

Interface density driven metal-to-insulator transition in nickelate based heterostructures

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Heterostructures made of alternating metallic layers of $\text{Nd}_{0.7}\text{La}_{0.3}\text{NiO}_3$ and layers displaying a metal-to-insulator transition (such as SmNiO_3) have been grown varying the period of the superlattices on top of LaAlO_3 substrates. Exploiting the phase boundary cost found between metallic and insulating phases of nickelates, it is shown that a metallic layer can be turned into an insulating one by means of heterostructuring in an intermediate thickness regime in which the single layers retain their metallic behavior.

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I. INTRODUCTION

Transition metal oxide perovskites, with chemical formula ABO_3 , constitute a vast playground towards creating quantum materials by design, i.e., with specific and unique properties [1–4]. Among properties of interest, metal-to-insulator transitions (MITs) have been deeply studied both at a fundamental and applied levels [5–10]. Rare-earth nickelates (RNiO_3 , $\text{R} = \text{Lu}, \dots, \text{Pr}$) are a family of materials undergoing such a phase transition as a function of temperature [11–14]. Depending on the size of the rare-earth cation, which in turn determines the distortion of the crystal structure and the bandwidth of the system, these compounds pass from a metallic, high symmetry, orthorhombic crystalline structure ($Pbnm$), to an insulating, lower symmetry, monoclinic one ($P2_1/n$), as the temperature is lowered below a critical metal-to-insulator transition temperature (T_{MI}) as displayed in the phase diagram in Fig. 1(a).

The MIT is commonly described in terms of an order parameter ΔN , which quantifies the difference in e_g occupancy between inequivalent Ni sites. In the metallic phase, ΔN is zero, as all nickel sites are equivalent and share the same nominal d^7 electronic configuration. Below T_{MI} , electronic and bond disproportionation occur, resulting in a rock-salt pattern of alternating expanded and contracted oxygen octahedra. This leads to two inequivalent Ni sites with different e_g occupancies, often denoted as $d^{7+\delta}$ and $d^{7-\delta}$ [15,16].

In previous work, the length-scale over which a metallic or insulating phase can be established was studied using a series of superlattices of $(m \text{ NdNiO}_3/m \text{ SmNiO}_3)_L$ grown in such a way that the total thickness of the heterostructure $2m \times L$ unit-cells (u.c.) stays constant, but the wavelength (or period) $\Lambda = 2m$ (u.c.) of the superlattice ranges from a value of 6 to a value of 60 [17,18]. By measuring the resistivity as a function

of temperature of these samples, it was possible to identify two different behaviors within the series. When below a critical wavelength Λ_c of ~ 16 u.c., the transport curves of the heterostructures display a single metal-to-insulator transition, occurring at a joint temperature T_j that lies between those of single compound films of either SmNiO_3 or NdNiO_3 . In contrast, when the thickness m of the nickelate layers exceeds the critical value of $\Lambda_c/2$, two different metal-to-insulator transition temperatures are observed, having values that approach those of the single compounds as Λ increases.

This behavior was explained in terms of a balance between an interfacial effect and a “bulk” one. While NdNiO_3 and SmNiO_3 individually favor metallic and insulating states, respectively, at intermediate temperatures, the formation of a metal-insulator boundary carries an energy cost proportional to $(\nabla(\Delta N))^2$. The energy cost for each interface is E_{PB} and thus the energy cost for the system goes as the interface density. As layer thickness m in a superlattice decreases, the density of interfaces in a superlattice increases, until, at $m = \Lambda_c/2$, the energy of the multiple interfaces becomes too costly for the system, and the different compounds transition instead together at an intermediate, joint metal-to-insulator transition temperature (T_j).

