



# Reconstruction of the polar interface between hexagonal LuFeO<sub>3</sub> and intergrown Fe<sub>3</sub>O<sub>4</sub> nanolayers

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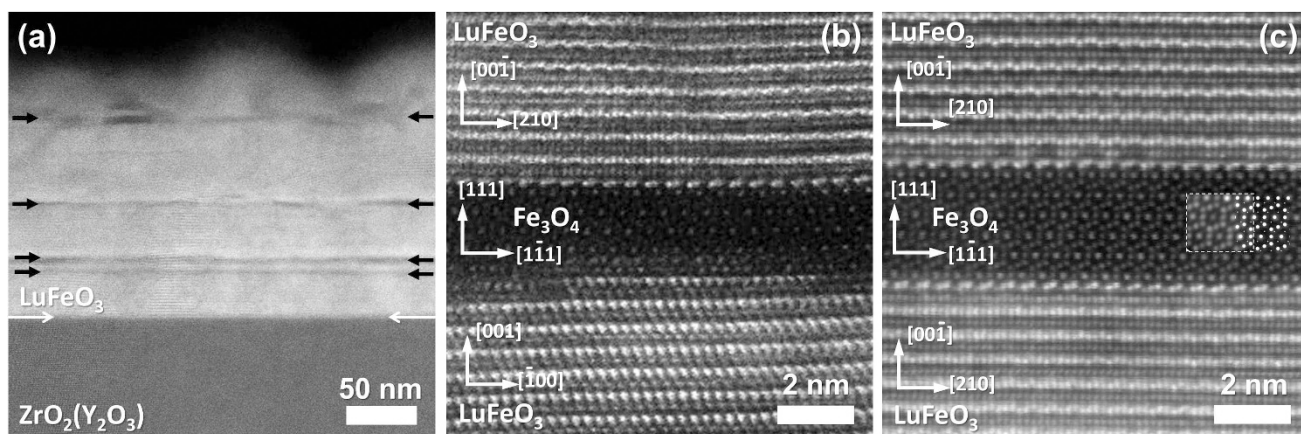
We report the observation of an unusual phase assembly behavior during the growth of hexagonal LuFeO<sub>3</sub> thin films which resulted in the formation of epitaxial Fe<sub>3</sub>O<sub>4</sub> nanolayers. The magnetite layers were up to 5 nm thick and grew under the conditions at which Fe<sub>2</sub>O<sub>3</sub> is thermodynamically stable. These Fe<sub>3</sub>O<sub>4</sub> nanolayers act as buffer layers promoting a highly epitaxial growth of the hexagonal LuFeO<sub>3</sub> thin film up to 150 nm thick. Using scanning transmission electron microscopy, we show that the interface between (001) LuFeO<sub>3</sub> and (111) Fe<sub>3</sub>O<sub>4</sub> can be reconstructed in two ways depending on the sequence in which these compounds grow on each other. We suggest the polarity of the interface is the reason behind the observed interface reconstruction and epitaxial stabilization of magnetite.

Interface engineering has recently become one of the most exciting topics of solid state sciences owing to numerous physical phenomena taking place at interfaces such as magnetism, superconductivity, and magnetoelectricity. These interface phenomena depend on epitaxy, strain, and reconstruction between the two phases forming the interface, as well as on their polarity, spin, orbital and electronic band structures<sup>1,2</sup>. These fascinating phenomena have been observed mainly at interfaces between perovskite oxides because their bulk properties are well-known, allowing for a relatively easy control of the physics at their interface<sup>3</sup>. Among the important aspects of interface engineering that are poorly explored are the polarity and reconstruction of the crystal surfaces and their influence on the physical properties of more complex interfaces<sup>4,5</sup>. Polarity is known to often cause a surface reconstruction when the polar catastrophe is not mitigated by absorption, yet its effect on the structure of interfaces is difficult to explore experimentally. Moreover, the polarity of the crystal surfaces has been also reported to strongly influence the growth of thin films on such surfaces, inducing a polymorphic phase transition or a phase separation on the polar substrates<sup>6–8</sup>.

Here we report an interesting phenomenon of spontaneous formation of magnetite nanolayers in thin films of hexagonal LuFeO<sub>3</sub> and describe the interface between these two phases. Hexagonal orthoferrites RFeO<sub>3</sub> (R is a rare earth element), the structural analogues of multiferroic hexagonal RMnO<sub>3</sub><sup>9,10</sup>, have been mainly obtained by epitaxial stabilization in thin-film state and possess a non-centrosymmetric (space group P6<sub>3</sub>cm) crystal structure that exhibits ferroelectricity along with weak ferromagnetism<sup>11–13</sup>.

