Defect landscape and electrical properties in solution-derived LaNiO_3 and NdNiO_3 epitaxial thin films

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ABSTRACT

In this work we evaluate the defects and the associated distortions present in tensile and compressive-strained chemical solution deposition (CSD) derived NdNiO_3 (NNO) and LaNiO_3 (LNO) thin-films by means of aberration corrected Scanning Transmission Electron Microscopy (STEM). We elucidate a fundamental link between strain and the most common defect observed in Nickelate films, the Ruddlesden-Popper fault (RPF), which will ultimately impinge on the electrical properties of the films. Overall, the concentration of RPFs defects increases with the lattice mismatch. More specifically, LNO films are always metallic, although transitioning from compressive to tensile strain results in the appearance of RPFs and an increase of the resistivity. On the other hand, NNO films always behave as insulators under tensile strain, whereas under compressive strain the increase of the thickness makes the onset of the metal-to-insulator transition (MIT) to shift to higher temperatures.

I. INTRODUCTION

The properties of transition-metal oxides (TMO) films strongly depend on epitaxial strain, which affects metal-oxygen bond lengths and angles and the kind of defects and densities, thus impacting their physical properties [1–3]. Besides, when these materials are fabricated in the form of thin films, it is easier to distort their crystal structure by epitaxial strain so it is possible to enhance their bulk physical properties or even generate new functionalities [4–6]. Among TMO, nickelate perovskites, RENiO_3 , where RE refers to a rare-earth, has centered a major interest since it is one of the few oxide materials that present metallic conductivity at room temperature and an abrupt metal-to-insulator transition (MIT) for a certain temperature [7–9] that make them very promising as elements for adaptative electronics [10–12]. In addition, in RNO compounds, it is possible to shift the MIT to lower temperatures when the ionic atomic number of the cation located at the vertex of the perovskite structure is increased [8,9]. Indeed, the Ni-O-Ni bond angle progressively decreases from 165° (maximum Ni-O-Ni bond angle observed in LaNiO_3 compounds) while reducing the

RE. As a consequence, the overlapping between the 2p oxygen and 3d Ni orbitals also diminishes affecting their electronic properties.

Likewise, it is possible to induce changes in RNO electronic properties by epitaxial strain [13–20], as well as by hydrostatic pressures [21,22]. Although it has been confirmed that these two mechanisms cause the MIT shifting to lower temperatures when the material is compressed, this effect is more pronounced when the distortions are generated by epitaxial strain [13]. This is why high quality epilayers grown on single crystal substrates are favoured for fundamental studies and for proof-of-principle device work. However, it still remains unclear how the ReNiO_3 films accommodate when they are epitaxially grown on different substrates. Here, we give new structural insights of tensile and compressive strained LaNiO_3 (LNO) and NdNiO_3 (NNO) thin films grown by the chemical solution deposition (CSD) technique, which is an easily scalable and low-cost deposition method. The confirmation that high quality RNO epilayers can be achieved by CSD is very promising since it opens the possibility to grow them faster in a longer length scale production. We have identified the presence of misfit dislocations in the 6nm-thick LaAlO_3 (LAO)/LNO heterostructure (where both the LAO and LNO have a rhombohedral structure) and the occurrence of Ruddlesden-Popper faults (RPFs) in the other heterostructures, which signals the importance of the chosen substrate structure. We also quantify a previously unforeseen polar-like distortion that appears on either side of the RPF.

II. EXPERIMENTAL RESULTS

RNO	a_{film} (Å)	Substrate	a_{subs} (Å)	Strain (%)	T_{MI} (K)	Thickness (nm)
NNO_{ort}	3.811	LAO_{rhom}	3.791	- 0.5	198	20
NNO_{ort}	3.811	LAO_{rhom}	3.791	- 0.5	112	6
NNO_{ort}	3.811	LSAT_{cub}	3.868	+ 1.5	Insulating	6
LNO_{rhom}	3.859	LAO_{rhom}	3.791	- 1.8	Metallic	6
LNO_{rhom}	3.859	LSAT_{cub}	3.868	+ 2.3	Metallic	6

TABLE 1. Structural properties of the films. NNO and LNO cell parameters were extracted from Ref. [8] and the ones from LAO and LSAT were directly given by the substrate supplier. The

nominal strain value (ϵ) is calculated by the common equation: $\epsilon = \frac{a_{\text{substrate}} - a_{\text{film}}}{a_{\text{substrate}}}$ ($\epsilon >$

0 means tensile strain).