In this work, we explore and exploit this mechanism as a knob to control the ground state of nickelate compounds. A series of $(m \text{ Nd}_{0.7}\text{La}_{0.3}\text{NiO}_3/m \text{ SmNiO}_3)_L$ superlattices is grown and characterized. In contrast to previous studies, while the single layer SmNiO_3 film shows a MIT, $\text{Nd}_{0.7}\text{La}_{0.3}\text{NiO}_3$ is instead fully metallic down to the lowest temperatures. A simpler choice for the metallic layers would have been to choose LaNiO_3 , which is the end-member of the nickelate family, and also metallic down to the lowest temperatures. However, LaNiO_3 has a rhombohedral crystalline structure, which would lead to an additional (structural) discontinuity at the interfaces in the superlattices. Also, density functional theory (DFT) calculations on NdNiO_3 show that relaxation of the structure reveals substantially larger Ni–O–Ni bond angles in the rhombohedral phase as compared to those in the orthorhombic phase, leading

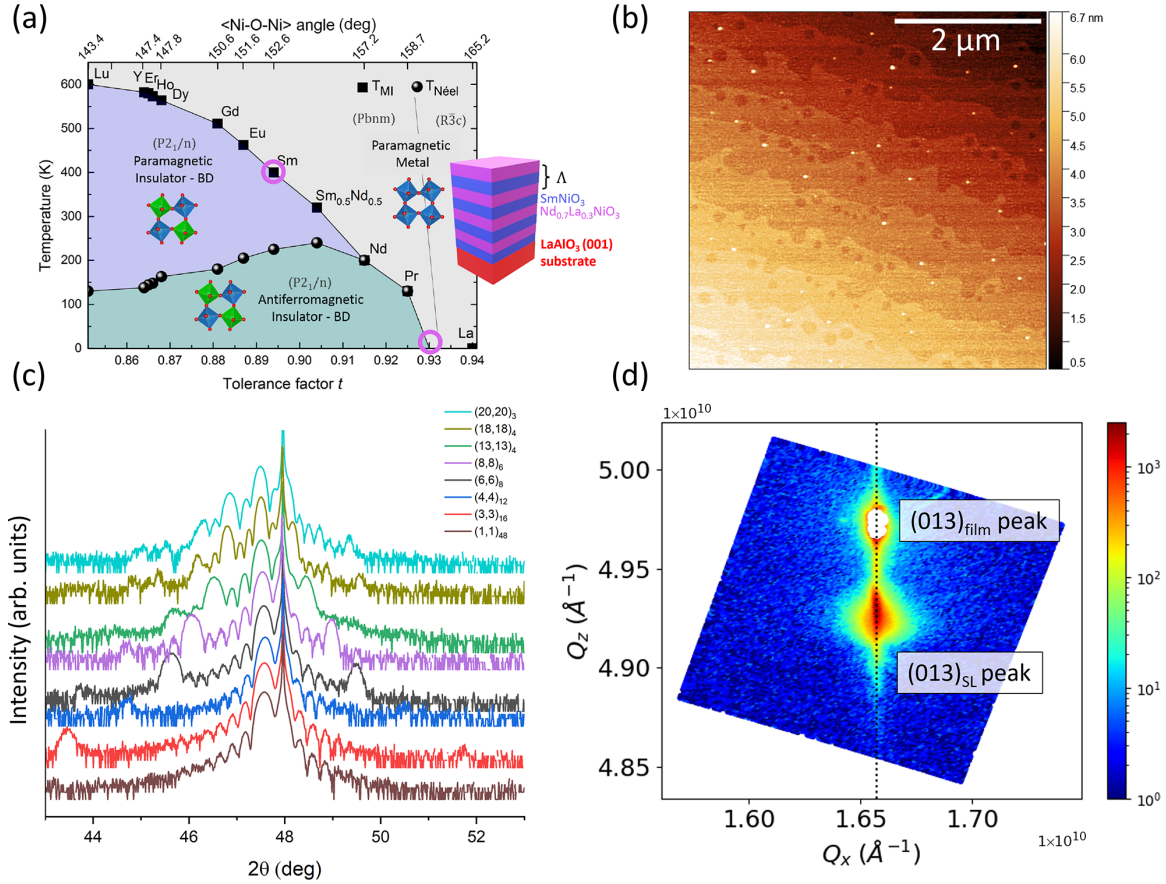


FIG. 1. (a) Nickelates phase diagram (adapted from S. Catalano *et al.* [13]) and sketch of a $\text{Nd}_{0.7}\text{La}_{0.3}\text{NiO}_3/\text{SmNiO}_3$ superlattice. (b) AFM scan of the surface of one of the superlattices of the series, showing a flat surface and revealing step and terraces. (c) X-ray diffraction scans around the $(002)_{\text{pc}}$ reflection of the superlattices confirm the high crystalline quality of the samples and the correct repetition number and thickness of the layers. (d) Example of a reciprocal space map around the $(013)_{\text{pc}}$ peak of the substrate, showing that the film is coherently strained to the substrate. A cutoff at 2500 cps has been introduced in the plot for clarity.

