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Optical Absorption in Ultrathin Silicon Oxide Film

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The reflectance spectra of ultrathin thermally grown silicon oxide films with thickness in the range from 6 to 18 nm were measured in the vacuum ultraviolet using synchrotron orbital radiation. From the modified Kramers-Kronig analysis of these reflectance, it has been found that the optical absorption of silicon oxide films below the optical absorption edge of fused quartz becomes appreciable with decreasing oxide film thickness or oxidation temperature.

1. Introduction

As a result of rapid advances in the microfabrication technology, the thickness of gate oxide film used in silicon based metal-oxide-semiconductor field effect transistor is now in the order of 10 nm. In such a case, the interfacial transition layer is expected to give appreciable effect on the chemical structures of gate oxide film. For this reason, the chemical structures near the SiO2/Si interface have been studied extensively¹⁾. The optical properties of silicon oxide have been investigated $^{2-5}$ and those near the optical absorption edge will be also influenced by the interfacial transition layer. However, the following two problems exist in these previous studies: Firstly, thermally grown silicon oxide films used for the transmittance measurement was prepared by removing substrate and is different in structure from as grown oxide films. Secondly, the refractive index of the thermally grown silicon oxide film must be different from that of fused quartz because of the difference in the method of formation. In order to determine the optical constants of as grown silicon oxide films, reflectance measurement, which is nondestructive measurement, was performed in the present study. In order to determine refractive index and extinction coefficient, the effect of multiple reflection in the silicon oxide film must be considered in the Kramers-Kronig analysis. As a result of this analysis the optical absorption in the ultrathin silicon oxide film below the optical absorption edge of fusued quartz was found to depend on the oxide film thickness or the oxidation temperature.

2.Experimental

The silicon oxide films used for the measurements were thermally grown on a ptype silicon (100) surface in dry oxygen at 800 °C and 1050 °C. The measurements were carried out at the Beam Line 1 (BL-1) of 0.38 GeV SOR ring of Institute for Solid State Physics by using a 1 m Seya-Namioka type monochromator in the photon energy range from 4 to 23 eV. The monochromatic light, which was incident on the silicon oxide film with an incident angle of 10 degrees, was polarized in the plane of the incidence. The absolute values of reflectance were determined so that the refractive index of thermally grown silicon oxide film in the photon energy range from 4 to 4.5 eV was equal to that of fused quartz.

3. Results and Discussion

The solid lines in Fig. 1 are the reflectance spectra measured for thermally grown silicon oxide films prepared at 1050°C with oxide film thickness as a parameter. The broken lines in Fig. 1 indicate



Fig. 1 Measured reflectance spectra of thermally grown silicon oxide films are shown by the solid lines with thickness of the oxide film as a parameter, while caluculated reflectance spectra using the optical constants of single crystalline silicon and fused quartz are shown by broken lines. The oxide films used for the measurements were grown in dry oxygen at 1050°C. curves calculated for each oxide film thickness by using the optical constants of single crystalline silicon and fused $quartz^{2}$. According to this figure, the measured reflectance is always smaller than the calculated one in the photon energy range from 6 to 9 eV. Therefore, in this photon energy range the optical properties of thermally grown silicon oxide films must be different from those of fused quartz. In the following, the discussion is mainly focussed on the spectra in this photon energy range.

In order to clarify the dependence of optical properties on the oxide film thickness, the optical constants of thermally grown silicon oxide films should be determined. The optical constants can be determined by including the additional term in the Kramers-Kronig relation. This additional term, which was introduced by Lupashko et al.⁶⁾ arises from a phase change on reflection at the boundarys of a thin silicon oxide film. The phase change thus determined and the reflectance were combined to calculate the optical constants of thermally grown silicon oxide films. The photon energy dependences of the refractive index thus determined are shown by solid lines in Fig. 2 for thermally grown silicon oxide films prepared at 1050°C with oxide film thickness as a parameter. The broken lines are the photon energy dependence of the refractive index of fused quartz. It is found that the refractive index of the silicon oxide film is different from that of fused quartz below the optical absorption edge of the fused quartz especially for thin oxide films. With increasing oxide film thickness, the refractive index of the silicon oxide film approaches to that of fused quartz.

The solid and broken lines in Fig. 3



FIg. 2 Photon energy dependence of refractive index shown by solid lines is obtained from modified Kramers-Kronig analysis of reflectance shown in Fig. 1. Photon energy dependence of refractive index shown by broken lines is those for fused quartz.

show the photon energy dependence of the extinction coefficient of the oxide films and that of fused quartz²⁾, respectively. Here, the refractive indexes shown in Fig. 2 were used to analyze. It can be seen from this figure that the extinction coefficient of the oxide film is larger than that of fused quartz in the photon energy range below the optical absorption edge of fused quartz. The extinction coefficient of the oxide film in this photon energy decreases with increasing oxide film thickness and approaches to that for fused quartz.

In Fig. 4 the solid line shows the



Fig. 3 Photon energy dependence of extinction coefficient shown by solid lines is obtained from modified Kramers-Kronig analysis of reflectance shown in Fig. 1. Photon energy dependence of extinction coefficient shown by broken lines is those for fused quartz.

optical absorption coefficient of 6.9 nm thick silicon oxide film thermally grown at 800°C, while the broken line shows that of 6.0 nm thick silicon oxide film thermally grown at 1050°C. The increase in the optical absorption near the photon energy of 7.6 eV may be correlated with the existence of the shallow bound states 1-2 eV below the conduction-band minimum⁷⁾. Furthermore, the optical absorption at photon energy range below the optical absorption edge of fused quartz extends to lower photon energy than 7.6 eV with decreasing oxidation temperature from 1050°C to 800°C.



Fig. 4 Photon energy dependence of optical absorption coefficient for oxide films thermally grown at 800 and 1050°C is shown by solid and broken line, respectively. An enlarged figure for the photon energy range from 7 to 9 eV is also shown.

4. Conclusion

The reflectance spectra of ultrathin thermally grown silicon oxide films with thickness in the range from 6 to 18 nm were measured in the vacuum ultraviolet. From the modified Kramers-Kronig analysis of these reflectance considering the multiple reflection in the oxide film, the optical absorption below the optical absorption edge of fused quartz becomes appreciable with decreasing oxide film thickness or oxidation temperature. This increase in optical absorption with decreasing the oxidation temperature may be correlated with the change in the structure of interfacial transition layer. The details of the analysis and the effect of exciton absorption⁸⁾ on the present study will be described elsewhere.

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