Atomic scale observation of interface defect formation processes between Si and SiO_2

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Due to the miniaturization of metal-oxide semiconductor (MOS) devices, SiO_2 thickness of the gate insulator is reduced to less than 2 nm. With such a thin SiO_2 film, leakage current due to the direct tunneling process severely degrades device performance. To overcome this problem, alternative high-k materials for replacing SiO_2 gate insulators are thought to be necessary. However, even in high-k materials, a well-controlled interfacial SiO_2 film of several 0.1 nm is necessary to maintain high channel mobility. Therefore, a dynamic oxidation process with a few Si layers is important, particularly creation mechanism of interface defects between Si and SiO_2. As a typical point defect at the Si/SiO_2 interface affecting electrical properties, a three-fold coordinated silicon atom with a neutral charge, the so-called P_b center, has been widely investigated. Electron spin resonance (ESR) is one of the most powerful tools available for investigating P_b centers. However, these studies have been limited to the static structure of Si/SiO_2 after Si oxidation, whereas microscopic information about the dynamic oxidation mechanism is required. For above purposes, we have developed an ultra-high-vacuum (UHV)-ESR system, which is a combination of an ESR system and a UHV chamber, and reported the dynamic oxygen and hydrogen termination processes on an Si clean surface. In this talk, we focus on the process of P_b center generation during silicon oxidation following oxygen termination on a clean Si surface, based on which we discuss the microscopic origin of P_b centers [1].

[1] W. Futako, N. Mizuochi, and S. Yamasaki, Phys. Rev. Lett. 92 (2004) 105505.

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