to larger bandwidth and metallicity, as described in detail in the Supplemental Material [19]. For this reason, a solid solution of $\text{Nd}_{1-x}\text{La}_x\text{NiO}_3$ with a La concentration $x = 0.3$ is employed. Indeed, previous studies showed that single compound thin films with this La concentration are both fully metallic and have an orthorhombic symmetry, that is therefore structurally compatible with the metallic phase of nickelates displaying a MIT [20,21]. As further confirmation, we present the characterization of newly grown $\text{Nd}_{0.7}\text{La}_{0.3}\text{NiO}_3$ single compound films in Fig. S1 of the Supplemental Material [19].

Remarkably, as the superlattice wavelength Λ is decreased, the $\text{Nd}_{0.7}\text{La}_{0.3}\text{NiO}_3$ layers develop a MIT at lower temperatures. A joint MIT is further observed below a critical wavelength, Λ_c . These results both demonstrate the importance of the metal-insulator phase boundary cost, and validate the model developed in [17].

II. RESULTS AND DISCUSSION

We grew a series of superlattices alternating layers of “metal-insulator” SmNiO_3 and metallic $(\text{Nd},\text{La})\text{NiO}_3$. The heterostructures were deposited on top of $(001)_{\text{pc}}$ -oriented

LaAlO_3 (pc: pseudocubic) through off-axis radio frequency (RF) magnetron sputtering, keeping the same geometry as that introduced by Eom *et al.* [22] and adopting the deposition conditions optimized in our previous work [23,24].

The resulting superlattice structure is sketched in Fig. 1(a), which also indicates end-member behavior on the accompanying nickelates phase diagram. Figure 1(b) shows a representative atomic force microscopy (AFM) image of a superlattice, which displays atomically flat surfaces. The high crystalline quality of the films can be further inferred from the analysis of 2θ x-ray diffraction (XRD) scans around the (002) reflection of the substrate, as shown for the full series of superlattices in Fig. 1(c). Finite size oscillations and superlattice peaks corresponding to the correct periodicity of each member of the series are observed. Reciprocal space maps around the asymmetrical (013) reflection of the substrate, as shown for one of the samples in Fig. 1(d), confirm an identical in-plane lattice constant for the substrate and the film throughout the whole thickness of the superlattice, indicating that the films are coherently strained to the substrates and that strain relaxation does not occur. A cutoff at 2500 counts per second (cps) has been introduced in the plot for clarity, and all the values exceeding this threshold are plotted in white.

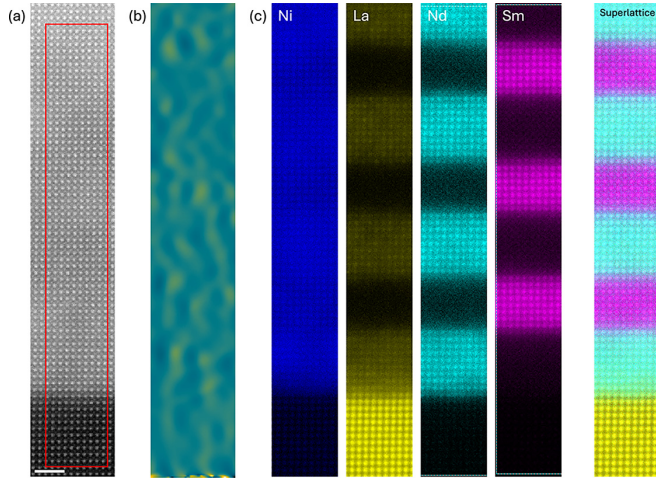


FIG. 2. STEM-EELS characterization of an example (m $\text{Nd}_{0.7}\text{La}_{0.3}\text{NiO}_3$ / m SmNiO_3) $_L$ superlattice. (a) Cross section HAADF image of a $(9,9)_4$ superlattice viewed along the $[100]_{\text{pc}}$ zone axis direction of the LaAlO_3 substrate. Scale bar: 2 nm. (b) GPA e_{xx} map indicating that the nickelate thin film is coherently strained to the substrate. (c) EELS compositional maps obtained from the region marked in red in (a). Intensity maps of background-subtracted La, Nd, and Sm M -edge signals are displayed, together with their overlay in the superlattice map.

