

A 500°C fabrication process for MIM capacitors—based on a Ta₂O₅/Nb₂O₅ bilayer with high permittivity—for DRAM and SoC applications

Yuichi Matsui, Masahiko Hiratani, and *Isamu Asano

Central Research Laboratory, Hitachi, Ltd., Kokubunji, Tokyo 185-8601, Japan

*Elpida Memory, Inc., Sagami-hara, Kanagawa 229-1198, Japan

Phone: +81-42-323-1111, Fax: +81-42-327-7773, E-mail: y-matsui@crl.hitachi.co.jp

1. Introduction

MIM capacitors are expected to find applications in embedded and RF devices as well as in Gbit-scale DRAMs. Tantalum pentoxide (Ta₂O₅) has been one of the promising dielectrics for the MIM capacitor. For example, the MIM-Ta₂O₅ has been investigated as a high-performance capacitor for SoC applications. Our previous work [1] developed the Ta₂O₅/Al₂O₃/Ta/Cu structure, where the Al₂O₃ layer was inserted between Ta₂O₅ and Ta to suppress the oxidation of the Ta barrier metal. To further increase the capacitance, the Ta₂O₅ must be formed on a metal electrode directly, and be crystallized to increase its permittivity. However, during the high-temperature process of crystallization, oxygen diffuses through the bottom electrode and oxidizes the barrier metal, forming a high-resistivity layer. To suppress the oxidation of the barrier metal, the fabrication temperature for the MIM capacitor must therefore be decreased to less than 500°C, even if a noble metal, such as Ru, is used as the bottom electrode.

The authors have previously shown that the hexagonal Ta₂O₅ has a permittivity higher than 50 [2]. In addition, another study found that a hexagonal polymorph of Nb₂O₅ exists at low temperatures, i.e., less than 600°C [3]. In response to these findings, we previously developed a niobia-stabilized tantalum pentoxide (NST) that enables crystallization temperature to be decreased and permittivity to be enhanced [4]. Following on from these previous works, the current study demonstrates the Ta₂O₅/Nb₂O₅ bilayer dielectrics.

2. Experimental

Nb₂O₅ and Ta₂O₅ thin films were formed by RF sputtering from sintered targets in an Ar/O₂ discharge gas at 300°C. After the deposition, the films were heat treated in N₂ or O₂ at temperatures from 500°C to 800°C. Capacitors were formed by Au evaporation through a metal mask with the substrates held at room temperature.

3. Results and Discussion

First, a Nb₂O₅ film was investigated as a nucleation layer for the low-temperature crystallization of Ta₂O₅. A 20-nm-thick Nb₂O₅ film was formed on Pt and Ru electrodes. On the Pt electrode, a 001 plane developed parallel to the electrode surface at 500°C and above [Fig. 1(a)]. On the Ru electrode, a polycrystalline film grew even in the as-deposited state [Fig. 1(b)]. These results indicate that the Nb₂O₅ film is crystallized at temperatures of less than 500°C, that is, lower than the Ta₂O₅ film by 200°C [4]. The permittivity increases from 30 to 60 at 500°C on the Pt electrode, while on the Ru electrode, even the as-deposited Nb₂O₅ film has a high permittivity of 60 (Fig. 2). These results show that the high permittivity is accompanied by the crystallization shown in Fig. 1.

Figure 3 is in-plane and cross-sectional views of the Nb₂O₅ film, which was heat treated at 500°C. The spot assignments based on the interplanar spacings of the

nano-area diffraction patterns (inset) show that the crystal structure of Nb₂O₅ film belongs to a hexagonal symmetry with *a* of 0.630 nm and *c* of 0.392 nm, which is similar to that of the Ta₂O₅ film [2]. The Nb₂O₅ film can therefore be considered suitable for a nucleation layer.

Next, the Ta₂O₅/Nb₂O₅ bilayer was investigated. A 5-nm-thick Nb₂O₅ film was deposited and heat treated at 500°C for 1 min, and then a 15-nm-thick Ta₂O₅ film was deposited on this film. Finally the bilayer was heat treated at temperatures between 500 and 700°C for 1 min. And single layers of 20-nm-thick Ta₂O₅ and Nb₂O₅ were formed for comparison. Figure 4 shows the dependence of permittivity of the bilayer and the single layers on heat-treatment temperature. It is clear that the permittivity of Ta₂O₅ increases at high temperature, i.e., 750°C and above; this permittivity increase is accompanied by crystallization [4]. The permittivity of the Nb₂O₅ single layer increased from 30 to 60 at 500°C (as shown in Fig. 2). On the other hand, the Ta₂O₅/Nb₂O₅ bilayer shows high permittivity of approximately 50 even when the Ta₂O₅ film was deposited on the Nb₂O₅ film at 300°C.