## Results

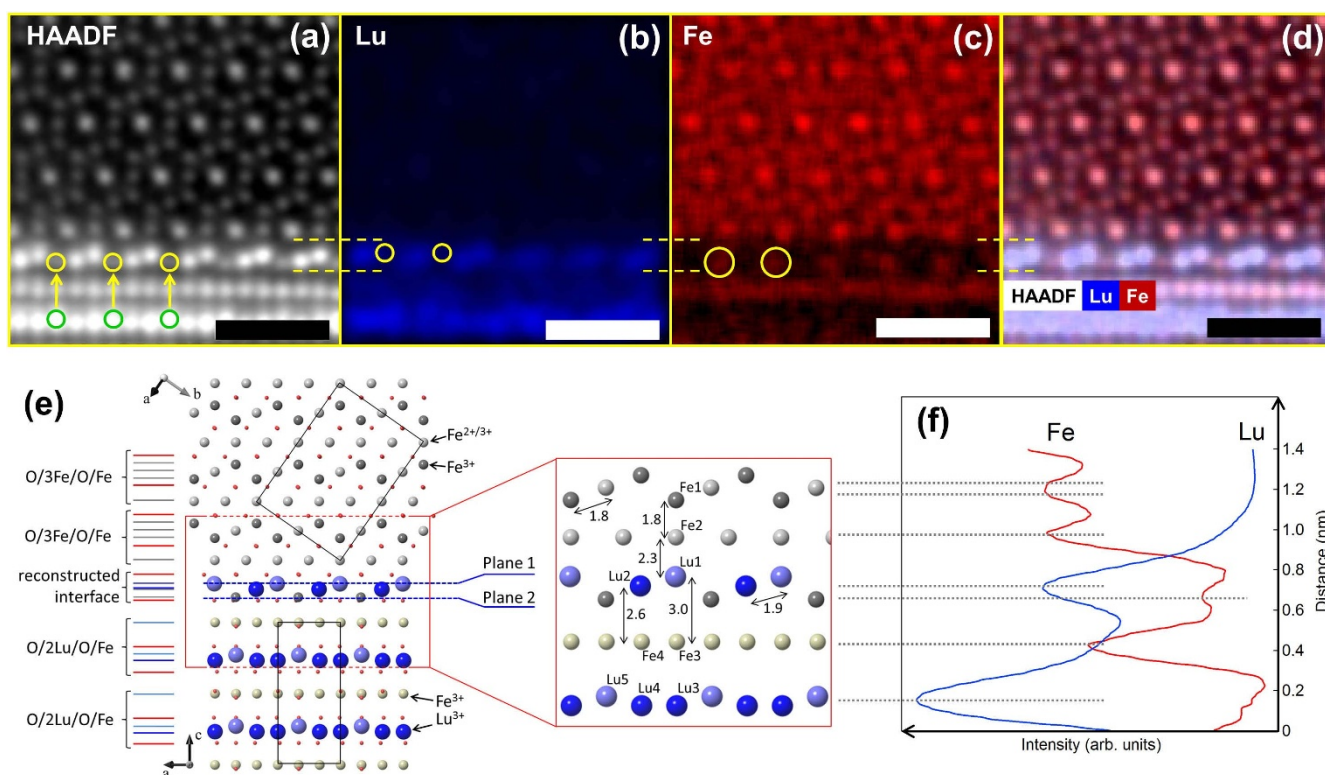
Hexagonal LuFeO<sub>3</sub> thin film was grown *c*-oriented on the (111) cut of cubic ZrO<sub>2</sub>(Y<sub>2</sub>O<sub>3</sub>) as confirmed by a detailed X-ray diffraction (XRD) study (see Supplementary material, Figure S1). In the in-plane XRD patterns of the films that were thicker than 50 nm the (110) LuFeO<sub>3</sub> peak appeared in addition to the (300) peak. The additional in-plane orientation results from a 30° rotation of the unit cell of hexagonal RFeO<sub>3</sub> around the *c* axis and has not been observed yet in thin films of hexagonal orthophases (RMO<sub>3</sub>, M = Al, Mn, Fe, Ga, In). To clarify the origin of the additional orientation, we performed a scanning transmission electron microscopy (STEM) study. In our earlier studies we reported the maximum thickness of epitaxially stabilized hexagonal RFeO<sub>3</sub> and RMnO<sub>3</sub> thin films to be approximately 70 nm<sup>12,14</sup>. However, STEM imaging showed that the thickness of our film exceeded ~150 nm (see Figure S3(a,b) in Supplementary material). Furthermore, low- and high-resolution high-angle annular dark-field (HAADF) STEM imaging revealed the presence of intergrown Fe<sub>3</sub>O<sub>4</sub> nanolayers in the LuFeO<sub>3</sub> film (Figure 1). The