The structural properties and chemical composition of the designed superlattice are further investigated by means of aberration-corrected scanning transmission electron microscopy (STEM). Figure 2(a) shows a high-angle annular dark field (HAADF) Z-contrast image of the $(9,9)_4$ superlattice viewed along the $[100]_{\text{pc}}$ zone axis direction of the LaAlO_3 substrate. No structural defects were observed in the sample, either within the layers or at their interfaces. The investigations also confirm that the superlattice is coherently strained to the substrate as shown in the Geometrical Phase Analysis (GPA) e_{xy} map in Fig. 2(b). Figure S2 in the Supplemental Material [19] provides a larger view area of the investigated sample. Electron energy-loss spectroscopy (EELS) compositional maps obtained from the area indicated in red in Fig. 2(a) are shown in Fig. 2(c). Sharp chemical interfaces between the $\text{Nd}_{0.7}\text{La}_{0.3}\text{NiO}_3$ and SmNiO_3 layers are observed throughout the sample. Some diffusion of La coming from the substrate into the first $\text{Nd}_{0.7}\text{La}_{0.3}\text{NiO}_3$ layer is however detected. Also, some degree of layer interdiffusion is identified through STEM-EELS and energy dispersive x-ray spectroscopy analyses, as discussed in the Supplemental Material [19].

We now discuss the transport properties of the (m $\text{Nd}_{0.7}\text{La}_{0.3}\text{NiO}_3$ / m SmNiO_3) $_L$ superlattices series. All samples were patterned into Hall bar geometries with a length