Figure 5 is a cross-sectional view of the Ta₂O₅/Nb₂O₅ bilayer. The inset Fourier transferred image of region A shows a 0.392-nm spacing in the vertical direction parallel to the *c*-axis and a 0.315-nm spacing in the horizontal direction perpendicular to the *c*-axis, and the diffraction spots are not separated. This result indicates that the hexagonal Ta₂O₅ is stabilized on the hexagonal Nb₂O₅ by incommensurate heteroepitaxy on the basal plane perpendicular to the *c*-axis. The crystallization temperature of the Ta₂O₅ film is therefore thought to be reduced from more than 700°C to less than 500°C on the crystallized Nb₂O₅.

The current-voltage characteristics of the capacitor were investigated (Fig. 6). The leakage current of the Nb₂O₅ film is larger than that of the Ta₂O₅ film by two orders of magnitude. However, the leakage current of the Ta₂O₅/Nb₂O₅ bilayer can be reduced to that of the Ta₂O₅ film. This suggests that the conduction mechanism in the Ta₂O₅/Nb₂O₅ bilayer is not predominated by the Schottky barrier at the Nb₂O₅/electrode interface but by the intrinsic nature of Ta₂O₅; thus, the Ta₂O₅/Nb₂O₅ bilayer is able to suppress the leakage current.

4. Conclusion

A novel dielectric using a layered combination of Ta₂O₅ and Nb₂O₅ was applied in MIM capacitors and experimentally investigated. The results of this investigation show that a Ta₂O₅/Nb₂O₅ bilayer has a low crystallization temperature of less than 500°C and high permittivity of 50, because the hexagonal Ta₂O₅ is stabilized on the hexagonal Nb₂O₅ by incommensurate heteroepitaxy. Although the Nb₂O₅ single layer is very leaky, the leakage current of the Ta₂O₅/Nb₂O₅ bilayer can be reduced to that of the Ta₂O₅ single layer. It can therefore be concluded that the Ta₂O₅/Nb₂O₅ bilayer is the most suitable dielectrics for MIM capacitors in DRAM and SoC applications.

References

- [1] T. Ishikawa *et al.*, Tech. Dig. IEDM, p.940, 2002.
- [2] M. Hiratani *et al.*, Appl. Phys. Lett., 81, p.2433, 2002.
- [3] D. Rosenfeld *et al.*, J. Vac. Sci. Technol., A12, p.135, 1994.
- [4] Y. Matsui *et al.*, Tech. Dig. IEDM, p.225, 2002.

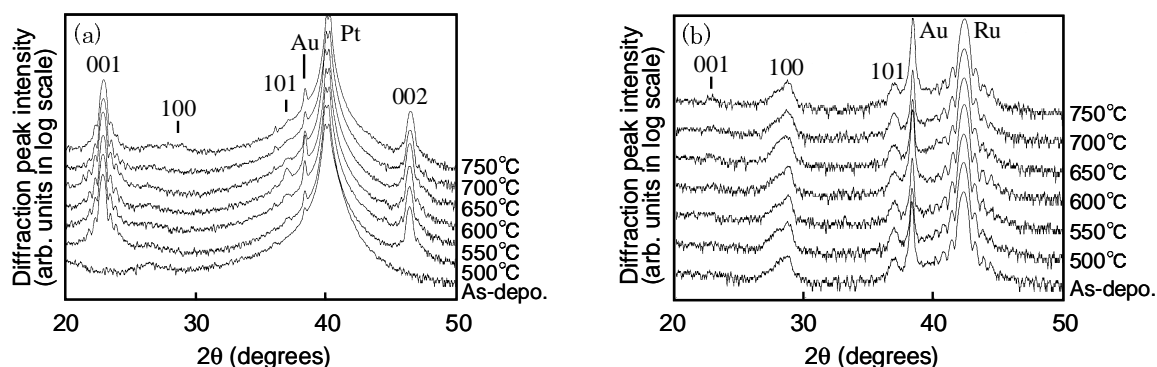


Fig.1 Change in the XRD patterns of 20-nm-thick Nb_2O_5 films with heat-treatment temperature. The Nb_2O_5 films were deposited on (a) Pt and (b) Ru electrodes.

