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First-Principles Calculation of High Strain-Induced Leakage Current in Silicon Dioxide used for Gate Dielectrics

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1. Introduction

Increasing capacitance of a gate dielectric and decreasing resistivity of a gate electrode are indispensable for improving electronic performance of MOSFETs. However, simple thinning of a gate oxide film causes high leakage current because of an increase in the tunneling current through the oxide film. In addition, it has been found that tensile stress higher than 1 GPa often occurs in new materials, such as metal-silicides and tungsten, that are used for a gate electrode [1]. Since it is well known that tensile strain in crystals reduces the bandgap of materials, such a high tensile stress may decrease the bandgap of the thin gate oxide and, thus, further increase leakage current [2].

In light of this background, we investigated the mechanical stress (strain)-induced leakage current through a SiO_2 gate dielectric. The change in the bandgap of SiO_2 caused by crystallographic strain was analyzed by a first-principles calculation. The leakage current was estimated by applying the Wentzel-Kramers-Brillouin (WKB) approximation [3]. A finite element method (FEM) was also used to analyze the strain field in a MOSFET structure. The increase in the leakage current caused by a tungsten gate electrode was evaluated quantitatively.

2. FEM Analysis

We analyzed the material dependence of a strain field in a gate oxide film by using FEM analysis. In this analysis, the gate-electrode-formation conditions such as film-deposition temperature and the shape change of the film deposited by etching were taken into account precisely. The intrinsic stress of thin films used for the gate structure was also considered in the analysis [4]. The measured values were 0.7 GPa for poly-Si, 2 GPa for tungsten, and -1 GPa for SiN_x used for the side wall of the gate electrode.

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. The maximum strain of about 1% develops when poly-Si is deposited on the oxide. The strain reaches about 3.5% when the gate material is changed to tungsten. It is thus concluded that the new gate material increases tensile strain in the gate oxide film and may increase leakage current.

3. First-Principles Calculation

The band structure of SiO_2 was analyzed by self-consistently solving the Hohenberg-Kohn-Sham (HKS) equations according to the framework of local density approximation (LDA) [5]. The structure of SiO_2 was assumed as the β-cristobalite. The positions of atoms in β-cristobalite SiO_2 are illustrated in Fig. 2. The measured lattice constant a is 0.716 nm. The pseudopotentials are generated using the method of Troullier and Martins [6]. The exchange-correlation potential of Ceperley and Adler [7] parameterized by Perdew and Zunger [8] was applied for this analysis. The wave functions are expanded in a plane-wave basis set with an energy cut-off of 60 Ry. The energy-band structure shown in Fig. 3 was calculated for unstrained SiO_2 (a = 0.716 nm). It is known that the energy bandgap calculated using LDA is smaller than the measured value. The calculated bandgap, E_g is 5.3 eV, which is about 34% smaller than the reported value of 8 eV.

To analyze the effect of strain on the bandgap, β-cristobalite SiO_2 was hydrostatically deformed and the change in the bandgap was calculated. Figure 4 shows the calculated strain dependence of the bandgap. Note that the value of the bandgap shown in Fig. 4 is modified from the original calculated value by adding 2.7 eV to compensate the calculation error. The bandgap of SiO_2 is a maximum near the unstrained state (zero strain) and decreases drastically with increasing in tensile strain.

The strain dependence of the leakage current was calculated by using WKB. Figure 5 shows the band diagram model for the strained SiO_2. ΔE_g is the difference between the unstrained bandgap, $E_g^{unstrain}$ and the strained bandgap, E_g^{strain}. The measured value of the barrier height, $\Phi_B^{unstrained}$, at Si/SiO_2 interface is 3.1 eV when the oxide is not strained. We assumed that the strained barrier height, $\Phi_B^{strained}$, is equal to $\Phi_B^{unstrained} - \Delta E_g / 2$.

Figure 6 shows the strain dependence of the leakage current density of 1.0-nm-thick oxide under an applied voltage of 1 V. The leakage current is minimum near the unstrained state (zero strain) and increases widely with increasing in tensile strain. The leakage current at 10% strain is about 16 times higher than that at zero strain. It is thus clear that reducing strain in the oxide is very important in terms of device reliability.

