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High Crystalline Quality Si Film Formation on Lattice-matched Mixed Oxide ($Sr_xBa_{1-x}O$)/Si(111) Stacked Structure

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Abstract

Epitaxial growth of mixed oxide ($Sr_xBa_{1-x}O$) films onto Si(111) substrates and growth of Si overlayers onto lattice-matched mixed oxide/Si structures are investigated. Rutherford backscattering/channeling spectroscopy reveals that a 3000-Å-thick mixed oxide film of the best quality (χ_0:surface channeling yield =0.037) grows at 780 °C, when the X-value is 0.32, and the Si overlayer's average dechanneling rate ($d\chi/dz$=0.08) near the surface is close to that of bulk-Si.

1. INTRODUCTION

Lattice-matched single crystalline insulators are attractive for use in semiconductor/insulator/semiconductor double heteroepitaxial structures, because they allow epitaxial growth of a high quality crystalline top semiconductor layer. Epitaxial growth of mixed alkaline earth fluorides matched with Ge, InP, and GaAs has been previously reported.[1)-4)]

However, these mixed fluorides do not match exactly with Si crystals. On the other hand, $Sr_xBa_{1-x}O$ mixed cubic crystals are closely lattice-matched to Si having a cubic structure with a=5.431Å, because SrO and BaO have cubic crystal structures with lattice parameters of 5.140 and 5.542 Å, respectively. Therefore, these alkaline earth oxides are expected to be useful as dielectric materials for Si/insulator/Si stacked structures with high-quality submicron-thick top Si layers.

This paper presents results of an investigation of the composition and growth temperature dependence of crystal quality for mixed oxide ($Sr_xBa_{1-x}O$) films grown on Si(111), and of the crystal quality of the top-Si layer grown on the lattice-matched $Sr_xBa_{1-x}O$/Si(111) structure.

2. EXPERIMENTS

Mixed oxide films and the top-Si layers were prepared in the same ultra high vacuum (UHV) growth chamber equipped with three electron-beam gun deposition systems. To grow $Sr_xBa_{1-x}O$ films, SrO and BaO-sources were alternately evaporated onto Si substrates at 600-830 °C. These growth stages were carried out by oxide deposition lasting 1 sec and exhaust lasting about 30 sec. This procedure was automatically repeated as many times as necessary. The pressures maintained during oxide deposition were less than 5.0×10^{-7} Torr. The top-Si films were deposited onto $Sr_xBa_{1-x}O$/Si kept at 700-800 °C by introducing a solid-phase-epitaxy (SPE) Si layer at the interface. The growth rate of the top-Si layer was typically 0.3 Å/sec.

The epitaxial growth process of $Sr_xBa_{1-x}O$ films on Si(111) and Si overlayers on the mixed oxide/Si(111) was monitored by in situ reflection high energy electron diffraction during deposition. The composition and crystallinity of $Sr_xBa_{1-x}O$ films and top-Si films were measured by Rutherford backscattering/channeling (RBS/C) spectrometry using 2.0 MeV $^4He^+$ ions in the glancing-exit geometry.[5)]

3.RESULTS AND DISCUSSIONS

3.1 Growth of $Sr_xBa_{1-x}O$ Films

Backscattering spectra for a 3000-Å-thick $Sr_xBa_{1-x}O$ film grown on a Si(111) substrate at 780 °C are shown in Fig.1. From the ratio of Sr to Ba-signal height at the surface in random spectra, the composition X (hereafter referred to as X-value) is determined as 0.32. The surface channeling yield, χ_0, which is defined as the ratio of aligned yield to random yield behind the surface peak, is 0.037 for the Ba portion.

