Extended Abstracts of the 2000 International Conference on Solid State Devices and Materials, Sendai, 2000, pp. 156-157

A-3-1 (Invited)

Influence of Lattice Distortion and Oxygen Defects in BST Films for Memory Capacitors

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$Ba_{1-x}Sr_xTiO_3$ (BST) have been intensively studied as a DRAM capacitor material, though, various technological problems still exist. Among them, lower dielectric constant and larger leakage current than those expected in bulk BST are most crucial problems for practical use of this material. In this report, we present the experimental results concerning the influence of lattice distortion and oxygen vacancies on the properties of BST capacitors, using the data obtained by epitaxially grown all oxide capacitors.

Influence of the lattice distortion on the dielectric constant can be interpreted by means of the Ti ion total energy change when the lattice distortion is introduced in BST (Fig.1); tetragonal elongation along electric field provides less energy increase and higher dielectric constant[1].

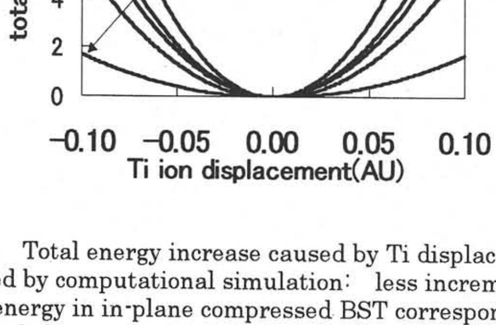

Fig.1. Total energy increase caused by Ti displacement derived by computational simulation: less increment of total energy in in-plane compressed BST corresponds to higher dielectric constant.

Such tetragonal distortion in BST dielectrics can be available utilizing the lattice mismatch between bottom electrodes and dielectrics in epitaxially-grown BST capacitors[2]. Polarization vs. applied voltage curves in epitaxial $SrRuO_3$/BST/$SrRuO_3$ capacitors with various mismatches are shown in Fig.2. Steep increment of polarization around the applied voltage=0V corresponds to high dielectric constant for appropriate BST/$SrRuO_3$ lattice mismatch. For further lattice distortion, dielectric constant decreases caused by emerging ferroelectricity.

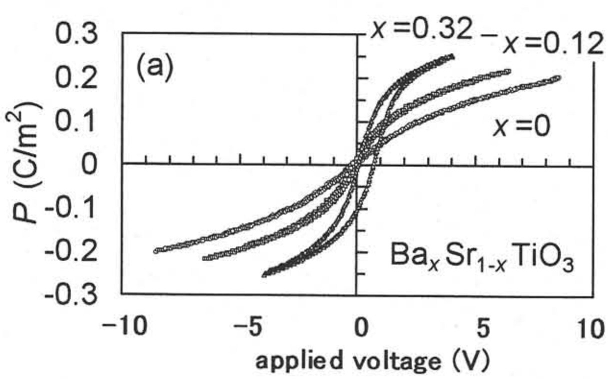

Fig.2. Polarization curves in epitaxial $SrRuO_3$/BST/$SrRuO_3$ capacitors (t=400A) with various mismatches.

Figure3 shows dielectric constant and leakage current of epitaxial $SrRuO_3/Ba_{0.12}Sr_{0.88}TiO_3/SrRuO_3$ capacitor (t=200A) and polycrystalline $Ba_{0.5}Sr_{0.5}TiO_3$ capacitor (t=200A). Dielectric constant as high as 1000 can be obtained in epitaxial BST capacitor by optimizing the lattice distortion[1]. Introduction of such lattice distortion will be a key issue to obtain a drastic improvement in charge accumulation ability in actual BST memory capacitors. Local epitaxial growth[3] onto polycrystalline perovskite electrodes will be a clue to such an ambitious technological challenge.

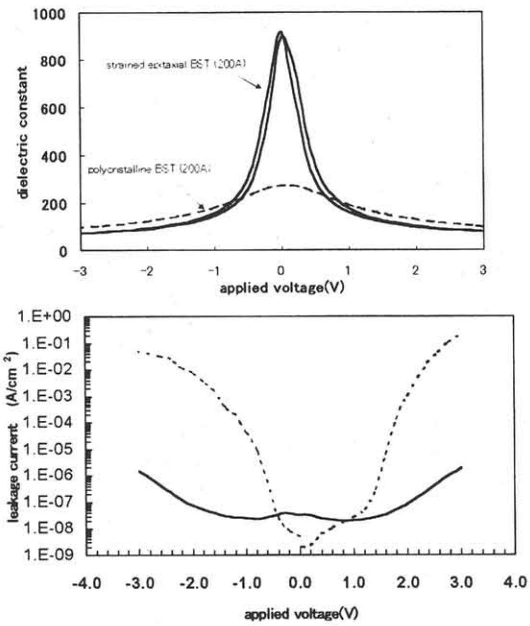

Fig.3. Dielectric constant and leakage current in epitaxial and polycrystalline capacitors.