4. Conclusions

It was shown that tensile strain in a gate oxide increases leakage current. The tensile strain concentrates at the edge of the gate electrode and it easily exceeds a few percent. It is therefore concluded that strain in the gate electrode materials must be reduced to improve reliability of devices.

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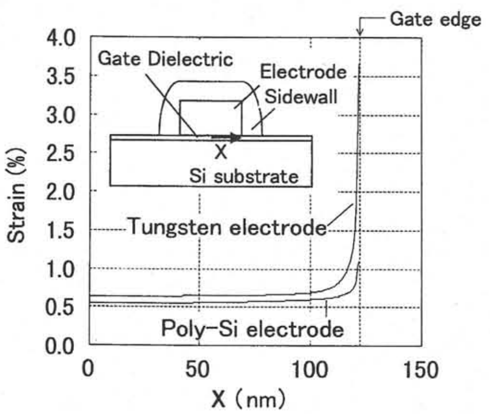

Fig. 1 Tensile strain distribution in gate oxide (SiO_2) on which poly-Si or tungsten is deposited as a gate electrode.

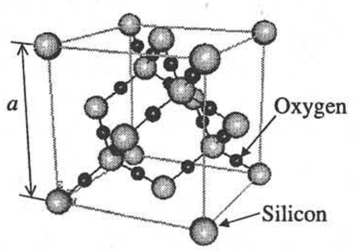

Fig. 2 Positions of atoms in β-cristobalite SiO_2.

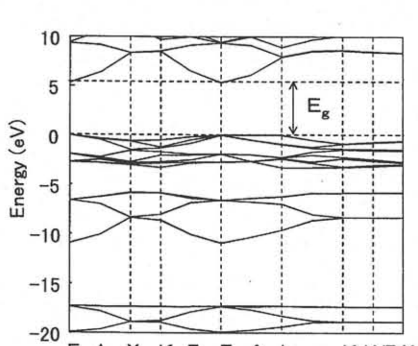

Fig. 3 Calculated band structure for unstrained β-cristobalite SiO_2 (a = 0.716 nm).

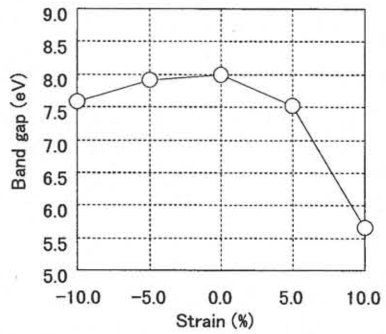

Fig. 4 Strain dependence of bandgap for β-cristobalite SiO_2.

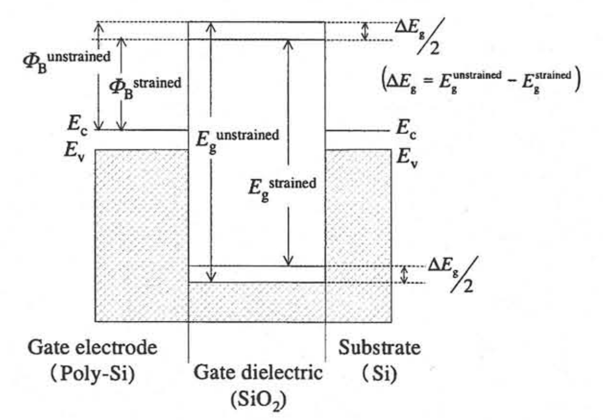

Fig. 5 Band diagram model for strained SiO_2.

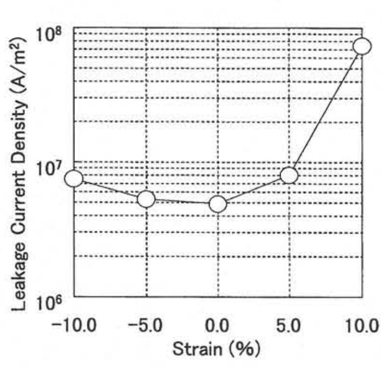

Fig. 6 Strain dependence of leakage current in β-cristobalite SiO_2.