The lattice parameters and strain values of LNO and NNO films grown onto (001)-oriented LaAlO_3 (LAO) and $(\text{LaAlO}_3)_{0.3}(\text{Sr}_2\text{TaAlO}_6)_{0.7}$ (LSAT) single crystal substrates are summarized in Table 1. Single phase and epitaxial films were grown following a CSD process with a solution based on metallorganic precursor salts. Later the layers are structurally, and morphologically characterized. See Ref. [23] for further details on solution synthesis, thermal treatment and structural and morphological films characterization. Even though NNO and LNO are orthorhombic and rhombohedral respectively (with larger cell parameters than conventional ceramic substrates), their pseudocubic structures are very close to those from LAO and LSAT substrates resulting in homogeneous and fully epitaxial thin films. Fig. 1 (a) shows the pseudocubic cell structure of both NNO and LNO phases. The oxygen octahedrons of both NNO and LNO compounds differ from the ideal perovskite structure. In the case of LNO compound, the octahedrons are tilted 165.2° along the $a^-a^-a^-$ pseudocubic axes (following Glazers' notation) [24], whereas the octahedrons are tilted are 157.6° and 156.1° along the $a^-a^-b^+$ axes in the NNO compound. This is not the only noticeable structural difference, as Nd cations are shifted up and down drawing a zig-zag-like pattern through the $[001]_{\text{PC}}$ direction (subscript PC for pseudocubic notation) in the NNO compound [25]. Accordingly, in the absence of strain, the $\text{Ni-O}_{\text{basal}}\text{-Ni}$ angles parallel to the substrate surface correspond to the 156.1° and 157.6° ones whereas the perpendicular $\text{Ni-O}_{\text{apical}}\text{-Ni}$ one is 157.6° .

The measured resistivity as a function of the temperature of each sample is illustrated in Fig. 1 (b). These measurements were performed using Van der Pauw configuration in a PPMS Quantum design system with variable temperature from 400K down to 5K. From the obtained curves, it is observed that both resistivity and metal-insulator transition temperature (T_{MIT}) are highly influenced by the substrate, film thickness and RE cation specie. In particular, the sharp metal-insulator transition (MIT) is only observed in NNO films grown onto the LAO substrate, which is shifted from 201K (in bulk) to lower temperatures when the film is compressed by epitaxial strain, as equally reported by Catalano *et al.* in magnetron sputtered thin films [13]. This is not occurring when NNO is grown onto LSAT substrate, which always behaves as an insulating material for the measured range of temperatures. On the other hand, LNO films remain always metallic (as in the case of bulk) regardless of the used substrate, even though the resistivity is different in each case. In order to better understand all these changes, we have studied the microstructure of our RNO films by means of scanning transmission electron microscopy (STEM). We used a FEI-TITAN low-base operated at 300 kV and a JEOL JEM ARM200cF operated at 200 kV, both equipped with a CEOS aberration corrector, which ensures sub-angstrom resolution. Electron energy loss spectroscopy (EELS) analyses were

performed with the JEOL JEM ARM200cF, which is equipped with a Gatan quantum electron energy-loss spectrometer. Specimens for STEM were prepared by conventional methods: grinding, dimpling and Ar ion milling.