Poor leakage current property and long-term reliability are another concern to overcome for the actual use of BST capacitors in advanced DRAMs. To establish the development strategy of such issues, fundamental mechanism for leakage current and stress leakage should be clarified. Epitaxially grown capacitors would provide important information concerning the electronic states and the origin of SILC and other leakage degradations in BST capacitors.

Leakage currents in epitaxially-grown $SrRuO_3/Ba_{0.12}Sr_{0.88}TiO_3/SrRuO_3$ capacitors of various thickness ranging 18nm to 36nm are shown in Fig.4. In each temperature, applied electric field dependence of various thickness samples fell onto a unique curve, which can be fitted by a simple Fowler-Nordheim equation. Thickness dependence of dielectric constant was quite small in these samples.

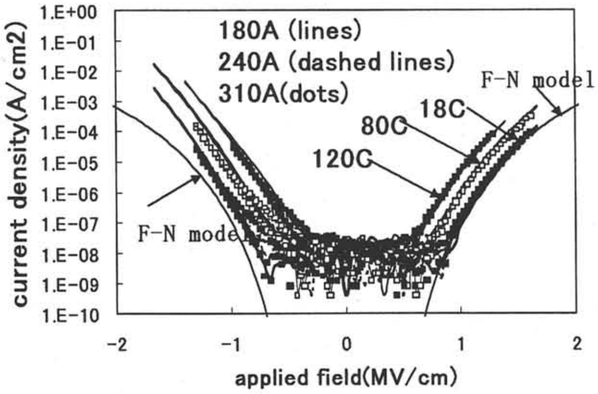

Fig.4. Leakage current of epitaxial BST capacitors with various thicknesses.

These results implied the full depletion model as a fundamental scheme for the electronic structure of these capacitors that have extremely clean interface and low defect concentration. It would be important to clarify how the leakage current degrades from such high-quality capacitors to ordinary polycrystalline BST capacitors. Figure 5 describes the variation of leakage current in epitaxial BST capacitors of same thickness (200A) with different degree of oxygen deficiency.

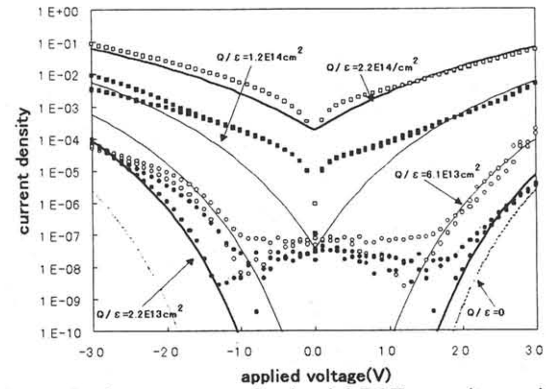

Fig.5. Leakage current of epitaxial BST capacitors with various oxygen deficiencies. Solid lines describe the expected leakage current assuming the existence of oxygen defect and consequent internal electric field.

As seen in Fig.5, leakage current exhibits extensive variation with introduction of oxygen deficiency. This variation was analyzed by means of internal potential caused by positive charge. Electric field enhancement at the electrode/dielectric interface was taken into account and the Fowler-Nordheim current was employed as leakage mechanism. The results shown in Fig.5 well describe the leakage variation observed in experiments.

As described above, oxygen defects in BST films play crucial role in leakage current in epitaxial capacitors, and also in polycrystalline capacitors, as well. It is strongly required to establish methods to evaluate and eliminate the defect concentration in BST capacitors. Ti_{LMV} measurement by Auger Electron Spectroscopy will provide sufficient information of oxygen deficiency and would be a tool to control the BST film quality[5]. Some of the conducting oxide electrodes would act as oxygen reservoir to compensate the oxygen defect at the interface[3], thus, employment of such electrodes is considered as a most practical solution to reduce the leakage current in BST capacitors.

References

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