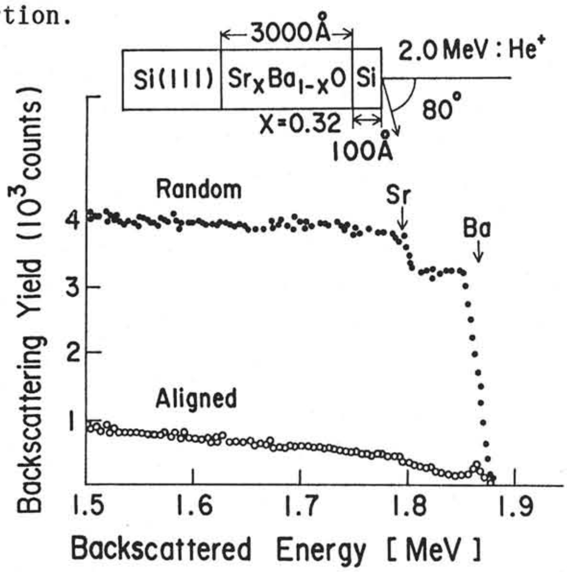

Fig.1 Random and aligned <111> backscattering spectra for the top half of a 3000-Å-thick $Sr_{0.32}Ba_{0.68}O$ film grown on Si(111)

The dependence of χ_0 on growth temperature for 600-Å-thick $Sr_xBa_{1-x}O$ (X=0.32) films is given in Fig.2. Good crystallinity is obtained at substrate temperatures higher than 780 °C. However, at temperatures over 820 °C, the growth rate fell off sharply, and it was found from RBS spectra that Oxygen-vacancies existed in the oxide films. Therefore, optimum growth temperature is shown to be in the 780-800 °C range.

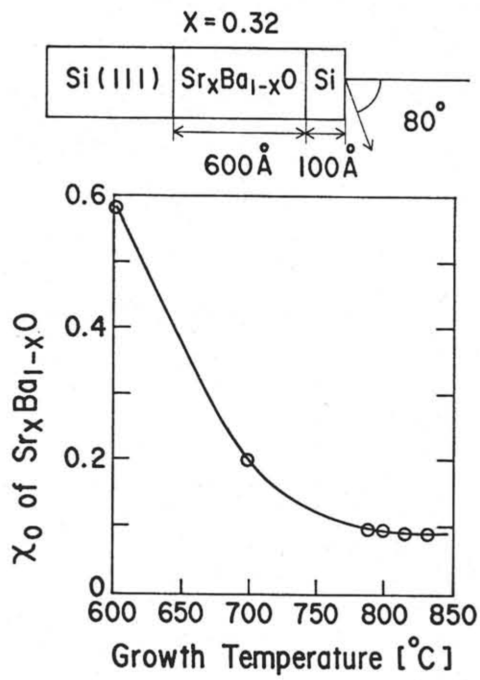

Fig.2 Growth temperature dependence of χ_0 for 600-Å-thick $Sr_xBa_{1-x}O$ films.

The dependence of χ_0 on composition for $Sr_xBa_{1-x}O$ films of various thicknesses grown on Si(111) substrates at 780 °C is shown in Fig.3. It is apparent from the figure that

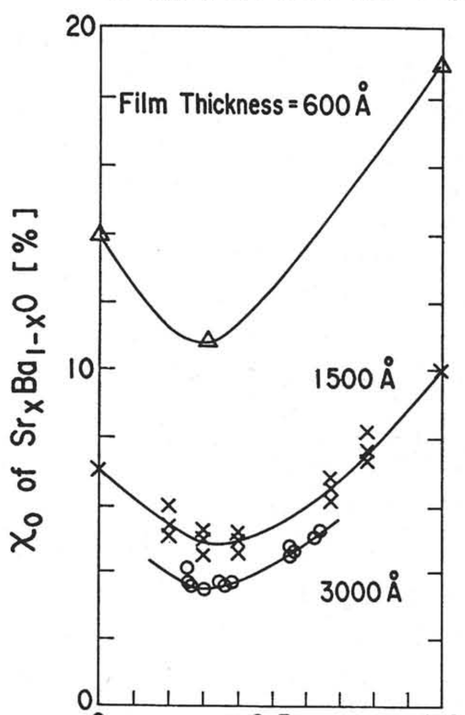

Fig.3 Composition dependence of χ_0 for $Sr_xBa_{1-x}O$ films with various film thicknesses grown on Si(111) substrates at 780 °C.

film crystallinity is strongly dependent on composition. Good crystalline quality (χ_0 less than 0.039) is obtained with X-values ranging from 0.25 to 0.39. Improved crystallinity with increased film thickness is also observed.

