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Depth Profiling of High-K Dielectric/Si Interfacial Transition Layer

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1. Introduction

High-K dielectrics have been studied extensively as an alternative to silicon oxide in the next generation of MOSFETs.[1] In the forming process of high-K dielectrics on Si substrate, the silicate layer is intentionally or inevitably formed between high-K dielectrics and Si substrate. The SiO_2/Si interfacial transition layer must be also formed between this silicate layer and Si substrate. Because the interface state density and the carrier transport in channel region are seriously affected by the structure of this transition layer(abbreviated as the TL hereafter), it is important to measure the compositional depth profile of this TL. The compositional depth profile of TL was determined on an atomic scale by EELS[3] and EDX[4] combined with finely focused electron beam. For these measurements, however, the sample for the cross sectional TEM studies must be prepared. In the present paper the nondestructive depth profiling method based on the angle-resolved photoelectron spectroscopy will be newly proposed and applied to the depth profile of TL between high-K dielectrics and Si substrate.

2. Experimental Details

In order to confirm the applicability of proposed depth profiling method to TL between high-K dielectric film and Si substrate, GdO_x films formed on n-Si(100) substate was used. For XRD studies GdO_x film with physical film thickness of 42 nm was deposited on Si(100) substrate by electron beam evaporation of Gd_2O_3(denoted as the sample A hereafter) and sample A was subsequently annealed by rapid thermal annealing at 400°C in O_2 for 5 min(denoted as the sample B hereafter). For angle-resolved photoelectron spectroscopy studies GdO_x film with physical film thickness of 2.8 nm was deposited on Si(100) substrate at room temperature by electron beam evaporation of Gd_2O_3 and subsequently annealed in 1 Torr dry oxygen at 400°C for 5 minutes(denoted as the sample C hereafter) and 0.55-nm-thick silicon oxide film was formed in 1 Torr oxygen at 600 °C(denoted as the sample D hereafter) through 0.35-nm-thick oxide film formed in 1 Torr oxygen at 300°C. Si 2p, Gd 4d, O1s and C 1s spectra excited by AlKα radiation arising from these films were measured at photoelectron take-off angle θ of 8, 15, 30, 40, 55 and 90 degrees with photoelectron acceptance angle of 3.3° at the entrance of electron energy analyzer using highly sensitive ESCA-300.

3. Experimental Results and Discussions

Figure 1 shows XRD patterns of the sample A and the sample B. According to this figure GdO_x film(sample A) is in amorphous phase, while GdO_x film(sample B) has cubic structure preferentially oriented to Si(222). Figs. 2(a) and 2(b) show Gd 4d and O 1s photoelectron spectra measured for the sample C at photoelectron take-off angle(TOA) of 15 degrees. Using values of photoionization cross sections and electron escape depths for Gd 4d and O 1s photoelectrons, a value of 0.67 was obtained for ratio of the number of Gd atom with respect to that of O atom. Hence, GdO_x can be identified as Gd_2O_3.[4]

Figure 3 shows Si $2p_{3/2}$ photoelectron spectra arising from the sample C, precisely, TL between Gd_2O_3 and Si substrate and those arising from the sample D, precisely, silicon oxide with TOA as a parameter. Because angle-resolved Si $2p_{3/2}$ photoelectron spectra arising from TL between Gd_2O_3 and Si substrate is different from those arising from silicon oxide, the depth profile in TL between Gd_2O_3 and Si must be quite different from that in silicon oxide. In other words, gadolinium silicate[5] in addition to silicon oxide must be formed between Gd_2O_3 and Si. Hence, the changes in the electron escape depth in the depth direction must be considered for TL between Gd_2O_3 and Si in order to explain the experimental data shown in Fig. 4 describing the photoelectron take-off angle dependence of Si $2p_{3/2}$ spectrum intensity measured for TL, which is normalized by Si $2p_{3/2}$ spectrum intensity measured for Si substrate.

Assuming that 1) the inverse electron escape depth in silicate can be expressed as the sum of p times inverse electron escape depth in SiO_2 and $(1 - p)$ times inverse electron escape depth in Gd_2O_3 and 2) silicon oxide can be effectively expressed as a mixture of SiO_2 and Si, from the analysis of Fig. 4 we obtained Fig. 5 exhibiting the changes in composition as a function of distance(x) from the oxide surface. Here,. p is defined as $0 < p < 1$. The concept of entropy[6] was used in the analysis of angle-resolved photo- electron spectra in order to determine the depth profile with minimum amount of informa- tion content. Fig. 5 indicates that TL between Gd_2O_3 and Si(sample C) consists of 0.29-nm-thick silicate layer, 0.45-nm-thick SiO_2 layer and 0.43-nm-thick suboxide(SiO_x) layer. The effect of non-uniformity of Gd_2O_3 layer on the analysis will be also discussed.

4. Conclusion

The method of determining the depth profile of transition layer was newly proposed and successfully applied to the transition layer formed between Gd_2O_3 and Si(100) substrate.

