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Atomic scale compositions across $DyScO_3/SrTiO_3$ interfaces

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Recently, highly conducting layers were reported at the interfaces between complex, insulating oxides of different polarity [1]. The polar discontinuity delivers the driving force for a charge accumulation in the interfacial region which has been demonstrated for $LaAlO_3$ interfaces with $SrTiO_3$. Here it is shown, that the polar discontinuity can be accommodated by variations in composition of cat ion lattice planes at the polar oxide interface between $DyScO_3$ and $SrTiO_3$, where $DyScO_3$ holds the same polarity as $LaAlO_3$. An intermixing extending over two monolayers at the interfaces for both, the Dy-Sr sublattice and the Sc-Ti sublattice is quantified. As a result, charge neutrality is established by electrical compensation between neighbouring atomic planes**.**

The atomic structure of a $DyScO_3/SrTiO_3$ multilayer system, which was grown by pulsed laser deposition, is revealed in the HAADF image shown in Figure 1. The positions of different types of atoms can be identified by inspection of the structure models displaying one orthorhombic unit cell of $DyScO_3$ and four cubic unit cells of $SrTiO_3$, respectively. Along the interfaces, i.e. in atom rows 4 and 14, the contrast at the Dy/Sr positions can be clearly observed to alternate between neighbouring atom columns. This is also seen in the concentration profile shown at the bottom, which was evaluated by quantification of the intensities through two-dimensional Gaussian fits to each atom position. I.e. an ordered interface structure is unambiguously detected, which can only be observed along the [101] direction seen here, which is one of two possible domain orientations of epitaxially grown $DyScO_3$ on $SrTiO_3$ [2].

The Sc and Ti composition of each atomic layer were determined by isochronous recording of EEL spectra (Fig 2 top) and of a HAADF image (fig 2 bottom). Details of the method are described elsewhere [3]. Sc and Ti concentrations are superimposed in the HAADF image in Figure 2. In addition, the average Dy concentration is displayed, i.e. the average of positions A and B shown in Figure 1. An intermixing extending over two monolayers at the interfaces is found for both, the Dy-Sr sublattice and the Sc-Ti sublattice. Furthermore, the valence of Ti is found to be constant throughout the layer system.

Employing the ionic model [1] the composition of the individual atomic layers can be translated into charges, which are displayed for the atomic layers 12 through 16 in Fig. 3. Considering a compensation between adjacent layers, which is denoted by the arrows, each of the layers is found to be neutral as indicated by the red diamonds. Hence, the interfaces are expected to be insulating, which is confirmed by electric measurements. From this result it is concluded that in addition to charge accumulations, intermixing of cat ions can contribute to counteract the interface dipoles associated with the polar discontinuity.

References

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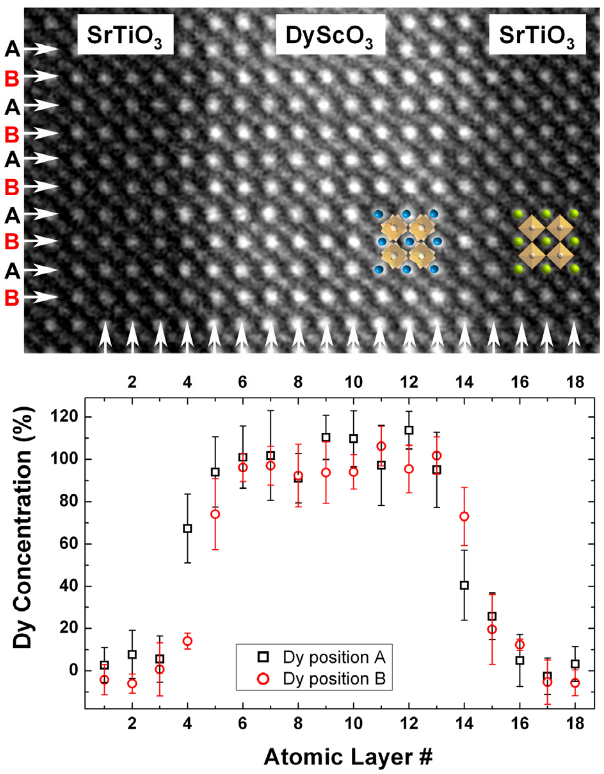

