Epitaxial $SrTiO_3$ thin films on silicon for electro-optical quantum devices

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Electro-optical (EO) quantum transducers will be key to quantum information processing as they are the gateway to transfer information between electronics (RF qubits) used for computation and photonics (optical qubits) used for communication. However, quantum applications require EO transducers that offer unity efficiency which is difficult to achieve with current materials. Perovskite oxides are an auspicious category, featuring high dielectric permittivity values at radio frequencies, strong nonlinearities and some materials such as $BaTiO_3$ can be integrated into standard silicon photonics. An overlooked material in the EO transducer community is strontium titanate ($SrTiO_3$, STO). Its intrinsic parameters allow a direct growth on silicon, it shows nonlinear optical behaviour and importantly, its dielectric permittivity of several hundred at room temperature is very high and increases further to ~10^4 at cryogenic temperatures thanks to its quantum paraelectric behaviour [1] making it an ideal transparent electrode material.

Molecular beam epitaxy (MBE) is one of the few techniques which allows epitaxial growth of STO directly on industry-relevant Si substrates. However, maintaining precise stoichiometry and high crystalline quality in this process remains a significant challenge. Establishing this is essential to obtain STO with bulk-like dielectric properties and to minimize leakage current and optical absorbance. In this study, the importance of cationic stoichiometry and the effect of thickness are investigated for STO thin films epitaxially grown on (001)-oriented silicon substrates.

High-temperature post-growth annealing treatments in O_2 were investigated to promote layer relaxation and reduce oxygen vacancy concentration, thereby improving the physical, electrical, and optical properties of stoichiometric STO. As a result, high-quality STO thin films exceeding 100 nm were successfully fabricated featuring a bulk-like out-of-plane lattice parameter and refractive index, as well as rocking curve full width at half maximum (FWHM) below 0.2°, smooth surface ($R_q < 0.2$ nm) and a leakage current density below 1E-7 A/cm^2 [2].

This epitaxy process for MBE growth of high-quality thick STO layers on silicon (001)-oriented substrates is essential for optimizing dielectric properties, such as the dielectric permittivity. By establishing a correlation between cationic stoichiometry, crystallinity, and STO thickness, we achieve significant enhancement of the effective permittivity at cryogenic temperatures, reaching values of over 2,500 for our stoichiometric 105 nm STO film. To our knowledge, this is the highest reported permittivity for STO thin films on silicon. This study paves the way for using STO thin films as active materials in advanced devices for various applications, including energy storage and quantum information technology.

References:

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[2] A. Boelen, M. Baryshnikova, A. Ulrich, K. Brahim, J. Van de Vondel, C. Haffner, and C. Merckling, "Stoichiometry and Thickness of Epitaxial $SrTiO_3$ on Silicon (001): An Investigation of Physical, Optical, and Electrical Properties," *APL Materials*, manuscript submitted for publication, 2025.

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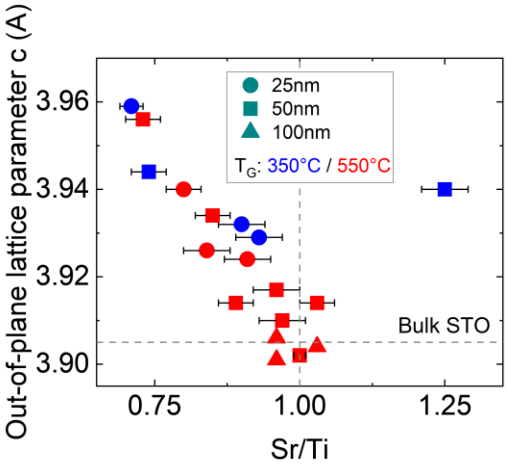

Figure 1: Out-of-plane lattice parameter (c) as a function of Sr/Ti ratio for STO films with varying thickness and growth temperature T_G. For obtaining a bulk-like lattice parameter, perfect cationic stoichiometry, high growth temperatures and layers > 50 nm need to be fulfilled.

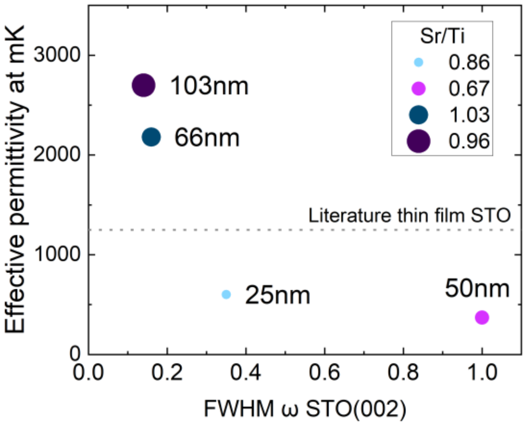

Figure 2: Effective permittivity ε_{eff} near 0 K as a function of the STO (002) rocking curve FWHM. Cationic stoichiometry (Sr/Ti = 1) and increasing STO thickness result in lower FWHM and higher effective permittivity.

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