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Effects of oxidation process on interface roughness of gate oxides on silicon: X-ray reflectivity study

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We report on the effects of the wet and dry oxidation processes on the interfacial roughness and time dependent dielectric breakdown (TDDB) characteristics of the poly-Si/SiO_2/Si(100) trilayer. The interface roughness of the oxide layers buried under a thick poly-Si electrode has been investigated using an x-ray reflectivity technique. Analysis of x-ray reflectivity data for the trilayer samples and for a bare oxide film shows that interface roughness of poly-Si electrode/SiO_2 interfaces depends on oxidation process while oxide layers have smooth SiO_2/Si-subtstrate interfaces. TDDB of the SiO_2 layer has also been observed to depend on the oxidation process, indicating that the interface roughness is a crucial factor affecting the TDDB characteristics. The wet oxidized SiO_2 film is more stable to dielectric breakdown and has smoother interfaces than the dry oxidized sample. © *1998 American Institute of Physics.* [S0003-6951(98)00704-9]

SiO_2 films are technologically very important for their application as a gate oxide material in dynamic random access memory (DRAM). The reliability of the device depends on the dielectric property of the oxide film. Hence, understanding the degradation of oxide films under electrical stress leading to dielectric breakdown is essential to fabricate highly reliable devices.[1] Recently many attempts have been made to determine the causes of the degradation of these films leading to device failures.[2–4] In an earlier study it was proposed that the failures of SiO_2 layers are mainly due to defects in the bulk rather than interface defects.[2] Some studies on the effect of interfacial structure of the oxide film on electrical characteristic have been reported.[3–5] It has been observed that the surface quality of the Si wafer plays an important role in dielectric stability of the devices, which is an indication that interface roughness affects the electrical characteristics.[5] Recently, electrical breakdown studies of $SiO_2/Si_3N_4/SiO_2$ (ONO) film showed that degradation of time dependent dielectric break-down (TDDB) is caused by interface roughness of silicon nitride (Si_3N_4) film.[3,4] In these studies interface roughness was measured with transmission electron microscopy and atomic force microscopy, and the degradation was attributed to local thinning of layer thickness.

It is well known that SiO_2 layers, grown thermally either in wet or dry oxygen ambient, show different TDDB characteristics.[2] However, quantitative comparison between interface roughness of the buried SiO_2 layer prepared by both oxidation processes with their effects on TDDB characteristics has not been reported to our knowledge. In this letter we present our investigation on the effect of oxidation in wet and dry oxygen atmosphere on interface roughness of the poly-Si/SiO_2/Si(100) trilayer, which is the structure of gate oxides in metal-oxide-semiconductor (MOS) devices, and their TDDB characteristics.

Two oxide samples with a nominal thickness of 100 Å were prepared on *p*-type Si(001) substrate by (a) wet oxidation and (b) dry oxidation methods at LG Semicon Co. After the oxidation process, the oxides were annealed under N_2 atmosphere for 30 min. Both oxide films were capped with 2000 Å thick *p*-type poly-Si electrodes by chemical vapour deposition. X-ray reflectivity data were collected using synchrotron radiation at Pohang Light Source (PLS) 3C2 beamline with a Huber four circle goniometer. A Si(111) double crystal monochromator was used to choose the x-ray wavelength of 1.6081 Å. For TDDB measurements capacitor cells of size 150 μm×150 μm were patterned on wafers. A failure rate was measured as a function of time when constant currents of 100 mA/cm^2 were injected into the capacitor cells.

In Fig. 1 x-ray specular reflectivity data of both wet and dry oxidized samples are shown along with the fit explained

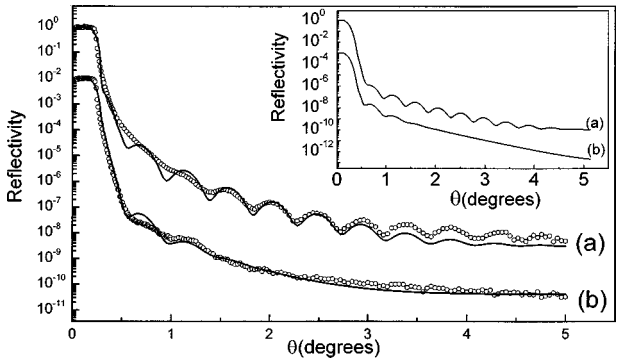

FIG. 1. X-ray reflectivity of poly-Si/SiO_2/Si(100) for thermally grown SiO_2 films using (a) wet oxidation and (b) dry oxidation process. Solid lines represent the fitting. Inset: Simulated x-ray reflectivity curves (a) for a layer with an AED contrast of 0.01 Å^{-3} and having smooth interfaces of 2 Å roughness, and (b) for a layer with an AED contrast of 0.06 Å^{-3} and having both smooth and rough interfaces of 2 Å and 8 Å roughness, respectively.