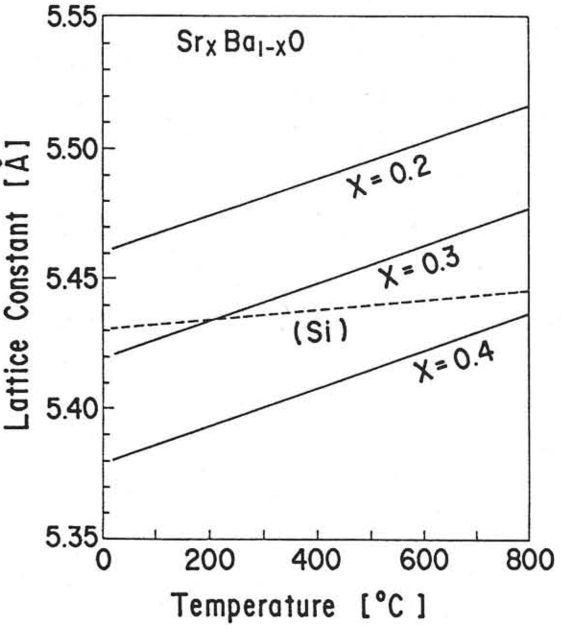

Fig.4 Calculated lattice parameters of $Sr_xBa_{1-x}O$ and Si as functions of temperature.

The calculated lattice parameters of $Sr_xBa_{1-x}O$ as a function of temperature, assuming that the mixed oxide satisfy the Vegard's law, are shown in Fig.4. In this calculation, the thermal linear expansion values for SrO, BaO, and Si are based on data recommended in refs. 6 and 7.

According to this calculation, the crystallinity improvement of mixed oxide films is thought to be caused by strain relaxation due to lattice mismatch reduction. In this experiment, the best quality (χ_0=0.037) was obtained from a 3000-Å-thick $Sr_{0.32}Ba_{0.68}O$ film. Figure 4 shows that this mixing ratio (X=0.32) is equivalent to the matching condition at 380°C, which is considerably lower than the growth temperature (780°C). In the following study, top-Si films were grown on 3000-Å-thick $Sr_{0.32}Ba_{0.68}O$ films.

3.2 Crystalline Quality of The Top-Si Layers

The energy spectra of 2.0 MeV $^4He^+$ ions backscattered at 100° from (1) a 0.5-μm-thick top-Si layer grown on SPE-Si(40Å)/$Sr_{0.32}Ba_{0.68}O$(3000Å)/Si(111) at 700 °C, (2) a 0.5-μm-thick homoepitaxial Si layer grown on SPE-Si(40Å)/Si(111) at the same temperature, and (3) bulk-Si(111), are compared in Fig.5. These spectra indicate that the surface crystal quality of the top-Si grown on a lattice-matched insulator is comparable to that of the homoepitaxial Si.

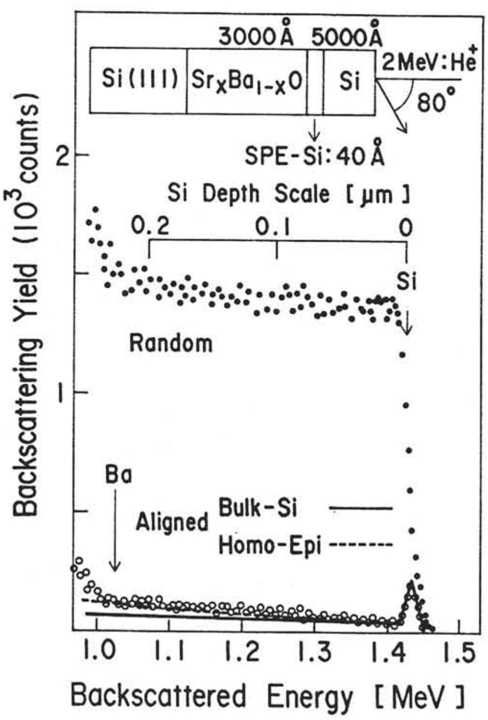

Fig.5 Backscattering spectra for (1) a 0.5-μm-thick top-Si layer grown on Si-SPE(40Å)/$Sr_{0.32}Ba_{0.68}O$(3000Å)/Si(111). The dashed and the solid lines indicate aligned spectra for (2) a 0.5-μm-thick top-Si layer grown on Si-SPE(40Å)/Si(111) and (3) bulk-Si(111), respectively.

