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Electrical Characterization of Atomic-Scale Defects in an Ultrathin Si Oxynitride Layer

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1. Introduction

The electrical properties of atomic-scale defects in ultrathin gate dielectric layers are an important factor for understanding the degradation of gate oxide layers. The initial degradation stage is actually triggered by a phenomenon on an atomic-scale (defect formation, electron trap, or positive charge). An atomic-scale damaged region is then formed in the gate oxide after the complete breakdown. However, the electrical properties of such a small region have not been separately investigated yet. Scanning tunneling microscopy (STM) and atomic force microscopy are effective techniques to study the local region of ultrathin dielectric layers [1-3]. In this work, we use STM and scanning tunneling spectroscopy (STS), and discuss the individual electrical properties of atomic-scale defects in an ultrathin Si oxynitride layer.

2. Experiment

We used an ultrahigh-vacuum STM system to prepare and observe the sample surfaces. An approximately 0.4-nm-thick oxynitride layer was grown on a clean Si(001)-2×1 surface under 2×10^{-6} Torr NO pressure at 650°C for 90 seconds. For comparison, we also investigated a 0.3-nm-thick Si oxide layer grown on a clean Si(001)-2×1 surface under 2×10^{-6} Torr O_2 pressure at 650°C for 600 seconds [4]. The STM images were observed at a sample bias, V, of +3.5 V with a tunnel current, I, of 0.1 nA. The I-V curves were measured by fixing the tip height for the same tunneling conditions.

3. Results and discussion

The atomic step on the initial Si surface is preserved after the oxynitridation [arrows in Fig. 1 (a)]. This result is consistent with a previous experiment using scanning reflection electron microscopy [5]. On the other hand, atomic-scale spots (0.3-2 nm in diameter) with various degrees of contrast are visible throughout the surface [Figs. 1 (a) and 1 (b)]. Most of these spots and the surrounding dark areas have normal dI/dV curves [Fig. 1 (c)]. A few spots, however, have clear peaks on their dI/dV curves [Figs. 1 (d) and 1 (e)]. We consider that the peak is caused by the defect state near the conduction band edge of oxynitride [Fig. 1 inset]. This is an atomic-scale defect, since its peak was observed around the center of spot (~1 nm in diameter).

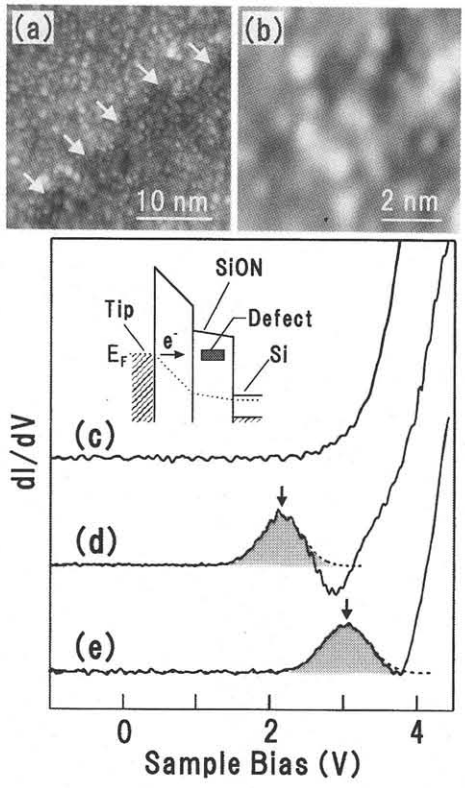

Fig. 1. STM images and dI/dV curves obtained from oxynitride layer; (a) and (b) are STM images, (c) is normal dI/dV curve, (d) and (e) are dI/dV curves of defects.

In addition, we obtained this type peak from the same spot many times. We, therefore, concluded that this structure remains stable under electrical stress caused by STM and STS observations.

We observe only a few unstable peaks from the same sample surface [Figs. 2]. At first this peak type is sharper than the stable type, it becomes broader after a few STS measurements [Figs. 2 (c) and 2 (d)]. We consider that this phenomenon corresponds to the damaging caused by electrical stress [Fig. 3]. The Si-Si bond in SiO_2 was predicted to have an empty state near the conduction band edge [6]. The sharp peak is, therefore, corresponded to this defect. The Si-Si bonds are thought to be unstable under electrical stress, and thus damaged easily. We