FIG 1 HAADF image of $SrTiO_3/DyScO_3$ multilayers. For each Dy layer the concentrations of positions A and B are deduced (bottom). Error bars denote the standard deviation of five equivalent positions within each Dy layer, i.e. positions A and B, respectively. The interface layers, rows 4 and 14, show a distinct difference in contrast between the neighbouring positions A and B. Error bars denote the standard deviation obtained from concentration values in regions of constant composition.

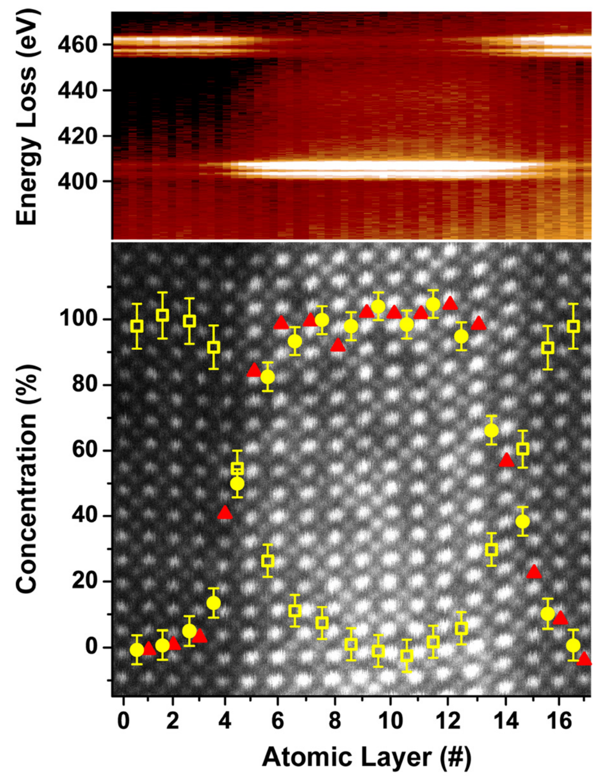

FIG 2 The spectroscopic image (top) showing the L_{23} absorption edges of Sc and Ti versus the lateral position and the HAADF image of $SrTiO_3/DyScO_3$ (bottom) were recorded simultaneously. The fast scan direction runs from bottom to top. Superimposed are the average Dy (red triangles), Sc (yellow circles) and Ti (yellow open squares) concentrations for each atom row, which were obtained from the HAADF image (FIG 1) and spectra extracted row by row from the spectroscopic image, respectively.

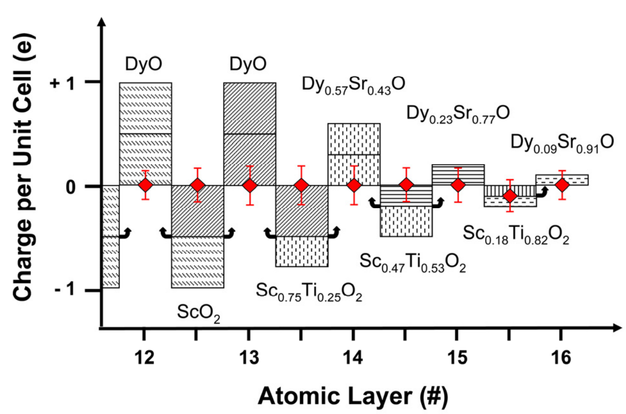

FIG 3. Summary of charges according to the composition for layers 12 through16 shown in Figs 1 and 2. Charge compensation with adjacent layers is indicated by the arrows and the hatching patterns. The resulting charge in each layer is shown as red diamonds. Error bars are calculated from the error estimates in composition.

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