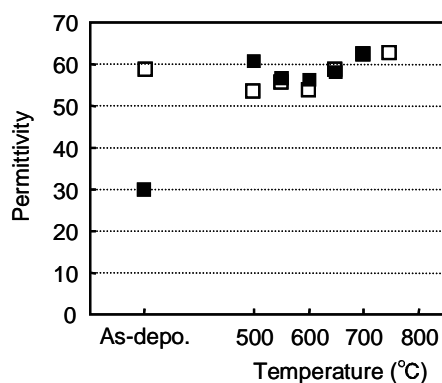


Fig.2 Dependence of the permittivity of Nb_2O_5 films on heat-treatment temperature. The Nb_2O_5 films were deposited on Pt (■) and Ru (□) electrodes.

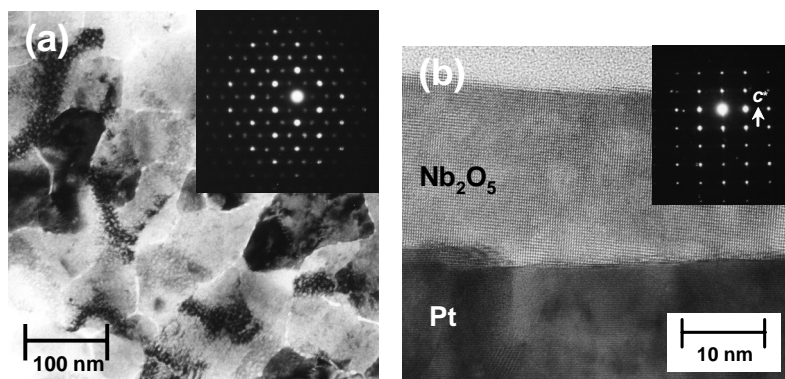


Fig.3 (a) In-plane and (b) cross-sectional views of Nb_2O_5 film, and nano-area diffraction pattern (inset) obtained when the electron beam is focused on a single grain and aligned normal or parallel to the film surface.

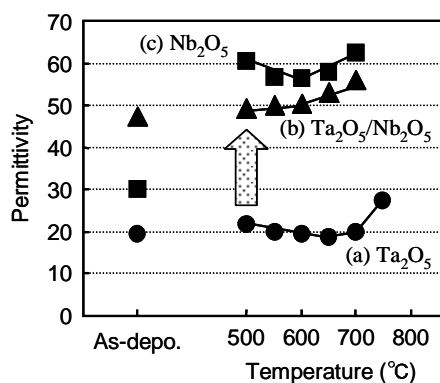


Fig.4 Dependence of the permittivity of Ta_2O_5 (circles), Nb_2O_5 (squares), and $\text{Ta}_2\text{O}_5/\text{Nb}_2\text{O}_5$ (triangles) films on heat-treatment temperature.

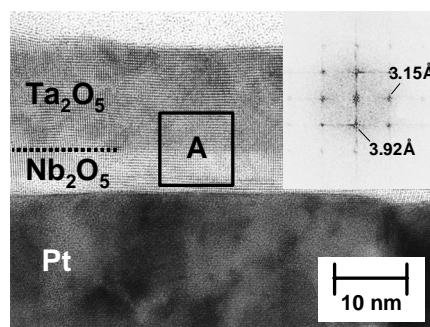


Fig.5 Cross-sectional view of $\text{Ta}_2\text{O}_5/\text{Nb}_2\text{O}_5$ structure deposited on a Pt electrode, and Fourier-transfer image of region A (inset). The Nb_2O_5 and Ta_2O_5 films were heat treated at 500°C.

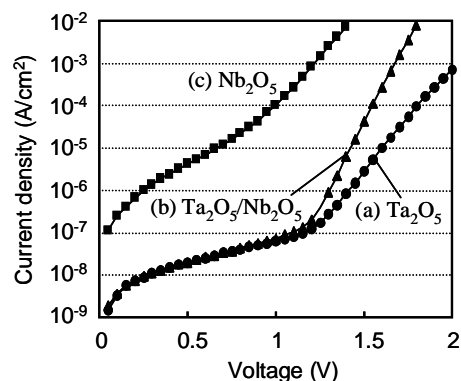


Fig.6 I-V characteristics of Ta_2O_5 (circles), Nb_2O_5 (squares), and $\text{Ta}_2\text{O}_5/\text{Nb}_2\text{O}_5$ (triangles) films. The Nb_2O_5 and $\text{Ta}_2\text{O}_5/\text{Nb}_2\text{O}_5$ films were heat treated at 500°C, and the Ta_2O_5 film was heat treated at 750°C.