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Functional Oxides Integrated Epitaxially onto Semiconductors

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1. Introduction

Oxides on semiconductors are becoming increasing important as more functionality on conventional semiconductor devices is being sought that can potentially lead to new applications. This can provide one of the pathways to extend the CMOS roadmap through the integration of added functionalities onto a silicon platform shifting to a *more-than-Moore* paradigm. The properties of oxides that include magnetic and ferroelectricity are enhanced with oxide crystallinity and methods to deposit epitaxial oxides on silicon and eventually compound semiconductors are the subject of research in many laboratories. Currently, the most successful growth of a crystalline oxide on semiconductors that has been achieved is the perovskite $SrTiO_3$ on both Si and GaAs using molecular beam epitaxy [1-3]. While a careful control of the oxygen during nucleation has been demonstrated to produce commensurate growth of $SrTiO_3$ on Si, the evolution of the oxide interface with the semiconductor and the oxidation states of the various elements in the films have not been studied, especially at the oxide/semiconductor interface. In this presentation we will discuss the use of *in-situ* photoemission spectroscopy to investigate of the STO/Si interface. X-Ray photoelectron spectroscopy will be used to determine the formation of interfacial SiO_2 and the oxidation states of Ti at various deposition parameters during the initial stages of growth and correlate the results with RHEED observations. STO on Si are used as virtual substrates to enable other functional oxides such as $BiFeO_3$ to be integrated onto Si.

2. Oxide growth

Oxide thin films are grown in an oxide MBE chamber by co-deposition using elemental sources and oxygen either in molecular or atomic form generated using a plasma source. For the growth of STO, co-deposition is used with the fluxes adjusted for stoichiometric growth and the growth rate determined using RHEED intensity oscillations. The native oxide form Si substrates are removed in-situ by deoxidation at around 750°C using a flux of Sr. The substrate is cooled to 500°C and additional Sr is added to form template with a (2x1) surface structure. The growth parameters are adjusted to nucleate crystalline oxides, and the formation of SiO_2 as a function of oxygen partial pressure is investigated by deposition of a thin layer of STO and transferring the sample, *in-situ* to the analysis chamber for XPS measurements. STO on Si is then used as virtual substrates to prepare other functional oxides. $BiFeO_3$ is deposited using Fe and oxygen plasma with an overpressure of Bi flux- the growth rate being controlled by the incoming Fe flux. Growth is monitored throughout using RHEED.

3. Results and discussions

Under optimized deposition conditions the STO grown on Si displayed a crystalline behavior as observed by RHEED which displayed a 2-dimensional (1x1) streaky pattern for stoichiometric films. To determine the chemical properties of the interface, XPS was used to investigate the oxidation states of the elements. Figure 1 shows the XPS spectra of the Si 2p peak for a 12Å thick STO layer grown under an optimized deposition temperature with varying

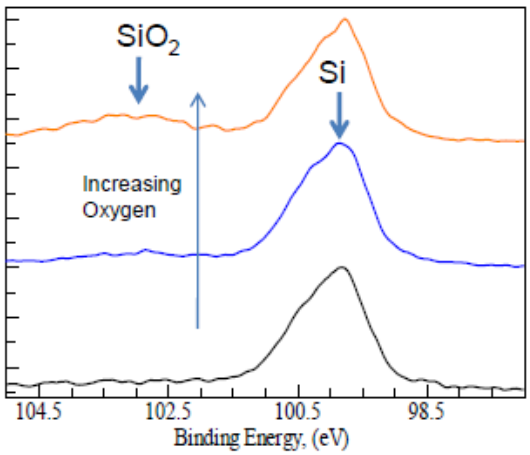

Fig. 1 Si 2p XPS spectra showing the effects of initial oxygen on the formation of SiO_2 during STO growth on Si

amount of molecular oxygen during the initial nucleation of the oxide films. The RHEED patterns observed after the growth of the STO film on Si(100) is indicative of a smooth crystalline film However the XPS data shown in figure 1 suggests that the oxygen level plays an important role during the formation of the interface, with higher oxygen levels leading to the formation of SiO_2. Such a layer would lead to incommensurate oxide deposition with degraded film properties. On the other hand, the use of very low oxygen pressure results in unoxidised Ti as determined by XPS.