The dependence of average dechanneling rate, $d\chi/dz$,[8] on SPE-Si layer thickness for the top-Si layers grown on mixed oxide at 700 and 800°C is shown in Fig.6. This figure shows that the crystal quality of the Si overlayers is improved by reducing SPE-Si layer thickness.

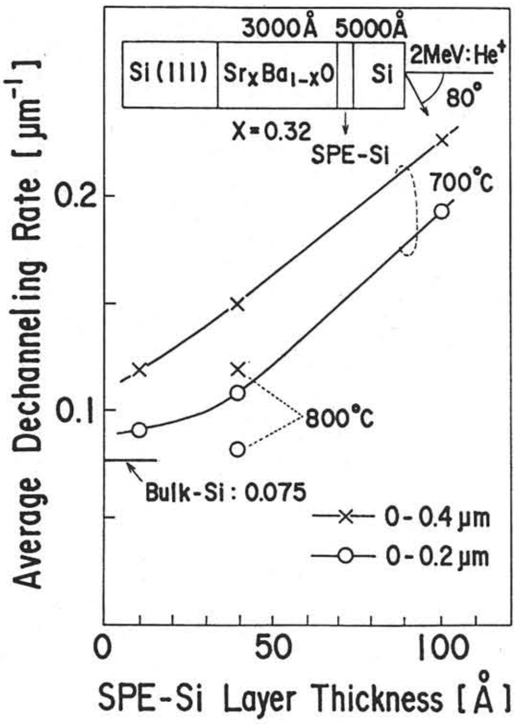

Fig.6 The dependence of the average dechanneling rate, $d\chi/dz$,[8] for the top-Si layers grown on mixed oxides at 700 and 800 °C, on SPE-Si layer thickness.

However, the precipitation of Sr and Ba on the surface was detected by RBS/S spectrometry from the Si overlayers with 10 and 6-Å-thick SPE-Si layers grown at 800 and 700 °C, respectively. This means that an SPE-Si of at least about 30-40 Å thickness is needed to prevent precipitation during growth of top-Si layers at 800 °C.

Conseqently, in this experiment, a 40-Å-thick SPE-Si layer is introduced at the interface. As a result, the best value of dx/dz equal to 0.08(0-0.2μm) obtained in the heteroepitaxial Si layer grown on lattice-matched oxides at 800 °C is close to the 0.075 of bulk-Si. This value is far superior to 0.7 and 1.1 for Si/YSZ film and typical commercial SOS films of similar thickness reported previously.[9]

4.CONCLUSION

Double heteroepitaxial growth of Si films and lattice-matched mixed oxide ($Sr_xBa_{1-x}O$) films onto Si(111) was investigated. The main results obtained were as follows.

1)$Sr_xBa_{1-x}O$) films with high crystalline quality (χ_0:surface channeling yield= less than 0.039) were grown epitaxially on Si(111) substrates at temperatures ranging from 780 to 800 °C, with X-values in the 0.25-0.39 range. In this experiment, the best quality (χ_0=0.037) was obtained from a 3000-Å-thick $Sr_{0.32}Ba_{0.68}O$ film.

2) High quality top-Si films with average dechanneling rates ($d\chi/dz$) of 0.08(0-0.2μm) were grown on lattice-matched $Sr_{0.32}Ba_{0.68}O$ film/Si(111) structures at 800 °C by introducing 40-Å-thick Si-SPE layers at the interface. This value ($d\chi/dz$) was close to the 0.075 found in bulk-Si near the surface.

Thus, it is concluded that lattice-matched epitaxial growth using $Sr_xBa_{1-x}O$ films on Si substrate is one of the most promising approaches for forming high quality submicron-thick top-Si layers.

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