figure 6 shows the band diagram model for the strained gate dielectric. $\Phi_B^{unstrained}$ is the barrier height between the electrode and the gate dielectric gotten from the Fermi level in the electrode. Thus, the leakage current can be calculated from the barrier height. ΔE_g is the difference between the unstrained bandgap, $E_g^{unstrained}$, and the strained bandgap, $E_g^{strained}$. We assumed that the barrier heights have the same strain dependence in the conduction and valence bands; that is, the strained barrier height $\Phi_B^{strained}$ is equal to $\Phi_B^{unstrained} - \Delta E_g/2$.

Figure 7 shows the strain dependence of the leakage current density of the 0.7-nm equivalent oxide thickness (EOT) high-k dielectric and 3.0-nm-thick SiO_2 dielectric under an applied voltage of 1 V.

The leakage current in each dielectric drastically increases as tensile strain increases. The leakage current in HfO_2 and ZrO_2 at 10% strain was about 100 times higher than at zero strain. In particular, the leakage current in TiO_2 at 10% tensile strain was about 10^5 times higher than at zero strain and exceeds the value for 3.0-nm-thick SiO_2 at 10% tensile strain.

The miniaturization of MOSFETs together with the use of new materials significantly increases strain in the gate oxide and thus increases leakage current. It is thus clear that reducing strain in high-k gate oxide will be very important for ensuring device reliability.

V. CONCLUSIONS

We analyzed the strain dependence of the leakage current of gate oxides by performing a first-principles calculation. The calculation showed that tensile strain in a high-k gate oxide increases leakage current. The tensile strain concentrates at the edge of the gate electrode, and it easily exceeds a few percent. We therefore concluded that

stress and strain in new gate electrode materials must be reduced to ensure device reliability.

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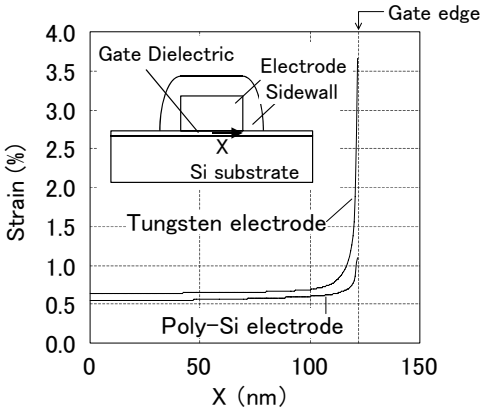


Fig. 1 Tensile strain distribution in gate oxide on which poly-Si or tungsten is deposited as a gate electrode.

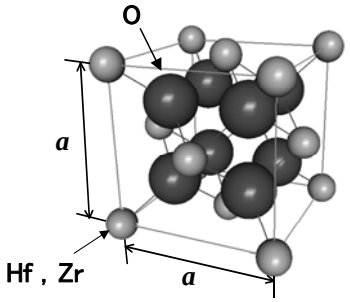
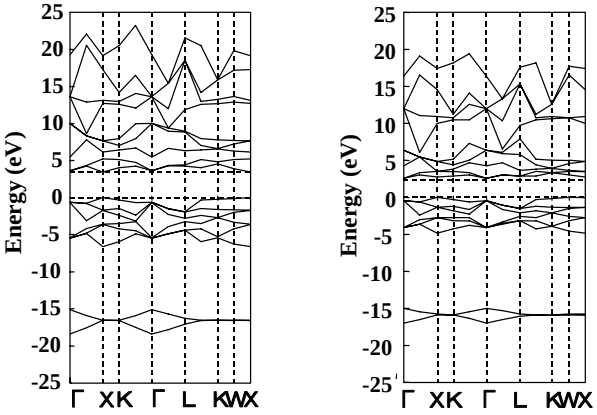
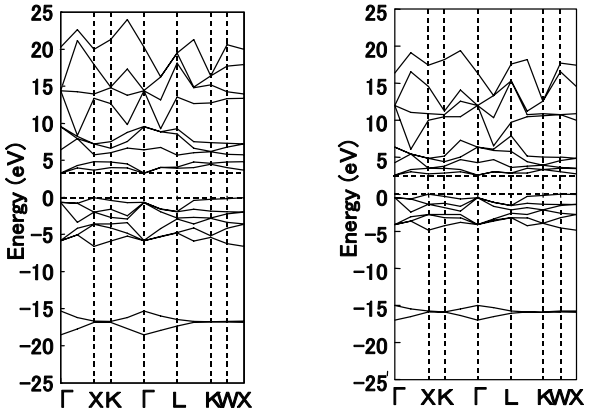


Fig. 2 Positions of atoms in fluorite HfO_2 and ZrO_2. (*a* : atomic constant)



(a) 0% strain (b) +10% strain

Fig. 3 Calculated band structure for HfO_2.



(a) 0% strain (b) +10% strain

Fig. 4 Calculated band structure for ZrO_2.

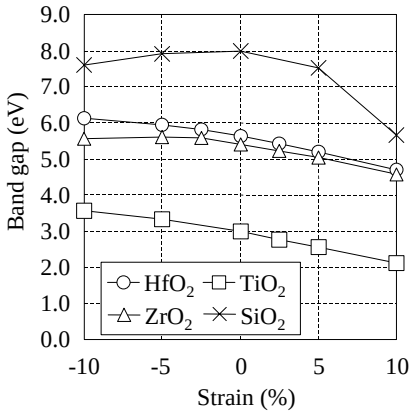


Fig. 5 Strain dependence of bandgap for HfO_2,

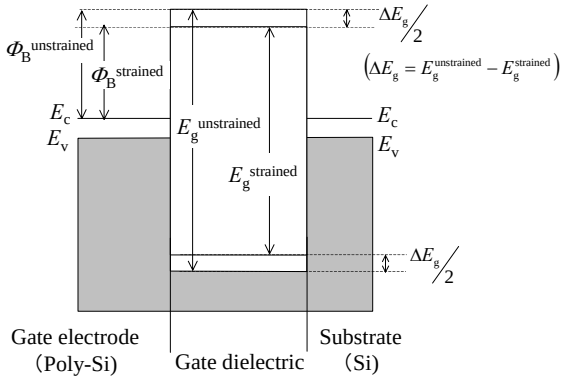


Fig. 6 Band diagram model for strained gate dielectric.

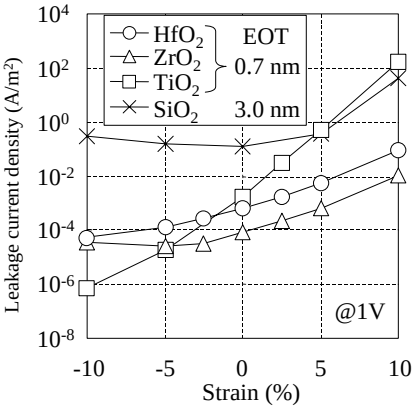


Fig. 7 Strain dependence of leakage current in HfO_2, ZrO_2, TiO_2, and SiO_2.