Having a crystalline oxide surface on Si is an enabler for deposition of other functional oxides that would not have been possible directly on silicon. STO/Si is used a

virtual substrate to deposit $BiFeO_3$, an oxide that can exhibit both ferroelectricity and antiferromagnetism with high transition temperatures [4], thus leading to the possibility for room temperature magnetoelectric coupling-based devices integrated onto Si CMOS circuitry. The growth of crystalline $BiFeO_3$ is accomplished by MBE and the RHEED image of figure 2 taken during deposition shows 2-D growth front with a 6-fold surface reconstruction.

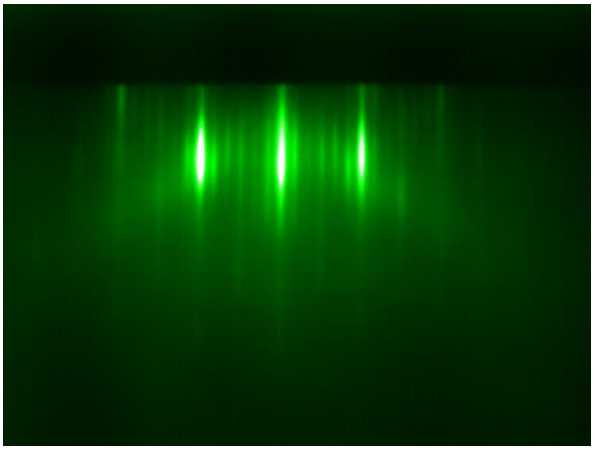

Figure 2 RHEED Image of a $BiFeO_3$ grown on Si using a thin STO buffer layer

The crystalline nature of the BFO film has been confirmed by X-Ray diffraction. Figure 3 represents the theta-2 theta scan for a thin BFO film deposited on STO/Si substrate showing the expected peak positions for a (100) oriented oxide films. AFM measurements of such films display rms values indicative of atomically smooth films. The ferroelectric and magnetic properties of the the BFO films are currently being determined.

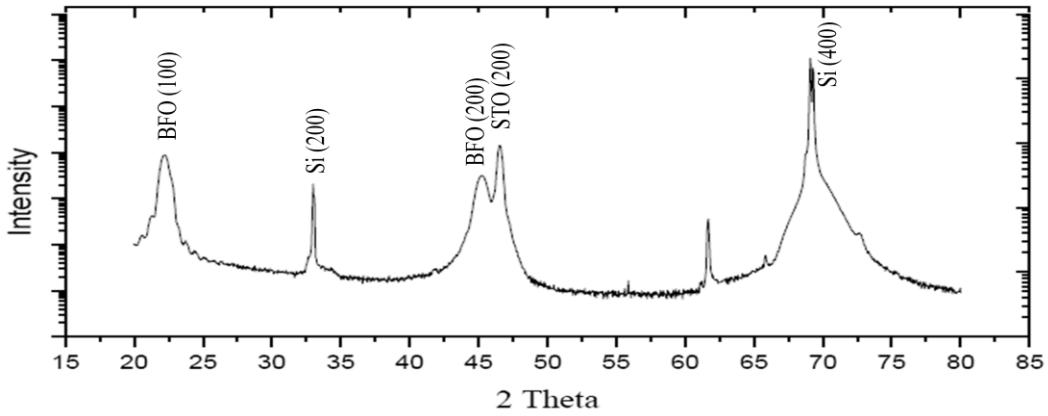

Fig. 3 XRD spectrum of a $BiFeO_3$ layer grown on STO/Si

3. Conclusions

The integration of crystalline oxides onto Si substrates is accomplished by molecular beam epitaxy and provide a pathway for the increasing functionality onto a Si CMOS platform. These oxides possess ferroelectric, magnetic and piezoelectric properties that are enhanced when the films are crystalline. Molecular beam epitaxy is a versatile deposition technique that, when optimized, can be used to engineer the oxide/semiconductor heterointerface for controlling the crystallinity of the oxide films.

Acknowledgements

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