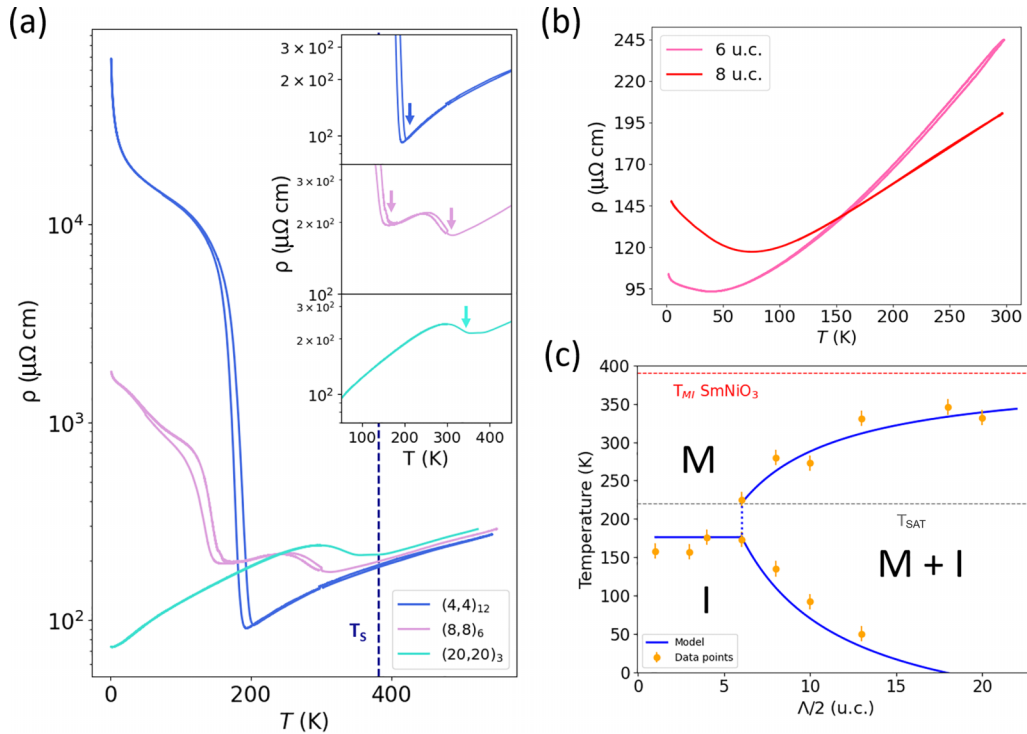


FIG. 3. (a) Resistivity versus temperature curves of three representative members of the superlattice series, displaying: a fully coupled behavior for short wavelengths (blue curve); a fully decoupled behavior for large wavelengths, with the $\text{Nd}_{0.7}\text{La}_{0.3}\text{NiO}_3$ layers remaining metallic down to the lowest temperature (aquamarine curve); and, for intermediate Λ values (pink curve), a situation for which the $\text{Nd}_{0.7}\text{La}_{0.3}\text{NiO}_3$ layers turn insulating at low temperatures, a behavior resulting from the increased density of electronic interfaces. (b) Resistivity versus temperature curves of two single, uncapped $\text{Nd}_{0.7}\text{La}_{0.3}\text{NiO}_3$ films, respectively 6 and 8 u.c. thick and grown on LaAlO_3 , displaying a metallic behavior and a small upturn below 70 K. (c) Electronic phase diagram of the full superlattice series, showing the T_{MI} values of the superlattices as a function of their half period (orange data points), compared to the fit that follows the theoretical model detailed in the text and in [17]. The red dotted line represents the T_{MI} of thick SmNiO_3 films and the gray dotted line indicates the saturation temperature T_{SAT} chosen as an input parameter for the model.

of approximately 300 μm by means of conventional UV photolithography and ion etching. Figure 3(a) displays the resistivity versus temperature curves of superlattices with increasing wavelengths, 8, 16, and 40 u.c., that, between them, illustrate the three different characteristic behaviors we observe (the resistivity versus temperature curves of all samples in the series are reported in the Supplemental Material [19]). As can be seen from the aquamarine curve for $\Lambda = 40$ u.c., for large wavelengths, the behavior of the two different layers is decoupled. Only one MIT at ~ 350 K can be identified, corresponding to the transition of the SmNiO_3 layers to the insulating phase, while the solid solution layer remains metallic all the way down to the lowest measurable temperature. In contrast, for the shortest wavelength superlattice having the highest density of interfaces (blue curve, $\Lambda = 8$ u.c.), we observe a sharp, single MIT at ~ 200 K, which suggests a complete coupling of the two layers with the initially metallic solid solution having becoming insulating in tandem with the SmNiO_3 layers. Interestingly, the pink curve in Fig. 3(a) for a $(8 \text{ Nd}_{0.7}\text{La}_{0.3}\text{NiO}_3/8 \text{ SmNiO}_3)_6$ superlattice ($\Lambda = 16$ u.c.) shows yet another behavior. Even though the resistivity of a single, uncapped $\text{Nd}_{0.7}\text{La}_{0.3}\text{NiO}_3$ film of an equivalent layer thickness of 6 or 8 u.c. displays a metallic behavior down to low temperatures [Fig. 3(b)], the resistivity of the 8 / 8 u.c. superlattice displays two MITs. The highest one at ~ 250 K is ascribed to SmNiO_3 , and the one at ~ 110 K to the solid solution. This in turn means that the solid solution layer is no longer metallic at low temperatures; a behavior possibly explained by the energetic cost of maintaining the metal-insulator phase boundaries.

One can also notice on Fig. 3(a) that, while the resistivities of the superlattices are very similar in the metallic state (where Q and ΔN are zero—no disproportionation), they are markedly different at low T , the shorter the wavelength the higher the resistivity. We ascribe this behavior to the evolution of Q and ΔN across the heterostructures (which creates a wavelength dependence of the low T resistivity). While Q and ΔN are essentially uniform at low T in short wavelength structures, they evolve in larger period samples (tending toward their bulk values as one moves away from the interface). Since the smaller Q and ΔN , the smaller the resistivity, one expects more conducting $\text{Nd}_{0.7}\text{La}_{0.3}\text{NiO}_3$ layers in large wavelengths samples, possibly explaining the observed behavior.