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below. For the analysis we incorporated correction of geometrical factors (foot-print correction) and substracted the offspecular diffuse background to obtain true specular reflectivity intensities. Figure 1 shows the corrected x-ray reflectivity data. We observe a sudden drop in reflectivity above the critical angle θ_c, indicating that both samples have large roughness amplitudes at the poly-Si electrode surfaces. However, we can see the difference between the two curves at the large angle of incidence (θ). For the wet oxidized sample oscillations in the reflectivity curve are clearly observable, while in the case of a dry oxidized sample the oscillations are not observed. The period of the oscillation corresponds to 102 Å which is the nominal thickness of the buried oxide layers. The oscillations in the reflectivity are due to a large contrast in the average electron density (AED) between the layers (i.e., a large difference in AED values of the layers) and smooth interfaces.[6,7] If either of these conditions are not satisfied then the oscillations in the reflectivity are not observed as illustrated for the dry oxidized sample in Fig. 1. The oscillation in reflectivity curve is observed only at large angles due to the large thickness of poly-Si layer on top of the oxide layer.

To analyze our x-ray reflectivity data quantitatively we have used a simple semi-kinematical approximation. The explicit formula for the reflectivity amplitude ($X=\mathrm{E}_{refl.}/\mathrm{E}_{inc.}$) can be expressed as

$$X=\sum_{l=1}^{N} r_l e^{-i\phi_l}, \quad \phi_l=-\sum_{j=1}^{l-1} q_j d_j, \tag{1}$$

where $N(=3)$ is the number of layers, r_l is the Fresnel coefficient of the lth interface which determines the amplitude of oscillation and depends on the contrast of AED, d_j is the thickness of the jth layer, and q_j is the normal component of the incident wave vector of the jth layer containing both real and imaginary components of the layer's refraction index. Hence, the above expression includes the effects of absorption and refraction. Roughness at each interface was introduced using a Debye–Waller like term such that r_l is multiplied by a factor of $\exp(-q_l q_{l-1}\sigma_l^2)$, where σ_l is the interface roughness amplitude.[8] We did not include multiple scattering effects since the reflected intensities are very weak (less than 10^{-4} of the incident beam intensity).

The parameters obtained from fitting the above expression to the specular x-ray reflectivity data are given in Table I. The top surface roughness of poly-Si is estimated to be about 30 Å for both samples. We observe that one of the interface roughness of SiO_2 in the dry oxidized sample is larger than that of the wet oxidized sample. We also observe smaller contrast in AED between poly-Si and SiO_2 of the dry oxidized sample than that of the wet oxidized sample. To pinpoint whether the large amplitude of roughness or the small AED contrast is responsible for the absence of oscillations in the reflectivity of the dry oxidized sample, we have simulated the reflectivity curves by varying the contrast in AED and the interface roughness. We show the simulated result in the inset of Fig. 1. We find that if both interface roughness of poly-Si/SiO_2 and SiO_2/sub-Si is 2 Å, then even with a very small AED contrast of 0.01 $Å^{-3}$ we still observe oscillation in the reflectivity curve as shown in curve (a) of the inset. We found that increased interface roughness for a layer even with a larger AED contrast reduces the oscillations in the reflectivity curve very rapidly. The reflectivity curve (similar to that of the dry oxidized sample) could be achieved as shown in curve (b) of the inset assuming a smooth interface ($\sigma\sim$2 Å) and a rough interface ($\sigma\sim$8 Å) for a buried SiO_2 layer with an AED contrast of 0.06 $Å^{-3}$. Thus we conclude that smooth interfaces of poly-Si/SiO_2/Si substrate for the wet oxidized sample gives rise to oscillations in the reflectivity curve at high angles while absence of oscillations in the reflectivity for dry oxidized sample is due to the large interface roughness at one of the SiO_2 interfaces.

TABLE I. Parameters obtained from the fit for wet and dry oxidised gate oxides.

Sample	Layer	Thickness (Å)	AED ($Å^{-3}$)	Roughness (Å)	Absorption ($\times10^{-6}$)
	poly-Si	2000±20	0.69	27	1.61
dry	SiO_2	98	0.65	8	0.87
	Si	⋯	0.70	2	1.61
	poly-Si	1980±20	0.69	34	1.61
wet	SiO_2	102	0.63	2	0.87
	Si	⋯	0.70	2	1.61
SiO_2/Si	SiO_2	77	0.667	3.37	0.84
(model A)[a]	Si	⋯	0.706	2.09	1.59
SiO_2/Si	SiO_2	77	⋯	2.38	0.84
(model B)[a]	Si	⋯	0.706	2.00	1.59

[a]Parameters of a bare oxide layer obtained using Parratt's recursion relation.

