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Contribution of Si/SiO_2 Interface Roughness in the Observation of Chemical Structure

Kenji ISHIKAWA, Hiroki OGAWA, Carlos INOMATA and Shuzo FUJIMURA

Process development division C850, Fujitsu Limited
1015 Kamikodanaka, Nakahara-ku, Kawasaki 211, Japan

Interfacial oxide structure was studied by infrared reflection absorption spectroscopy (IR-RAS). Interfacial structure was found to arise from the height and width of the longitudinal optical phonon mode and was analyzed. In order to account for interface roughness, we used a four phase model (ambient/bulk SiO_2/inter-layer/Si) and an the inter-layer based on the effective medium approximation (EMA) in which interface roughness is assumed to be a physical mixture of Si and SiO_2. The results are in satisfactory agreement with experimental data and thus interface roughness is found to be relevant in the discussion of the Si/SiO_2 interface chemical structure.

1. Introduction

In gate oxide fabrication of silicon metal-oxide-semiconductor devices, the evaluation of the chemophysical oxide structure is required in order to assess the influence of film formation method on device performance.

As device dimensions shrink, gate oxide thicknesses reach under 5 nm and the oxide structure is probably different in this region. In previous publications[1], the shift in wave number of the IR transmittance absorption peak due to the transverse optical phonon polariton (TO) arising from Si-O stretching vibration correlated to intrinsic stress at the Si/SiO_2 interface. These studies did not consider interface roughness, however.

The effects of interface roughness on stress relief is of interest, as is a new oxide growth mechanism that includes interface morphology formation since interface roughness entails the definition of thickness to be ambiguous. Both chemical structure and interface roughness are important considerations.

In this study, the effects of interface roughness on IR spectra are investigated through simulation using the effective medium approximation model which assumes interface roughness to be a physical mixture of Si and SiO_2.

2. Experimental procedure and results

IR-RAS was done with p-polarized light at oblique angles of incidence. This method detects the longitudinal optical phonon polariton (LO) arising from Si-O stretching vibration and can be applied to industrial wafers with lapped back surfaces.

Substrate material used was Si(111) wafers of 1kΩcm resistivity. Following wet cleaning, chemical oxides were stripped by NH_4F and the samples were then oxidized in a standard furnace at 1100°C in dry O_2.

In a previous study[2], we compared bulk structure with interfacial structure by incrementally etching back the oxide and performing RAS. Spectra simulation was done using the actual dielectric function derived from the bulk oxide since measured spectra is distorted if the optical path and thickness change.

Figure 1 shows the actual spectrum (solid) of the interfacial oxide and the simulated spectrum

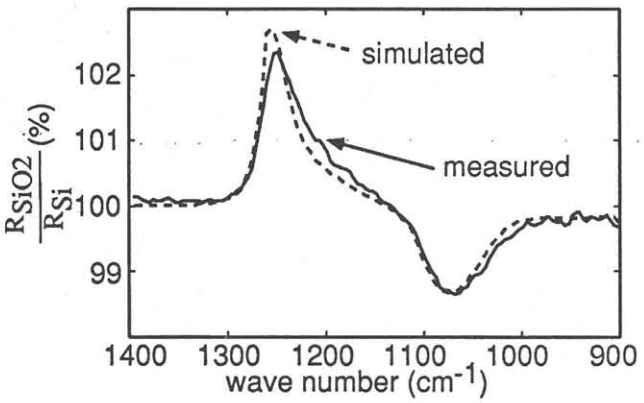

Fig. 1 RAS spectra of actual (solid) interfacial oxide of less than 3 nm and simulated (dotted) bulk oxide of less than 3 nm.

(dotted) of the bulk oxide of less than 3 nm. From comparison of the two spectra, the interfacial structure arises from the height and width of the LO mode (at ~1255cm^{-1}) and from the swollen features in the spectral region between the LO and TO modes (at 1060-1080cm^{-1}). These features can be considered to be due to differences in structure near the interface and this study examines the contributions by interface roughness.

Cross-sectional transmission electron microscopy measurement (XTEM) of the Si/SiO_2 interface was done. Figure 2 shows the XTEM topograph of a sample oxidized with the same process parameters as the IR-RAS samples. The interface was observed to be rough but a quantitative discussion of size and periodicity of roughness is not possible from the representation of quasi-cross-section.

3. Models for data analysis and discussion

We assume the existence of an inter-layer at the Si/SiO_2 interface due to roughness and describe the dielectric function (ε_{int}) of the inter-layer using the effective medium approximation which assumes a physical mixture of silicon and spherical oxide embedded into silicon (Fig. 3)[3]. This is valid when the sphere size is smaller than the wave length of light, about 10 μm. ε_{int} is described as

$$L = \frac{a}{a+2} \qquad g = \frac{\varepsilon_{Si}}{L\,\varepsilon_{bulk} + (1-L)\,\varepsilon_{Si}} \qquad (3.1)$$

$$\varepsilon_{int} = 1 + \frac{(1-f)\,(\varepsilon_{Si}-1) + f\,(\varepsilon_{bulk}-1)\,g}{(1-f)+fg}$$

where L is the depolarization factor and f is the volume fraction.

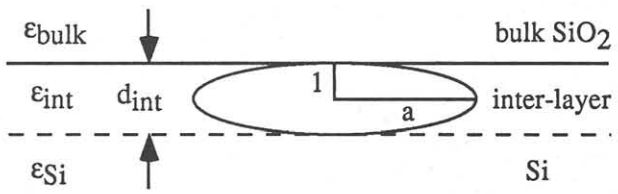

Fig. 3 Schematic diagram of effective medium approximation for interface roughness.

