Thermodynamic Optimization of OMCVD Deposition of $SrTiO_3$

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$SrTiO_3$ is a potential candidate in the search of novel high K oxides that could replace silica in electronic devices. The thermodynamic study of the Sr-Ti-O and Sr-Ti-O-Si systems revealed multiple voids and incompleteness of data. Nevertheless, the existing values have been used to determine the compounds that are supposed to be in equilibrium with $SrTiO_3$ in the Sr-Ti-O-Si system. A first result is, that $SrTiO_3$ is not in equilibrium with pure silicon on which it is supposed to be deposited (Fig. 1). This means that interface reactions are likely to occur and the phase diagram is therefore a valuable tool to understand the behaviour.

Thin $SrTiO_3$ films are currently deposited starting from organometallic precursors and an Ar/O2 mixture. Therefore the CDV diagrams for a $Ti(i\text{-}Opr)_2(thd)_2$ – $Sr(thd)_2$-tetraglyme – Ar – O_2 mixture have been determined. With these diagrams, the parameters that are favourable for the deposition process can be identified to avoid co-deposition of unwanted carbon or carbonates (Fig.2).

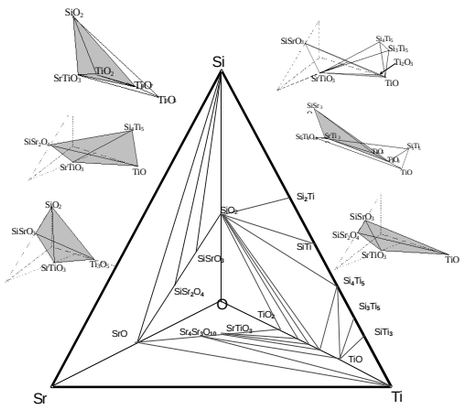

Fig. 1.The Sr-Ti-O-Si phase diagram calculated at 973.15K and 1 bar, showing some of the 9 four phase equilibria which are formed with $SrTiO_3$. The tetrahedron presents all condensed phases which have been taken into account for the calculations.

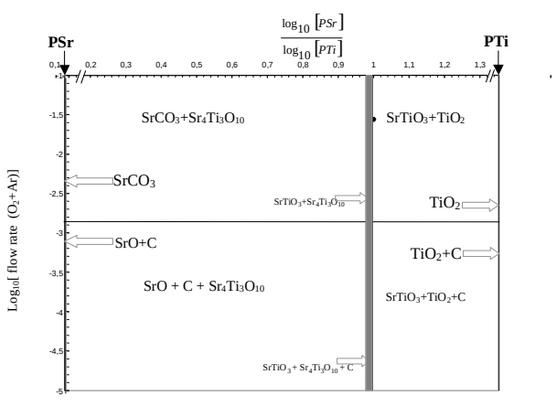

Fig 2.- Equilibrium deposited compounds as a function of precursor and Ar/O_2 pressure at 973.15K and 6.7 mbar