The epitaxial growth of the 6nm-thick NNO and LNO films onto LAO and LSAT substrates is confirmed by the high angle annular dark field images (HAADF) images, also known as Z-contrast images, shown in Fig. 2. They show a cube-on-cube relationship between film and substrate. The sharp and coherent substrate-film interfaces (marked with white arrows) are easily identified in this imaging mode as the brightness associated to each atomic column scales with its atomic number [26]. Moreover, the images also show two distinct defects within the films depending on the used RE specie and substrate. In the case of LNO grown onto LAO substrate, misfit dislocations are generated at the substrate-film interface (pointed by an orange arrow). If the film is fully relaxed by the misfit dislocations, it is possible to estimate the separation (S) between them by this simple expression: $S = b/\varepsilon$, where ε refers to the nominal strain value and b to the modulus of the Burgers vector associated to the misfit dislocation [27–30]. Considering that $b = (100)$ and $\varepsilon = -1.8\%$, misfit dislocations are expected to be 21 nm apart. However, the measured distance (50nm in average) indicates that the film is partially strained. It is worth mentioning that, from all set of samples studied, we have only observed misfit dislocations in the LNO/LAO heterostructure, in which both substrate and film share the same structural symmetry (rhomboedral). In other scenarios, RNO crystal prefers the generation of another kind of defect: the Ruddlesden-Popper fault (RPF) (yellow arrows in Figure 2).

The RPF is characterized by suppressing one Ni plane and shifting half unit cell the crystal structure along the $\langle 111 \rangle$ direction [31,32]. In the fault, both the RE and O atoms from the RNO perovskite structure are ordered like half unit cell of a rock salt structure which runs along one of the three crystallographic directions. Indeed, we have additionally acquired atomic resolution EELS maps and planar view Z-contrast images to confirm the atomic composition of RPF structures and that they are oriented parallel to any crystallographic axis, see Ref [23] for further details. Yet, in some areas there is no contrast between Nd and Ni atomic columns because two different nano-sized regions shifted by the rock salt fault are superimposed along the viewing axis. When this happens, the RE and the Ni atomic columns lay one upon another and the difference in contrast is cancelled [31,33].

Still, it is possible to identify the same Nd rippling present in NNO bulk crystals [25]. This Nd rippling feature is also detected by the appearance of additional spots in the

corresponding fast-fourier transform (FFT) pattern (yellow circles), as shown in Fig. 2 (b). For the particular thickness of 6nm, we observe that the Nd rippling always runs parallel either to the $[100]_{pc}$ or $[010]_{pc}$ substrate directions, thus defining different grain domains. However, this zig-zag feature also runs along the out-of-plane direction when the film thickness is enlarged [23]. In contrast, these spots are not observed in the LNO thin film's FFT, as no La rippling is present in this compound. It is important to note that the presence of RPFs poses a stoichiometric issue, however, we have observed that the systems studied solve it forming NiO nanoparticles that are aggregated at the surface of the films [23].

The fact that the concentration of RPFs increases with the substrate mismatch suggest that the occurrence of RPFs is a strain relief-like mechanism that helps to accommodate the strain of the RNO films. In order to confirm that, a strain analysis has been carried out in all the LNO and NNO layers. We have used the Geometrical Phase Analysis (GPA) software, which allows for measuring, strain, or deformation, with respect to some reference area, in our case the substrates. Circular masks with radii producing a lateral resolution ≈ 1 nm in the GPA images were defined around the (200) and the (002) reflections in order to minimize possible artifacts upcoming from the RPFs and LSAT substrate. The resulting in-plane and e_{xx} and out-of-plane e_{yy} strain maps are shown in Figure 3. Regarding LNO films (a,d), the in-plane distortion maps (e_{xx}) show no color depth-wise variations in defect-free areas, meaning that the substrate in-plane parameter is completely transferred to the film. On the other hand, the observed color change, in the out-of-plane distortion map (e_{yy}), is associated to an out-of-plane parameter expansion (compression) in the compressive-strained (tensile-strained) LNO layer when grown onto LAO (LSAT). The resulting strain is homogeneous within the layer with values around 2% (-1.5%) in samples grown onto LAO (LSAT). These results confirm that both films are still partially strained with similar values to those reported in previous studies [32].