Interface roughness was characterized by EMA parameter and RAS spectra simulation using the schematic diagram of the four phase model

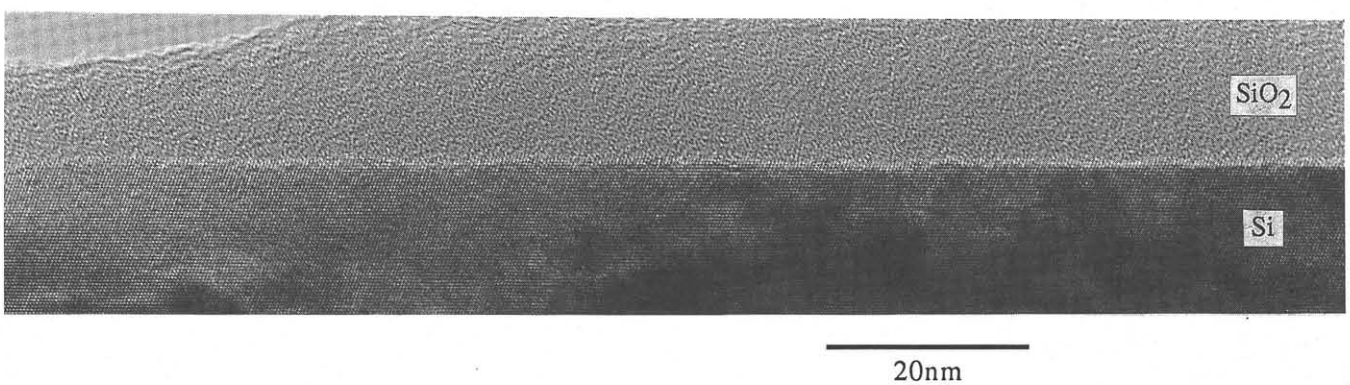

Fig. 2 XTEM topograph of the Si/SiO2 interface.

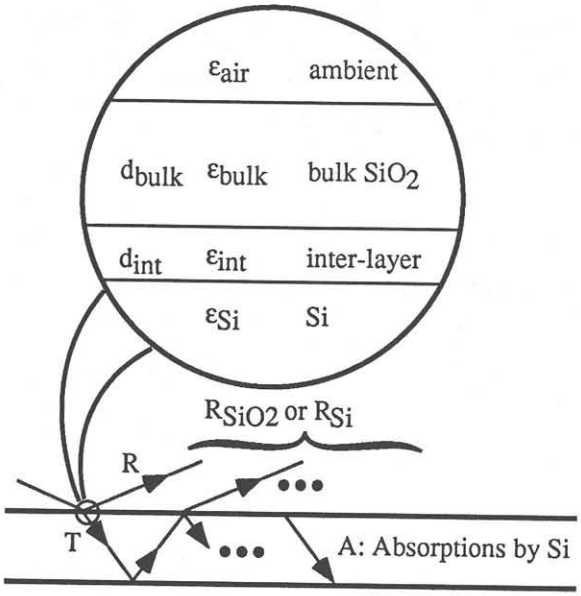

Fig. 4 Schematic diagram of multiple internal reflections of silicon substrate and phase system for RAS spectra simulation.

(ambient/bulk SiO_2/inter-layer/Si) and the multiple internal reflections in the silicon substrate (Fig. 4). Figure 5 shows the simulated result (solid) of the best fit to the spectrum (solid line in Fig. 1) of the interfacial oxide. As reference, the thin dotted line shows the spectrum of the bulk oxide. L, f, and d_{int} values of the best fit results are 0.5, 0.9 and 0.6 nm, respectively. This estimation, however, can be misleading if in fact the result contains the distinct chemical structure near the interface. If another method of roughness measurement enables unambiguous identification of the parameters of EMA, the chemical properties of the oxide are characterized by this method.

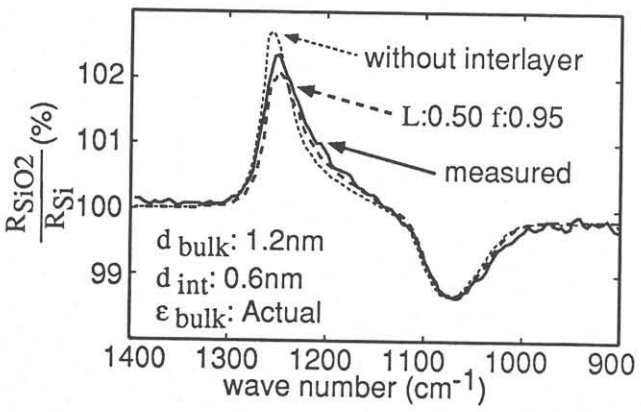

Fig. 5 Simulated RAS spectrum (dotted) of the best fit to measured spectrum {(solid), solid line in Fig. 1} As reference, the simulated spectrum of bulk oxide (thin dotted).

4. Conclusion

Interfacial oxide structure was studied by IR-RAS. The LO mode of the observed spectra of interfacial oxide arose with lower frequency and wider width. These changes were assumed to result from interface roughness. XTEM observation and analysis by the EMA model and by RAS spectra simulation were done. The results are in satisfactory agreement with experimental data. Quantitative interface roughness needs to be assessed due to the possibility of inclusion of chemical structure difference.

Acknowledgments

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References

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