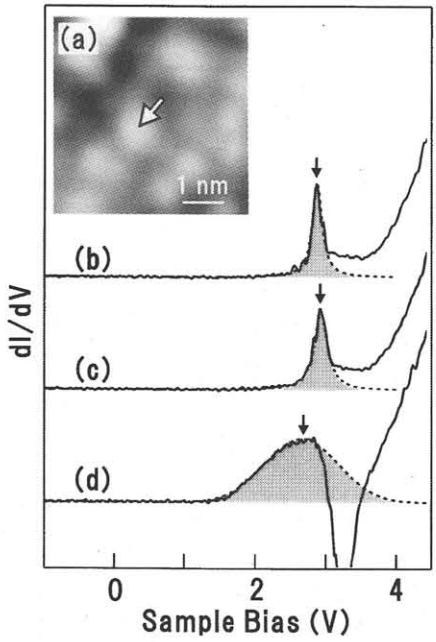

Fig. 2. Unstable *dI/dV* curves observed from defect in STM image (a); (b), (c), and (d) are first, second, and seventh STS measurements.

consider that the observed structures [Fig. 1] have already been damaged before the STS measurements. We also consider that an atomic-scale Si cluster have been formed after the damaging, because a nanometer-scale Si structure has a wider band gap than a bulk Si crystal, and its conduction band shifts toward a higher energy. In addition, the atomic-scale Si dots formed on an oxide by a Si deposition showed similar broad peaks depending on the dot size. Consequently, the unstable and stable peaks correspond to the Si-Si bond and the damaged structure, respectively.

Finally, we compare the properties of the damaged structures in the oxynitride layer to those in the oxide layer. We observed similar damaged structures in the oxide layer, however, the defect density is about one order smaller than that in the oxynitride layer [Fig. 4]. *Unfortunately* N incorporation enhances the defects. On the other hand, the energy distribution of the oxynitride shifts toward a higher energy compared to that of the oxide. This result suggests that the size of the damaged structure in the oxynitride is smaller than that in the oxide, because the energy gap of the Si cluster increases with decreasing size. The *fortunate* outcome of this work is that N atoms suppress the expansion of the damaged region.

4. Conclusion

We demonstrated that the electrical properties of atomic-scale defects in ultrathin dielectric layer were individually evaluated using STM and STS. We also observed the Si-Si bonds and the damaged structures formed by electrical stress of the observation. Incorporation of N atoms suppresses the expansion of damaged region, but it enhances the defect density.

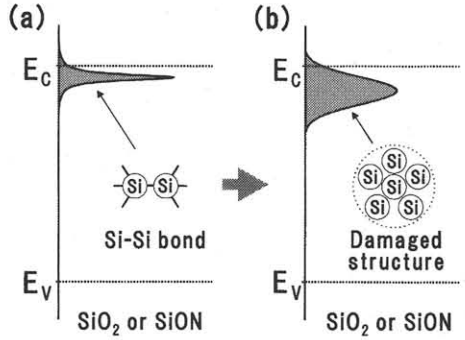

Fig. 3. Model for structural change of defect due to electrical stress.

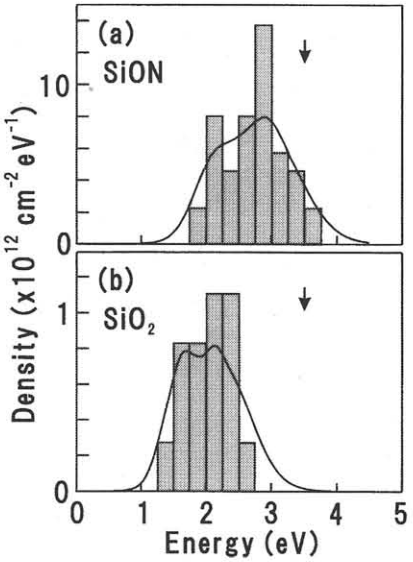

Fig. 4. Energy distributions (we set $E_F = 0$ eV) of defect states for oxynitride (a) and oxide (b). The arrows indicate the conduction band edge of SiO_2.

Acknowledgments

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References

[1] K. Fujita, H. Watanabe, and M. Ichikawa, J. Appl. Phys. **83**, 3638 (1998)

[2] H. Watanabe, T. Baba, and M. Ichikawa, J. Appl. Phys. **85**, 6704 (1999).

[3] R. Hasunuma, A. Ando, K. Miki, and Y. Nishioka, Surf. Sci. Lett., **443**, L1055 (1999).

[4] H. Watanabe *et al.*, Phys. Rev. Lett. **80**, 345 (1998); N. Miyata, H. Watanabe, and M. Ichikawa, Phys. Rev. Lett. **84**, 1043 (2000).

[5] N. Miyata, H. Watanabe, and M. Ichikawa, Appl. Phys. Lett. **76**, 3561 (2000).

[6] E.P. O'Reilly and J. Robertson, Phys. Rev. B **27**, 3780 (1983).