Figure 3(c) shows a T_{MI} versus $\Lambda/2$ electronic phase diagram for the whole superlattice series. Similarly to the previous study on $\text{NdNiO}_3/\text{SmNiO}_3$ superlattices, we identify a fully coupled behavior and joint MIT for the thinnest layers, occurring at temperature $T_j \sim 170$ K and below a critical wavelength $\Lambda_c = 12$ u.c. The data are modeled by means of the simple energy considerations introduced in Ref. [17]. The energy of the layers in the metallic state is $E_M = 0$, whereas the energy of the insulating state for the SmNiO_3 [$E_1^S(T)$] and solid solution layers [$E_1^{\text{NLNO}}(T)$] can be written as a function of temperature,

$$E_1^S(T) = K_S \frac{(T - T_S)}{T_S}$$

$$E_1^{\text{NLNO}}(T) = -K_{\text{NLNO}} \frac{(T - T_{\text{NLNO}})}{T_{\text{NLNO}}},$$

with K_S and K_{NLNO} being positive constants specific to the two materials and T_S and T_{NLNO} being the thick films transition temperatures. To account for the metallic state of the $\text{Nd}_{0.7}\text{La}_{0.3}\text{NiO}_3$ layers, a T_{MI} with a formally negative value of ~ -100 K is used in the fit. This negative T_{MI} is a proxy for the “level” of metallicity of the solid solution compound. It is worth noticing that the T_{MI} values of the upper and lower branches asymptotically approach the T_{MI} value of, respectively, the single SmNiO_3 [red dotted line in Fig. 3(c)] and the chosen T_{NLNO} value for the $\text{Nd}_{0.7}\text{La}_{0.3}\text{NiO}_3$ layer. Furthermore, as proposed in Ref. [17], to better capture the physics of the system, the linear dependence in temperature of the energy of the SmNiO_3 insulating layers is restricted to a range close to the T_{MI} value of SmNiO_3 . For this reason, an additional parameter T_{SAT} [gray dotted line in Fig. 3(c)] has been introduced, and, for $T < T_{\text{SAT}}$ the energy of the insulating state is constant, with a value $E_1^S = K_S \frac{(T_{\text{SAT}} - T_S)}{T_S}$.

As shown in Fig. 3(c), the model set out above fits the data well across the whole wavelength range. The fact that this is achieved when applying a single set of parameters across the full sample series suggests that the degree of chemical intermixing and hence stoichiometry of the two layers does not change meaningfully in function of the superlattice wavelength.

Beyond the validation of the energetic model, the results unambiguously point to another finding: the phase boundary cost of forming a metal-insulator interface can induce a phase change in $\text{Nd}_{0.7}\text{La}_{0.3}\text{NiO}_3$ layers from the metallic nature of the uncapped thin film to insulating in the sandwiched layers of a superlattice. This is demonstrated both by the fully coupled superlattices with period $< \Lambda_c$, where the SmNiO_3 and $\text{Nd}_{0.7}\text{La}_{0.3}\text{NiO}_3$ layers show a joint $T_{\text{MI}} = T_j$, and in particular the intermediate period superlattices (for instance $\Lambda = 12$ or 16 u.c.) which display two metal-to-insulator transitions, one for each layer type. This coupling represents a fundamental shift in the order parameters of the $\text{Nd}_{0.7}\text{La}_{0.3}\text{NiO}_3$ layers, that cannot be explained by considering them in isolation from the neighboring SmNiO_3 layers, and illustrates the potential of interface energetics for inducing and controlling phase changes.

III. CONCLUSIONS

In conclusion, high crystalline quality heterostructures of SmNiO_3 and $\text{Nd}_{0.7}\text{La}_{0.3}\text{NiO}_3$ were grown using off-axis RF magnetron sputtering on $(001)_{\text{pc}}$ LaAlO_3 substrates, fully characterized by means of XRD, AFM, and STEM, and subsequently patterned for transport measurements. This heterostructure design and the measured transport properties as a function of individual layer thicknesses confirm the importance of the phase boundary cost picture proposed in Ref. [17]. In the heterostructures presented here, such phase boundary cost is exploited to induce a phase change in the quantum state of the $\text{Nd}_{0.7}\text{La}_{0.3}\text{NiO}_3$ solid solution layers, suppressing, for short and intermediate wavelength superlattices, their natural metallic ground state and inducing an insulating one at low temperature when sandwiched in between SmNiO_3 layers. This work gives an example of how phase boundary energetics can be used for controlling electronic phases in correlated oxides.

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DATA AVAILABILITY

The data that support the findings of this article are openly available [32], embargo periods may apply.

