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Stoichiometric analysis of superficial Ba doped Strontium Titanium Oxide layers using APT: the case of the missing Oxygen!

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Oxides play a significant role in the semiconductor field. This includes SiO2 through to HfO2 for insulating gate layers [1]; to the more complex transition-metal oxide perovskites (e.g. SrTiO3, BiFeO3) [2] which are now being explored for future memory and quantum computing applications. Sub-stoichiometric oxygen has been shown to increase the leakage current while accurate characterization of these layers is challenging but remains a crucial step in their evolutionary process. Given their scale (a few nm) and evolving complexities, few techniques offer the spatial resolution combined with mass analysis capabilities required, hence atom probe tomography (APT) [3] is now being explored.

In this study, atomic layer deposited (~7 nm) Ba doped SrTiO3 layers have been analyzed using APT (see figure 1). Additionally, Rutherford backscattering spectrometry (RBS) was used to determine the ratio between Ba:Sr:Ti and Time-of-Flight/Energy elastic recoil detection (ERD) the Sr:O ratio. The objective was to establish the correct layer stoichiometry, a critical parameter for tailoring device performance, from a single analysis. A LEAP 5000 XR was used for the APT analysis of the sample, and from the mass spectra obtained, apparent layer stoichiometries determined. APT showed an excellent Ba:Sr:Ti ratio agreement to RBS (see Table I), however, from the APT Sr:O ratio compared with the ERD, a significant oxygen underestimation was observed.

In conclusion, given that APT is expected to have the same detection efficiency for all ions, it was found through comparison with RBS and ERD that the oxygen quantification in APT from Ba doped SrTiO3 layers was underestimated by ~20 at.%. The excellent agreement in Ba:Sr:Ti ratio between APT and RBS would indicate that any potential loss mechanism(s) present has (have) an equivalent impact for all three elements. Correspondingly, the loss mechanism(s) is (are) either larger for oxygen, or there is an additional influence, which suppresses the generation/detection of the oxygen ions in APT.

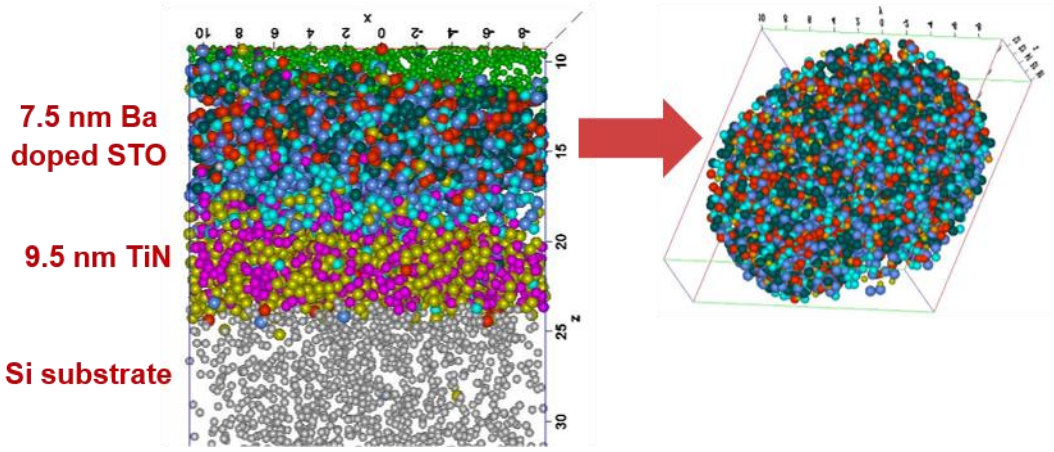

Figure 1. Figure 1. (a) Reconstruction of data taken from a thin film of Ba doped SrTiO3 on TiN and (b) The isolated Ba doped SrTiO3 region of interest used for the stoichiometric analysis.

Element	APT	RBS
	Element ratio	Element ratio
Ba	8.1	9.5
Sr	30.0	28.4
Ti	61.9	62.1

Figure 2. Table I. The Ba:Sr:Ti ratio found from APT and RBS where an excellent agreement for APT with the well-established RBS technique is attained.

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