Effect of oxygen coadsorption on titanium silicide formation on Si(001)

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Introduction
Recently, the application of high-\textit{k} gate dielectrics poses several problems, such as reduction of mobility, regardless of the dielectric material [1]. Mechanisms involving surface optical phonons and remote charge scattering (RCS) have been proposed. Ultrathin SiO\textsubscript{2} film with a thickness of about 1 nm is of vital importance since it can be used as a buffer layer for the growth of high-\textit{k} materials [2]. It is well recognized that the structure of SiO\textsubscript{2}/Si interface affects the device performance in the metal-oxide-semiconductor (MOS) structures. Hence, precise control of the thickness and interface morphology of the SiO\textsubscript{2} interlayer below the high-\textit{k} oxides appears to be critical.

Experimental
The x-ray photoemission spectroscopy (XPS) measurements were performed at BL-18A of the Photon Facory at the Institute of Materials Structure Science, High Energy Accelerator Research Organization (KEK-PF). All experiments were performed in an ultrahigh vacuum (UHV) chamber. Prior to oxidation and subsequent annealing, a titanium thin film with the thickness of 0.3-0.4 nm was grown in situ on Si(001) using an e-beam evaporator. The sample was heated by applying direct current. We determined the titanium thickness from the intensity ratio of Ti 2p state and Si 2p state determined by XPS on sputter-cleaned Si(001) [3].

Results and discussion
Fig. 1 shows the Si 2p spectra. After deposition at room temperature (RT), a broad peak was formed at around -0.4 eV, as shown in Fig. 1(b). No well-crystallized silicide island was observed just after deposition of titanium at RT, as confirmed in our scanning tunneling microscopy (STM) studies [4, 5]. According to the valence band measurements, only weak bonding between Ti and Si is possible through hybridization of Ti 2p and Si 3p states at this stage [3]. The large binding energy shift to 3.30 eV occurs after subsequent oxygen exposure of 60 L at RT (Fig. 1(c)). After oxidation, almost all the Si 2p component is shifted close to the Si\textsuperscript{4+} region. On the other hand, the surface component at around -0.5 eV diminishes after a larger amount of oxygen exposure at 750 L on clean Si(001), while only a weak tail is observed at the suboxide (Si\textsuperscript{+}, Si\textsuperscript{2+}, Si\textsuperscript{3+}) region. In contrast, no distinct peak is discernible at the Si\textsuperscript{4+} region (Fig. 1(d)).

Using parameters for \(h\nu=130\) eV, the thickness of the SiO\textsubscript{2} formed by oxidation at RT is estimated to be 1.2 nm, indicating formation of three to four oxide layers. In contrast, the thickness of oxide after oxygen exposure of 750 L at RT is estimated to be below 0.2 nm, corresponding to limited growth in the monolayer regime. At a similar amount of oxygen exposure, Si(001) is known to be oxidized only up to the backbond site at RT [6]. Hence, the role of catalytic properties of titanium thin films for oxidation of the silicon surface was suggested from the present experimental findings.

References

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\[ \text{Fig. 1 A series of Si 2p PES spectra obtained at RT for (a) a clean Si(001) surface, (b) titanium-deposited surface at the coverage of 0.3-0.4 nm, (c) followed by an oxygen exposure of 60 L, and (d) the oxidized Si(001) surface at 750 L.} \]