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- [1] D. I. Khomskii, *Transition Metal Compounds* (Cambridge University Press, Cambridge, 2014).
 - [2] P. A. Cox, *Transition Metal Oxides: An Introduction to their Electronic Structure and Properties* (Oxford University Press, Oxford, 2010).
 - [3] H. Y. Hwang, Y. Iwasa, M. Kawasaki, B. Keimer, N. Nagaosa, and Y. Tokura, Emergent phenomena at oxide interfaces, *Nat. Mater.* **11**, 103 (2012).
 - [4] N. F. Mott, The basis of the electron theory of metals, with special reference to the transition metals, *Proc. Phys. Soc. A* **62**, 416 (1949).
 - [5] N. F. Mott, Metal-insulator transition, *Rev. Mod. Phys.* **40**, 677 (1968).
 - [6] J. A. Alonso, M. J. Martínez-Lope, M. T. Casais, M. A. G. Aranda, and M. T. Fernández-Díaz, Metal-insulator transitions, structural and microstructural evolution of RNiO_3 ($\text{R} = \text{Sm}, \text{Eu}, \text{Gd}, \text{Dy}, \text{Ho}, \text{Y}$) perovskites: Evidence for room-temperature charge disproportionation in monoclinic HoNiO_3 and YNiO_3 , *J. Am. Chem. Soc.* **121**, 4754 (1999).
 - [7] J. A. Alonso, J. L. García-Muñoz, M. T. Fernández-Díaz, M. A. G. Aranda, M. J. Martínez-Lope, and M. T. Casais, Charge disproportionation in NiO_3 perovskites: Simultaneous metal-insulator and structural transition in YNiO_3 , *Phys. Rev. Lett.* **82**, 3871 (1999).
 - [8] J. del Valle, R. Rocco, C. Domínguez, J. Fowlie, S. Gariglio, M. J. Rozenberg, and J.-M. Triscone, Dynamics of the electrically induced insulator-to-metal transition in rare-earth nickelates, *Phys. Rev. B* **104**, 165141 (2021).
 - [9] J. Son, S. Rajan, S. Stemmer, and S. J. Allen, A heterojunction modulation-doped Mott transistor, *J. Appl. Phys.* **110**, 084503 (2011).
 - [10] A. Parihar, M. Jerry, S. Datta, and A. Raychowdhury, Stochastic IMT (insulator-metal-transition) neurons: An interplay of thermal and threshold noise at bifurcation, *Front. Neurosci.* **12**, 210 (2018).
 - [11] G. Catalan, Progress in perovskite nickelate research, *Ph. Transit.* **81**, 729 (2008).
 - [12] M. L. Medarde, Structural, magnetic and electronic properties of perovskites ($\text{R} = \text{rare earth}$), *J. Phys.: Condens. Matter* **9**, 1679 (1997).
 - [13] S. Catalano, M. Gibert, J. Fowlie, J. Íñiguez, J.-M. Triscone, and J. Kreise, Rare-earth nickelates: thin films and heterostructures, *Rep. Prog. Phys.* **81**, 046501 (2018).
 - [14] J. B. Torrance, P. Lacorre, A. I. Nazzari, E. J. Ansaldo, and Ch. Niedermayer, Systematic study of insulator-metal transitions in perovskites RNiO_3 ($\text{R} = \text{Pr}, \text{Nd}, \text{Sm}, \text{Eu}$) due to closing of charge-transfer gap, *Phys. Rev. B* **45**, 8209 (1992).
 - [15] A. Subedi, O. E. Peil, and A. Georges, Low-energy description of the metal-insulator transition in the rare-earth nickelates, *Phys. Rev. B* **91**, 075128 (2015).
 - [16] O. E. Peil, A. Hampel, C. Ederer, and A. Georges, Mechanism and control parameters of the coupled structural and metal-insulator transition in nickelates, *Phys. Rev. B* **99**, 245127 (2019).
 - [17] C. Domínguez, A. B. Georgescu, B. Mundet, Y. Zhang, J. Fowlie, A. Mercy, A. Waelchli, S. Catalano, D. T. L. Alexander, P. Ghosez, A. Georges, A. J. Millis, M. Gibert, and J.-M. Triscone, Length scales of interfacial coupling between metal and insulator phases in oxides, *Nat. Mater.* **19**, 1182 (2020).
 - [18] B. Mundet, C. Domínguez, J. Fowlie, M. Gibert, J.-M. Triscone, and D. T. L. Alexander, Near-atomic-scale mapping of electronic phases in rare earth nickelate superlattices, *Nano Lett.* **21**, 2436 (2021).
 - [19] See Supplemental Material at <http://link.aps.org/supplemental/10.1103/syz5-9cbc> for details of the growth and characterization of single-layer and superlattice nickelate films; high-resolution STEM, EDXS, and EELS analyses of layer structure, composition, and interdiffusion; strain and domain mapping using geometric phase analysis; quantification of interface intermixing; resistivity versus temperature curves for all superlattices; DFT calculations of crystal symmetry and Ni–O–Ni bond angles; and a full description of experimental methods, which includes Refs. [25–31].
 - [20] J. Fowlie, B. Mundet, C. Toulouse, A. Schober, M. Guennou, C. Domínguez, M. Gibert, D. T. L. Alexander, J. Kreisel, and J.-M. Triscone, Crossover between distinct symmetries in solid solutions of rare earth nickelates, *APL Mater.* **9**, 081119 (2021).
 - [21] J. Fowlie, Electronic and structural properties of LaNiO_3 -based heterostructures, PhD. thesis, Université de Genève, 2018.
 - [22] C. B. Eom, J. Z. Sun, B. M. Lairson, S. K. Streiffer, A. F. Marshall, K. Yamamoto, S. M. Anlage, J. C. Bravman, T. H. Geballe, S. S. Laderman, R. C. Taber, and R. D. Jacowitz, Synthesis and properties of $\text{YBa}_2\text{Cu}_3\text{O}_7$ thin films grown *in situ* by 90° off-axis single magnetron sputtering, *Physica C: Supercond.* **171**, 354 (1990).
 - [23] L. Varbaro, B. Mundet, C. Domínguez, J. Fowlie, A. B. Georgescu, L. Korosec, D. T. L. Alexander, and J.-M. Triscone, Electronic coupling of metal-to-insulator transitions in nickelate-based heterostructures, *Adv. Electron. Mater.* **9**, 2201291 (2023).
 - [24] L. Varbaro, B. Mundet, S. Bandyopadhyay, C. Domínguez, J. Fowlie, L. Korosec, C.-Y. Hsu, D. T. L. Alexander, P. Ghosez,