As to NNO films, different scenarios are observed, see Fig. 3. (b-c,e). First, the e_{xx} map corresponding to the NNO film grown onto LAO (low compressive strain) shows a coherent strained film with a homogenous out-of-plane expansion (2%), which is much higher than what was expected for the reference mismatch value, a compressive -0,5% deformation. Second, the NNO film shows two differentiated regions when grown onto LSAT substrate: a three-unit cell thick defect-free slab close to the interface, and a dense network of rock-salt faults above it. The yellow dashed line in Fig. 3(e) marks the interface between these two different regions of the NNO film. The e_{xx} map reveals a fully strained and coherent defect-free slab region, i.e. an expansion of the in-plane NNO cell parameter. Besides, as expected for a Poisson-like deformation, the e_{yy} map shows there an out-of-plane compressed cell. However, in the upper

layer, strong contrast variations are observed in e_{xx} & e_{yy} maps, stemming from a large concentration of rock salt faults. Interestingly, the 25 nm-thick NNO film grown onto LAO also shows a 6 nm-thick defect-free layer that is compressed (expanded) along the in-plane (out-of-plane) direction, growing up to the first 6 nanometers of the film, see Fig. 3(c). Yet, in the upper region of the film, with larger amount of RPFs defects, the in-plane parameter is expanded, suggesting that the crystal partially accommodates the strain in this region.

We have additionally evaluated the density of RPFs (R) for each 6nm-thick RNO film by summing the perimeter length of all the RPFs that are identified in several Z-contrast images and dividing the resulting number by the total film areas viewed in the images, as done in Ref. [34]. The obtained R values for the NNO films are 0.22 nm^{-1} and 0.70 nm^{-1} when they are grown onto LAO ($\epsilon \sim -0.5$), and LSAT ($\epsilon \sim 1.5$), respectively, whereas, the obtained R values for LNO films are 0 and 0.044 nm^{-1} when grown onto LAO ($\epsilon \sim -1.8$), where misfit dislocations are observed, and LSAT ($\epsilon \sim 2.3$), respectively. These R values evidence that the density of RPFs tend to increase with the substrate mismatch value in both RNO compounds. The residual resistivity of each RNO film is also observed to increase with R .

Besides, our work also reveals a structural distortion on either side of the rock salt fault, see Figure 4. These structural changes were quantified using a center of mass refinement on the Z-contrast image shown in Fig. 4 (a) to determine the atomic positions of the Re and Ni sub-lattices. We obtained a detailed real-space map of the in- and out-of-plane (d) parameter and the distance δ from the center of mass of the unit cell. As shown in Fig. 4 (b) and (c), the substrate in-plane parameter is transferred to the whole film. The elimination of the NiO plane at rock salt fault structure reduces the Nd-Nd spacing along the out-of-plane direction up to a value of $2.891 \text{ \AA}$ ($a_{\text{NNO}} = 3.812 \text{ \AA}$). The cells located at either side of the rock salt fault are also compressed an approximate value of -5 or -6% along this direction, taking as a reference the film or substrate, which is tantamount a reduction of the unit cell volume. Interestingly, the LNO unit cell expands along the out-of-plane direction before and after the fault. This might explain the negative Poisson coefficient obtained from the XRD Q-plot measurements associated to the tensile-strained NNO samples [23]. Concomitantly to these structural changes, the Ni atomic columns shift towards the fault, thus generating a polar-like distortion. These polar-like distortions are always observed pointing at the rock salt fault, regardless of its orientation, parallel or perpendicular to the substrate [23]. It is worth noting that both effects are confined only at the very first unit cells surrounding the RPF, and that are observed in all the studied heterostructures. These out-of-plane distortions are similar to those observed in LNO/LAO heterostructures direction [35,36], but different in orientation to those recently

reported oxide systems such as the $\text{Sr}_{n+1}\text{Ti}_n\text{O}_{3n+1}$ Ruddlesden-Popper oxide [37], which show a polar distortion parallel to the rock salt fault plane.

