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Atomic Structure and Chemistry of Defects in non-stoichiometric $SrVO_3$ Thin Films

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Strontium vanadate, $SrVO_3$, is a transition-metal oxide with the potential for emergent behaviour at oxide-oxide interface. It is of particular interest in the fabrication of highly conductive oxide films where its interface with the substrate plays a key role [1,2]. Furthermore, controlling the precise composition of the film is critical to achieve desired properties. Otherwise, several types of defects are introduced in the films that lead to property degradation through charge compensation. Detailed characterization of atomic-scale structure and chemistry are thus required to completely understand the film and interface behaviour [3].

In this talk, we will examine grown $SrVO_3$ (SVO) films on the (001) $(LaAlO_3)_{0.3}(Sr_2AlTaO_6)_{0.7}$ (LSAT) substrates by a combined chemical beam epitaxy/molecular beam epitaxy approach [4]. We will show that the latest advances in aberration correction and x-ray detectors proved essential to fully characterize the substrate/film interface. For this study a probe corrected FEI Titan G2 60-300 S/TEM with ChemiSTEM technology was used for both high-angle annular dark-field (HAADF) imaging and atomic resolution energy dispersive x-ray spectroscopy (EDS). For stoichiometric films, see Figure 1(a), a defect free perovskite SVO film is observed. Controlled deviations from stoichiometric growth conditions resulted in films that accommodated various types of defect, predominately misfit dislocations and Ruddlesden-Popper defects, see Figure 1(b-c). We will discuss the type of defects formed at the interface and within the film when grown under Sr-rich and V-rich conditions. For a complete characterization of these defects, we will demonstrate the power of atomic resolution EDS to simultaneously explore the distribution of *all* constituent atoms.

We will also show that the atomic structure of SVO/LSAT interfaces prove to be difficult to interpret using solely HAADF STEM. Figure 2(a) shows that A- and B-site atom columns of the perovskite LSAT cannot be readily distinguished due to insufficient Z-contrast. This is particularly critically as bright atom columns are observed at the interface. We will discuss the results from atomic resolution EDS that provide an unambiguous interpretation of the interface, as shown in Figure 2(b). Finally, our results will emphasize the latest advances in STEM imaging and EDS reveal new insights into the atomic structure of the SVO/LSAT interface and the chemistry of the defects present in the films.

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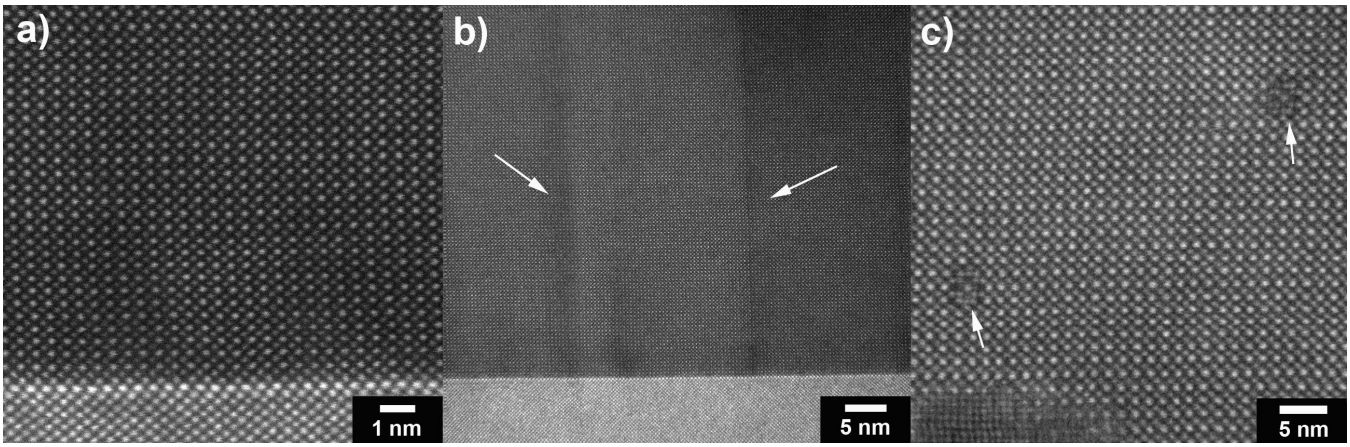

Figure 1. (a) STEM image of the atomically abrupt SVO/LSAT interface in the stoichiometric sample, (b) STEM image of an RP fault in Sr-rich films in a cross-section TEM sample, (c) the same RP faults in a plan-view TEM sample.

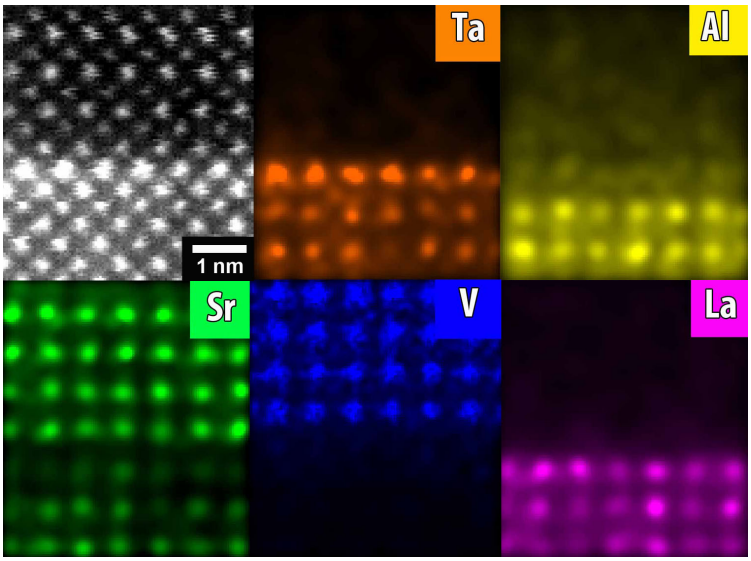

Figure 2. Atomic-resolution imaging and EDS maps at the SVO/LSAT interface. Z-contrast for the substrate is ambiguous. EDS (3-pixel Gaussian filter applied) shows that the A- and B-site columns form an abrupt interface.

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