References

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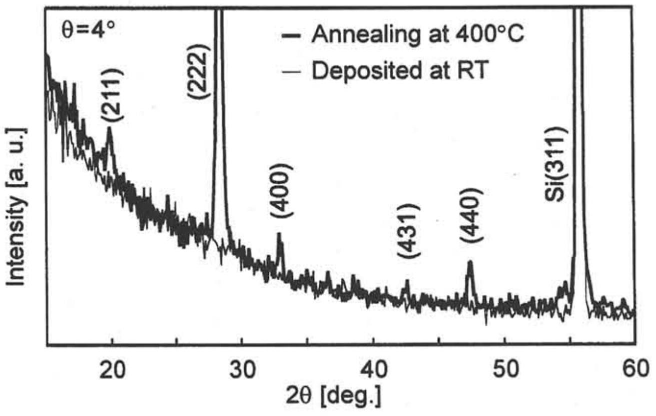

Fig. 1 XRD patterns of sample A and sample B. Here, X-ray is incident on the film surface with incident angle(θ) against film surface of 4°

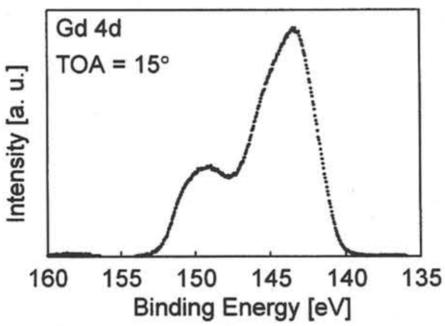

Fig. 2(a) Gd 4d spectrum measured for GdO_x film.

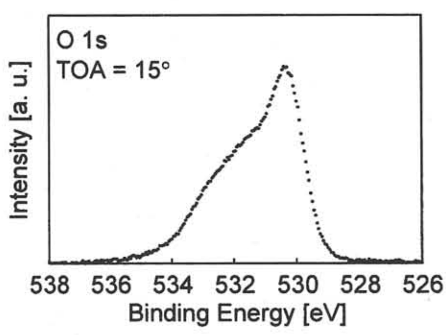

Fig. 2(b) O 1s spectrum measured for GdO_x film.

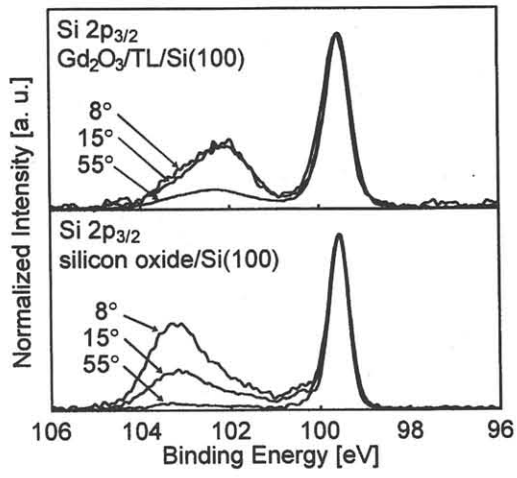

Fig. 3 Angle-resolved $Si2p_{3/2}$ spectra arising from TL between Gd_2O_3 and Si(100) is quite different from those arising from silicon oxide with photoelectron take-off angle as a parameter.

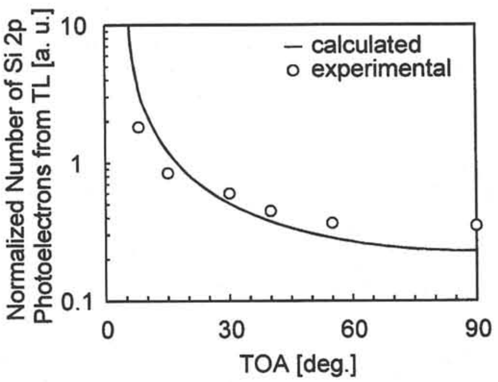

Fig. 4 Normalized number of Si $2p_{3/2}$ photoelec -trons arising from TL between Gd_2O_3 and Si.

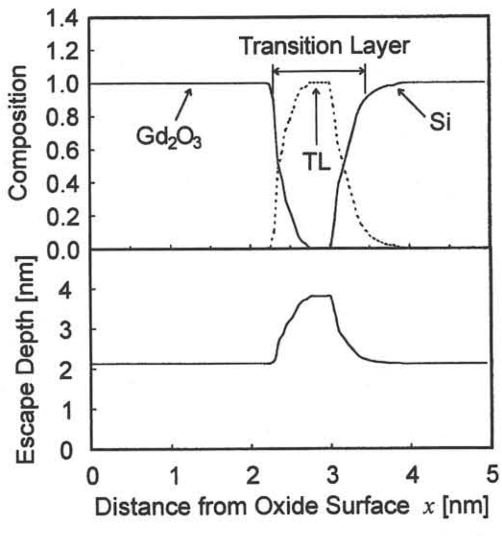

Fig. 5 Composition and elctron escape depth as a function of distance from oxide surface