The Effects of Lanthanum-Doping on Strontium-Titanate Thin Films Grown on Si <001> Substrates

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Abstract:
Lanthanum-doped strontium titanate (La:STO) films were grown on silicon <001> substrates at a thickness range of 6-25 nm. Atomic layer deposition was used to grow the films after buffering the substrate with four unit cells of STO deposited via molecular beam epitaxy. La:STO films were successfully grown on silicon (Si) while maintaining a single-crystal structure and achieving good conductivity, in comparison to the insulating properties of undoped STO. The charge density of the La:STO film was calculated to be $2.18 \times 10^{21}$ cm$^{-3}$. Charge densities obtained for varying La concentrations ranged from $6.72 \times 10^{20}$ to $3.86 \times 10^{21}$. Only 6% La-doping would be required to obtain the IBM specification of $1 \times 10^{21}$ charges/cm$^3$ for use in a transistor [1]. When tested electrically, a 15% La-doped thin film had a resistivity of about $1.6 \times 10^4 \, \Omega$-cm; however, this is still more resistive than bulk La:STO at the same La-doping concentration (~ $1 \times 10^4 \, \Omega$-cm) [2].

Introduction:
In the fast-paced, ever-developing silicon industry, research is being done to grow crystalline oxides on silicon. Strontium titanate (STO) is one of the few oxides that is chemically stable when deposited on silicon and would be useful in a variety of applications when integrated with other oxides such as the ferroelectric barium titanate [1]. Although research has been successful in such integration, there is a need to find better and more efficient deposition methods. The commonly used molecular beam epitaxy (MBE) process is costly and impractical for large-scale production. This research focuses on using a chemical deposition method, known as atomic layer deposition (ALD), to deposit La:STO thin films.

Experimental Procedure:
Silicon wafers were obtained and diced into 20 $\times$ 20 mm$^2$ pieces. They were solvent cleaned and exposed to ozone radiation to remove carbon contamination, according to the procedure outlined by McDaniel et al. [3]. Using MBE growth methods, four unit cells of crystalline STO were grown on the Si interface to provide a crystalline template for the La:STO. The samples were transported in vacuo to the ALD chamber, where La:STO films were grown at thicknesses of 6-20 nm. Before removal from the vacuum system, these films were analyzed by x-ray photoelectron spectroscopy (XPS) to determine if the ALD was successful in depositing the correct stoichiometric amounts of the elements. After removal, the crystalline structure and film thicknesses were analyzed by x-ray diffraction (XRD) and x-ray reflectivity (XRR) methods. Contacts for electrical testing were made by gold sputter deposition and liquid gallium-indium metal. Electrical measurements were performed using a four-point probe station.

Results and Conclusions:
The XPS data revealed that the ALD growth method was successful in growing perovskite-structured La:STO. It also showed that increased lanthanum activation occurred after annealing at a substrate temperature greater than 600°C; this further corresponded to a decreased resistivity of the film when tested electrically. High doping concentrations (~30%) distorted the crystal, as was discovered in analysis of the XRD data. The rocking curve was an XRD analysis performed at a set angle to show the degree of crystallinity; it revealed that increasing film thickness as well as high doping concentrations
(>30%) contributed to crystalline defects. Because the STO was compressively strained to match the lattice structure of Si, increasing film thickness would require greater energy to keep the crystals strained. Therefore, thicker films were unable to maintain this higher energy order and the STO relaxed back to its original lattice constant.

XRR analysis was used to determine the thicknesses of the films according to the relationship between the x-ray reflectivity and the film thickness given by Bragg’s law: \( \lambda = 2d \sin \theta \). It was estimated that the film thickness grown by ALD was the total thickness determined minus \( \sim 1.5 \) nm from the MBE template growth.

**Future Work:**

Future work would be required to study the electrical properties of thin film La:STO. Because a proposed transistor model by IBM would use a thin La:STO film of only 3 nm, it would be important to understand the impact of such a small scale on the mobility of the films [1].

Furthermore, it was hypothesized that uniform, perovskite crystallinity played an important role in the conductivity of these films since thicker, polycrystalline films had a higher measured resistance. Further research would need to be done to validate this supposition. In order to further the purpose of this research to eliminate the need for MBE growth methods, growth on a different substrate such as germanium may be necessary.

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**References:**