For the structure of gate oxides it is very difficult to determine which interface of the dry oxide layer has a larger roughness amplitude. This is evident from $|X|^2$ of Eq. (1) which contains a symmetric oscillatory term with respect to the exchange of roughness amplitudes. In order to determine which interface is rough, we prepared a dry oxide thin film on a Si substrate without a cap layer to avoid symmetric interfaces; the interfaces are now those of air/SiO_2 and SiO_2/Si-substrate. The x-ray reflectivity data of this sample are shown in Fig. 2. We have used Parratt's formalism[9] to analyze the x-ray reflectivity data. First we considered a single layer of SiO_2 with no variation in AED in the layer (model a); the result of the fit is presented by a solid line. We tried to improve the fit by including variations in AED in the oxide layer[10,11] (model b); and got consistent values for

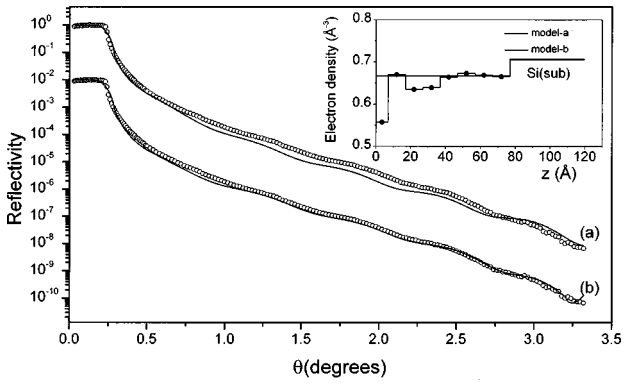

FIG. 2. X-ray reflectivity of a thermally grown SiO_2 film by dry oxidation process. Solid lines represent the fit using Parratt's recursion relation for model a (a), and model b (b). Inset: Electron density profiles for model a and model b. Sizes of errors are equivalent to those of symbols.

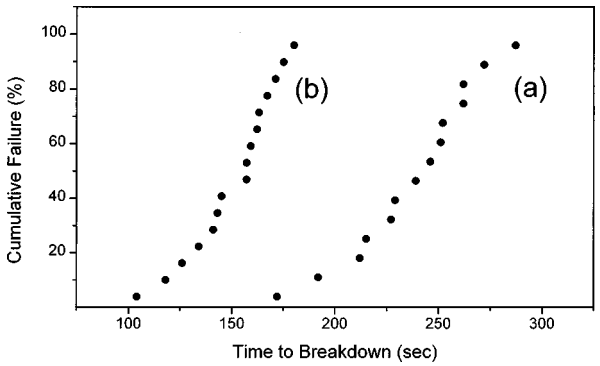

FIG. 3. TDDB plot of poly-Si/SiO_2 /Si(100) of thermally grown SiO_2 film using (a) wet oxidation and (b) dry oxidation process.

roughness amplitudes. The variation in AED is shown in a magnified scale in the inset of Fig. 2. In model b interface widths at air/SiO_2 and SiO_2/Si were only considered and the total thickness of the SiO_2 film was kept the same as model a. The parameters obtained from the fit are given in Table I. We estimate roughness amplitudes of the SiO_2/Si-substrate interface in dry oxides as ~2 Å, which is consistent with values obtained by others.[12–16] By taking a clue from this study, we have attributed the smooth interface to the SiO_2/Si-substrate interface for the dry oxidized sample.

In Fig. 3 we show TDDB characteristics of the samples. Accumulative failure rates in percentages are plotted as functions of time. We observe that for the wet oxidized samples the failure occurs later than the dry oxidized samples, indicating that wet oxidized samples are more stable compared to dry oxidized samples. This has been observed in earlier studies.[2] We attribute this stability of wet oxidized sample to its smooth interfaces. Since interface roughness amplitude even for the dry oxidized sample is very small (~8 Å) compared to the layer thickness (~100 Å), it is not clear whether dielectric breakdown of the layer is caused mainly by local thinning of the layer thickness, as reported for ONO films[4] or by interface defects.[2] Further study of the oxide layers with various thicknesses is required to clarify this point.

In summary, we have demonstrated that interface roughness of the gate oxide layer buried under a thick electrode can be quantitatively characterised by x-ray reflectivity measurements with a simple semikinematical analysis. It is also shown that there is a clear difference between x-ray reflectivity curves of wet and dry oxidized samples. The wet oxidized layer has smoother interfaces and, as a result, is more stable under electrical stress than the dry oxidized one. Similar analysis can be used to study interfaces and dielectric stability of other oxides which are considered as candidates for a charge storage material for the next generation memory devices.

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