NUCLEATION OF SrTiO₃ (STO) NANOSTRUCTURES ON Si SUBSTRATES PREPARED BY METALORGANIC DECOMPOSITION (MOD)

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Presently, the semiconductor industry faces several technological challenges which must be addressed to preserve their competitiveness. To reduce the leakage current through the conventional gate oxide, SiO_2, this material has been replaced in recent years by high-k dielectrics which exhibit high thermal stability interfaces with Si, dielectric constants higher than that of SiO_2 and high bandgap energies. But the introduction of high-k oxides in complementary-metal-oxide-semiconductor (CMOS) devices causes a carrier mobility reduction in the transistor channel. The replacement of the Si channel by a III-V compound semiconductor, which possess much higher electron mobilities than Si, has been proposed as an alternative to improve the circuit characteristics. But direct growth of a III-V semiconductor (e.g., GaAs) on Si presents very difficult technical problems derived from the nucleation of a polar material (GaAs) on a non-polar one (Si), the high lattice mismatch (4.1%) and the high difference in thermal expansion coefficients (60%), which leads to the formation of a high defect density in the III-V channel. One of the most promising techniques to tackle this problem is selective epitaxy of GaAs on Si using the so-called epitaxial lateral overgrowth (ELO) [1-3].

The aim of this work is to develop a new process to obtain self-organized nanostructures of strontium titanate (STO) on Si by metalorganic decomposition (MOD) which act as a buffer template for subsequent selective growth of GaAs by molecular beam epitaxy (MBE). There is an extensive bibliography describing the deposition of STO layers on various substrates, such as glass, STO or $LaAlO_3$ using MOD [4-7], MBE [8-11], chemical vapor deposition (CVD) [12] and liquid phase deposition (LPD) [13]. However, the deposition of STO layers on Si substrates by MOD has only been reported by Ng. [14].

The precursor solutions were prepared in dry Ar atmosphere due to the hygroscopicity of the precursor, $SrTi(OCHMe_2)_6$. The solvent was isopropanol. The solutions, with concentrations between 1.0x10-3 and 1.0x10-2M, were deposited over Si (001) substrates in a clean room by spin coating and, subsequently, drying, pyrolysis and crystallization steps were applied. The crystallization was carried out by two alternative heating procedures: (i) rapid thermal annealing (RTA), which was performed in O_2 atmosphere at 650, 750 and 800ºC, and (ii) conventional heating in air to 900ºC. The surface morphology of the STO deposits and the chemical state of surface species were studied by atomic force microscopy (AFM) and infrared spectroscopy (IRS), respectively.

In the samples crystallized at 650ºC, the STO phase coexists with organometalic macromolecules due to incomplete reaction. In the other series, the STO self-organizes by the formation of three kinds of nanostructures. Low precursor solution concentrations lead to the formation of islands grouped in two populations with diameters of ≈65 and ≈35nm and heights of ≈9 and ≈6nm, respectively. The estimated density have been found to be between $3.0x10^8$ and $2.0x10^{10}$ cm^{-2}. Medium concentrations favor the appearance of rings with external and internal diameters of ≈50nm and ≈20nm, respectively, and an average height of ≈4nm. Full uniform layers were obtained for the highest concentrations. The circular islands became rectangular when the annealing temperature increased due to an improved crystallization process (STO phases crystallize in cubic and rectangular systems). The island size was found to increase with precursor solution concentration up to a critical value (5.0x10⁻³M), where an island to ring transition takes place. This nucleation mechanism agrees with the growth models proposed by Doudevski [15] and Lorke [16] for other material systems. The island formation begins with the adsorption of organometalic molecules on the substrates constituting a matrix of crystallization nucleus. When the temperature is increased the solvent evaporates and molecules diffuse on the surface interacting among them. As concentration increases, the nuclei density increases and surface collisions become more frequent. At this stage the aggregation of new atoms to the nuclei is the limiting step. When the islands reach a critical dimension the upper atoms are in an energetically unfavourable state and they migrate out of the island re-incorporating to the surrounding substrate where the ring is formed.

The IR spectra prove the absence of water or solvent residues. The $SrTrO_3$ phase was present in both 800 (RTA) and 900ºC (conventional oven) samples. By contrast the 900ºC samples exhibit bands corresponding to secondary crystalline phases (SiO_2, TiO_2 and $SrCO_3$).

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Figures

Figure 1 AFM ($1.0 \times 1.0 \mu m^2$) images of the surface morphology of (a) islands and (b) rings. 3D and 2D details ($50 \times 50 nm^2$) of an island (c, e) and a ring (d, f) with their cross-sectional profiles (f,g) for samples crystallized at 750ºC from a 1.0×10^{-3} M solution.

Figure 2 Graphic representation of island size (a) and (b) island density vs precursor solution concentration for the samples crystallized at 800ºC in O_2 (RTA oven) and at 900ºC in air (conventional oven).

Figure 3 IR spectra of samples for precursor of 1.0×10^{-2} M, crystallized at 900 and 800ºC with band attributed to **STO**, **SiO₂**, **SrCO₃** y **TiO₂** phases.