Strain Optimization to Reduce Gate Leakage Current in MOS Transistors with Silicon Oxynitride Gate Dielectrics by Use of First-Principles Calculations

Yoshiharu Kanegae, Hiroshi Moriya and Tomio Iwasaki

Mechanical Engineering Research Laboratory, Hitachi, Ltd., 502 Kandatsu, Tsuchiura,
Ibaraki 300-0013, Japan
E-mail: kanegae@gm.merl.hitachi.co.

Abstract

We developed a method for optimizing strain to reduce gate leakage current in metal-oxide-semiconductor (MOS) transistors by using first-principles calculations. This method was used to investigate the possibility of decreasing gate leakage current by controlling the strain on gate dielectric materials. We found that compressive strain decreases drastically the leakage current through silicon oxynitride (SiON) gate dielectrics. This change reflects strain-induced change in the band gap of the material. Using finite element analysis to estimate the strain in MOS transistors, we showed the usability of SiON in terms of gate leakage currents and the importance of controlling the strain on the gate dielectric materials.

1 Introduction

The performance of semiconductor devices has been improved by reducing pattern size, but the gate dielectrics in metal-oxide-semiconductor (MOS) transistors become thinner as patterns become finer. The leakage current passing through the thin gate dielectrics because of the tunneling effect thus increases and so does power consumption. Silicon oxide (SiO_2) has been being conventionally used as the gate dielectric material in MOS transistors. However, the SiO_2 gate dielectric in the present mass-produced 0.1-μm devices is now becoming close to its physical limit, and silicon oxynitride (SiON) gate dielectrics are beginning to be used. This material has a relative dielectric constant about 1.5 times higher than that of SiO_2 and its use in place of SiO_2 reduces the gate leakage current in MOS transistors because it would be about 1.5 times thicker with the same capacitance as SiO_2 gate dielectrics. The SiON gate dielectrics should therefore be used as long as possible until so-called high-*k* (high-dielectric-constant) gate dielectrics like hafnium oxide (HfO_2) and zirconium oxide (ZrO_2) gate dielectrics can be put to practical application in mass-produced devices.

Controlling the strain on thin films used in fine-structured devices like semiconductors is often important, and strain-induced leakage current has been confirmed in a semiconductor device [1]. Since this current might be due to strain decreasing the band gaps of gate dielectric materials [2], the strain dependence of the band gaps of various gate dielectric materials should be investigated. Thus, in this work, we used first-principles calculations to investigate the strain dependence of the band gap of SiON and of the leakage current in MOS transistors with SiON gate dielectrics.

2 Strain Dependence of Band Gaps

To calculate the band structures of SiON by first-principles calculations, we first assumed the crystal structures of this material. We assumed the structure of SiON to be that of the Si_2N_2O, which is the only known crystal structure of SiON [3]. We put periodic boundary conditions on this crystal, and calculated the band structure based on the density-functional theory (DFT) with the generalized gradient approximation (GGA). We also calculated the band structure of SiO_2 assuming the β-cristobalite structure [4] by use of the same method. To calculate the strain dependence of leakage current in MOS transistors, we needed the strain dependence of the band gaps of the SiON and SiO_2 used as gate dielectric materials. We explored the effects of strain on these band gaps by calculating band structures with hydrostatic strains on these crystals. This hydrostatic strain was expressed by increasing and decreasing the lattice constants of these materials, increasing them to model tensile strain and decreasing them to model compressive strain. To perform the first-principles calculations, we used the Cambridge Sequential Total Energy Package (CASTEP) in Materials Studio by Accelrys Inc.

The strain dependence of the band gaps of SiON and SiO_2 is shown in Fig. 1, where positive strains are tensile and negative strains are compressive. Since the band gaps calculated by DFT are known to be smaller than the measured values, we corrected the calculated values using the measured ones under no strain by our X-ray photoelectron spectroscopy (XPS) measurement. We can see in Fig. 1 that the band gap of SiO_2 shows little change under compressive strain and decreases under tensile strain. The band gap of SiON, on the other hand, increases under compressive strain and decreases under tensile strain. We can thus expect that if the SiON gate dielectrics in MOS transistors are under compressive strain, the leakage current will be decreased. Furthermore, the rate-of-change in band gap of SiON is larger than that of SiO_2. Therefore, we think that the bandgap of SiON gate dielectrics can be controlled by strain more easily than can that of SiO_2 dielectrics.

3 Strain Dependence of Gate Leakage Current

The gate leakage current in a MOS transistor was evaluated using the formula under the Wentzel-Kramers-Brillouin (WKB) approximation [5, 6]. Since a strain changes the band gaps of materials, we expressed the effect of strain as the change of band gap shown in Fig. 2. We considered the change of band gaps ΔE_g to change the work functions as $\Phi_\mathrm{B}^\mathrm{strained} = \Phi_\mathrm{B}^\mathrm{unstrained} - \Delta E_\mathrm{g}/2$, where $\Phi_\mathrm{B}^\mathrm{strained}$ and $\Phi_\mathrm{B}^\mathrm{unstrained}$ are the work functions with strain and that without strain respectively. We determined the $\Phi_\mathrm{B}^\mathrm{unstrained} = E_\mathrm{g}^\mathrm{unstrained} - E_\mathrm{g}^\mathrm{Si} - E_\mathrm{of}$, using measured values of $E_\mathrm{g}^\mathrm{unstrained}$, E_g^Si and E_of as shown in Fig. 3, where E_g^Si (= 1.1 eV) is band gap of Si.