The films' microstructure described so far allows establishing some correlations with the resistivity measurements. As shown in previous studies, the electrical transport of RNO films is influenced by the mismatch [13,17], orientation [14,38] and symmetry [39] of the chosen substrate, and by the film thickness [17] and termination [35,40]. All of these parameters play a role on the stabilization of the Ni-O-Ni bond angles and lengths and therefore on the intrinsic RNO electronic configuration [8,9,20]. From the transport measurements of our films, shown in Fig.1(b), it is observed that compressive strain shifts the MIT to lower temperature values in NNO films as a direct consequence of the Ni-O bond narrowing [9,13,16,20]. Besides, tensile strain increases the film resistivity more than one order of magnitude, in both LNO and NNO films, compared to the compressed films. On the one hand, this increase of the resistivity might be ascribed to the enlargement of the Ni-O bond lengths. However, the lower resistivity measured in the PLD-derived LNO/LSAT [41] suggests that the RPFs also influence the electrical transport, as the RPFs might act as blocking barriers agents to the current flow due to the NiO plane suppression. This is more evident in the case of the NNO/LSAT heterostructure, where the high concentration of RPFs, with only two or three defect-free monolayers, not only substantially enhances the film resistivity but it also enlarges the insulating behavior out of the measured range of temperatures (5-400K). Besides, when comparing the resistivity vs. temperature curves of RNO films grown by chemical and physical methods, one realize that CSD-derived RNO films have a less abrupt MIT [13,14,31,42], which we ascribe to their larger concentration of defects.

In conclusion, our work has revealed that the lattice mismatch accommodation/strain relief mechanism in epitaxial CSD-derived LNO and NNO thin films is not driven by the formation of mismatch dislocations alone, but by formation of RFPs, which turn to be their most common defect. We demonstrate that the concentration of RPFs defects increases with the lattice mismatch. Misfit dislocations are more favorable when both the Nickelate films and the substrate have the same structural symmetry. Additionally, distortions in the RPFs' neighboring unit cells have also been identified. The RNO cell is compressed in the range of one unit cell next to the rock-salt fault, while the Ni atoms are displaced far from the center of the unit cell and towards the rock salt fault. Both the strain and the presence of the RPFs affect the electrical conductivity and the MIT of the RNO films. In LNO films the transitioning from compressive to tensile strain results in the appearance of RPFs and an increase of the resistivity in otherwise metallic films. On the other hand, NNO films always behave as

insulators under tensile strain, whereas under compressive strain the increase of the thickness makes the onset of the metal-to-insulator transition (MIT) to shift to higher temperatures. Our results show that the presence of a large amount of RPFs is clearly detrimental to the conductivity, and that their generation and concentration depend on the used substrate, strain and growing conditions.

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FIGURES

FIG .1. (a) Pseudocubic structure of the NdNiO_3 (left) and LaNiO_3 (right) bulk phases. La, Nd, Ni and O atoms are plotted in orange, green, blue and red, respectively. (b) Resistivity measurements as a function of the temperature for the studied samples.

FIG. 2. Z-contrast images of LNO and NNO thin films grown onto LAO (a,c) and LSAT (b-d) substrates. Misfit dislocations and RPFs are pointed out with orange and yellow arrows, respectively. Inset shows the spots appearing at the Fourier Transform (FFT) pattern associated to the Nd rippling. One of them is marked with a yellow circle. Scale bar: 5 nm.

FIG. 3. Strain analysis where the GPA software is applied to Z-contrast images from 6nm-thick LNO/NNO films grown onto LAO (a-b) & LSAT(d-e) substrates, and from (c) 25nm-thick NNO/LAO film. The in-plane and out-of-plane strain maps are generated by selecting the g_{200} (e_{xx}) and g_{002} (e_{yy}) Bragg reflexions, which minimize artifacts coming from the RPFs. A region from the substrate has been selected as a strain-free reference area. Color fluctuations up to $\pm 0.5\%$ are attributed to statistical error. The intensity is correlated with

the strain value which is represented by a temperature scale whose contrast limits are $\pm 20\%$. Substrate/film interface is highlighted by blue dashed lines. Areas below yellow and dashed lines are clean of defects. Scale bars: 2nm.

FIG. 4. (a) Z-contrast image from a LNO/LSAT heterostructure with a horizontal RPF within the film. Inset, schematics of LNO structure showing the distortions and the out-of-plane parameter d and the distance δ from the center of mass of the unit cell (marked with the cross). The yellow arrow marks the LNO-LSAT interface. Scale bar 1nm. (b) out-of-plane spacing map obtained from (a). Each pixel represents one unit cell and its intensity is proportional to the measured out-of-plane value. (c) Top, averaged values of the out-of-plane (red) and in-plane (black) spacing, and bottom, averaged values of the distance δ as a function of the position. The dashed line marks the interface between LNO and LSAT.