- and J.-M. Triscone, Structural study of nickelate based heterostructures, *APL Mater.* **12**, 031104 (2024).
- [25] G. Lucas, P. Burdet, M. Cantoni, and C. Hébert, Multivariate statistical analysis as a tool for the segmentation of 3D spectral data, *Micron* **52–53**, 49 (2013).
- [26] Y. Zhu and C. Dwyer, Quantitative position-averaged K-, L-, and M-shell core-loss scattering in STEM, *Microsc. Microanal.* **20**, 1070 (2014).
- [27] M. J. Hÿtch, E. Snoeck, and R. Kilaas, Quantitative measurement of displacement and strain fields from HREM micrographs, *Ultramicroscopy* **74**, 131 (1998).
- [28] P. Giannozzi, O. Andreussi, T. Brumme, O. Bunau, M. B. Nardelli, M. Calandra, R. Car, C. Cavazzoni, D. Ceresoli, M. Cococcioni, N. Colonna, I. Carnimeo, A. Dal Corso, S. de Gironcoli, P. Delugas, R. A. DiStasio, A. Ferretti, A. Floris, G. Fratesi, G. Fugallo, R. Gebauer *et al.*, Advanced capabilities for materials modelling with QUANTUM ESPRESSO, *J. Phys.: Condens. Matter* **29**, 465901 (2017).
- [29] D. Vanderbilt, Soft self-consistent pseudopotentials in a generalized eigenvalue formalism, *Phys. Rev. B* **41**, 7892 (1990).
- [30] J. P. Perdew, K. Burke, and M. Ernzerhof, Generalized gradient approximation made simple, *Phys. Rev. Lett.* **77**, 3865 (1996).
- [31] B. Mundet, M. Hadjimichael, J. Fowlie, L. Korosec, L. Varbaro, C. Domínguez, J.-M. Triscone, and D. T. L. Alexander, Mapping orthorhombic domains with geometrical phase analysis in rare-earth nickelate heterostructures, *APL Mater.* **12**, 031124 (2024).
- [32] <https://doi.org/10.26037/yareta:mzfaokbfr5e6hoxnowsgjt62fe>