To estimate the order of strain on gate dielectrics in MOS transistors, we used a finite element method (FEM) analysis in which the formation conditions such as film-deposition temperature and the shape change of the film by deposition were taken into account precisely. The intrinsic stress of thin films used for the gate structure was also considered in the analysis. We clarified by the analysis that the principal strain concentrates at the bottom edge of the gate electrode and that the maximum strain is about 3 %. Thus, we assumed that the realistic and controllable strains in MOS transistors are up to 3 % and calculated the corresponding strain dependence of gate leakage current.

The strain dependence of gate leakage current in MOS transistors with SiON and SiO_2 gate dielectrics are shown in Fig. 3. In calculating the values plotted there, we assumed the gate bias $V_G = 1.1$ V and equivalent oxide thickness of gate dielectrics $T_{OX} = 1.2$ nm. We can see that the leakage current through the SiO_2 gate dielectric is relatively very large and does not change much under strain. Thus, we think that the leakage current through a SiO_2 gate dielectric can hardly be controlled by controlling the strain on the dielectric. On the other hand, the leakage current through the SiON gate dielectric decreases under compressive strain and increases under tensile strain, reflecting an increased and a decrease of the band gap of SiON (Fig. 1). The difference between the leakage current under a tensile strain of 3 % and that under a compressive strain of 3 % is more than one order of magnitude. Therefore, we think that controlling the strain on a SiON gate dielectric will decrease the gate leakage current in a MOS transistor more than will controlling the strain on a SiO_2 dielectric. We suggest that if SiON is used as the gate dielectric in MOS transistors and the strain on the SiON gate dielectric is controlled to be compressive, the gate leakage current can be decreased drastically.

4 Summary

Using first-principles calculations, we investigated the strain dependence of the band gaps of SiON and SiO_2 and of the gate leakage current in MOS transistors with SiON and SiO_2 gate dielectrics. We found that the leakage current through a SiO_2 gate dielectric does not change much under changes in strain on the dielectric. Thus the leakage current through a SiO_2 gate dielectric can hardly be expected to be reduced by adjusting the strain on the dielectric. The leakage current through a SiON gate dielectric, on the other hand, decreases under compressive strain and increases under tensile strain. We suggested that the gate leakage current in MOS transistors can be decreased drastically by using SiON as the gate dielectric and controlling the strain on the dielectric to be compressive. We think the results of this study can contribute to the production of more reliable semiconductor devices.

References

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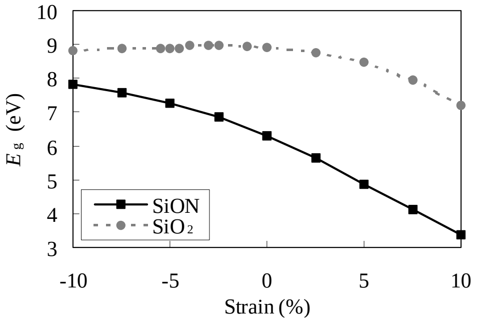

Figure 1: Strain dependence of band gap E_g for SiON and SiO_2. (1 eV = 1.6×10^{-19} J).

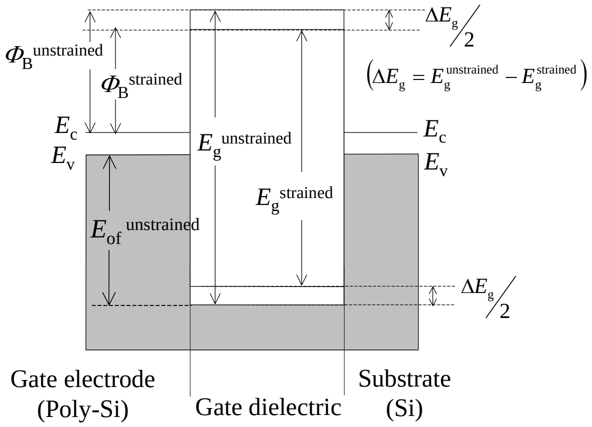

Figure 2: Band diagram model for a strained gate dielectric in a MOS transistor. $E_g^{\text{unstrained}}$ and $\Phi_B^{\text{unstrained}}$ are respectively the band gap and the work function with no strain. Under strain these change to E_g^{strained} and Φ_B^{strained}.

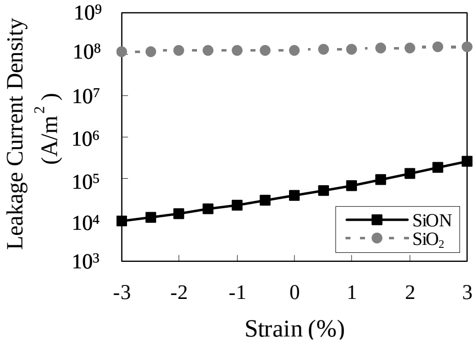

Figure 3: Strain dependence of gate leakage current in MOS transistors with SiON and SiO_2 gate dielectrics.