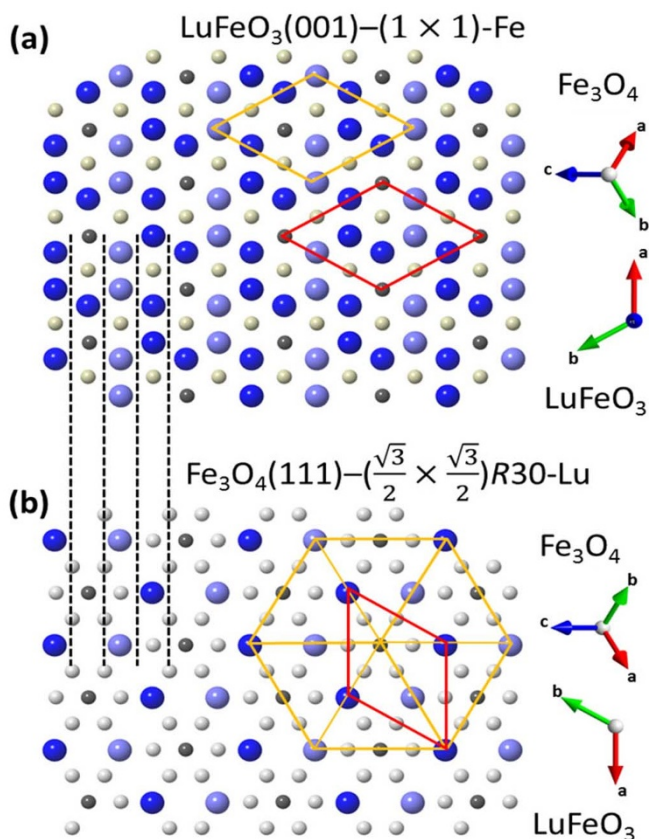
**Figure 1** | (a) Low-resolution HAADF STEM of hexagonal LuFeO<sub>3</sub> thin film grown on ZrO<sub>2</sub>(Y<sub>2</sub>O<sub>3</sub>) substrate; black arrows indicate Fe<sub>3</sub>O<sub>4</sub> nanolayers. High-resolution HAADF STEM images of a continuous nanolayer (b) that imposes the reorientation of LuFeO<sub>3</sub> and an isolated nanolayer (c) that does not reorient LuFeO<sub>3</sub>. The framed inset in (c) represents the simulated HAADF STEM image of Fe<sub>3</sub>O<sub>4</sub>; white dots in (c) are real atomic positions of Fe atoms in the magnetite structure. The (b) image was taken from the region, where the underlying LuFeO<sub>3</sub> layer is not reoriented, while the same orthoferrite sublayer in the (c) image is reoriented by the previous Fe<sub>3</sub>O<sub>4</sub> nanolayers.

magnetite layers grew within the LuFeO<sub>3</sub> film matrix parallel to the substrate surface and were up to 5 nm thick. Two types of Fe<sub>3</sub>O<sub>4</sub> layers can be distinguished: continuous (at least several  $\mu\text{m}$  long) and isolated island-like ( $\sim 50$  nm long) ones shown in Figure 1(b) and (c), respectively. The continuous Fe<sub>3</sub>O<sub>4</sub> layers change the in-plane orientation of the upper LuFeO<sub>3</sub> layer by 30° and the isolated layers do not reorient the hexagonal LuFeO<sub>3</sub> layers grown on top of it (Figure S2 in Supplementary material).

At first sight a reasonable explanation of our observations seems to lie in epitaxial stabilization of Fe<sub>3</sub>O<sub>4</sub> (space group Fd-3m,  $a=8.396$  Å) on top of the (001) surface of RFeO<sub>3</sub> (Figure S5 in Supplementary material). The  $a$  lattice parameter of hexagonal LuFeO<sub>3</sub> is 5.90 Å, which is very close to half of the distance  $a_{\text{magnetite}}/\sqrt{2}=11.874$  Å between the oxygen positions on the (111) surface of Fe<sub>3</sub>O<sub>4</sub>. Such a close lattice match at the interface between hexagonal LuFeO<sub>3</sub> and Fe<sub>3</sub>O<sub>4</sub> favors epitaxial growth. However, according to the temper-



**Figure 2** | (a) HAADF STEM image of the reconstructed interface between LuFeO<sub>3</sub> and Fe<sub>3</sub>O<sub>4</sub>. Open green circles mark the present Lu atoms in LuFeO<sub>3</sub> structure and yellow circles show the corresponding position at the interface, where Fe is located. (b–c) Corresponding atomic resolution EDX maps of Lu and Fe, open yellow circles mark the same position with Fe. (d) Combined HAADF STEM image and Fe+Lu map, where the colors of Lu and Fe remain the same as in (b–c). The scale bar is 1 nm. (e) A model interface between LuFeO<sub>3</sub> and Fe<sub>3</sub>O<sub>4</sub> and the sequence of atomic layers forming polar (001) LuFeO<sub>3</sub> and (111) Fe<sub>3</sub>O<sub>4</sub> surfaces. Black rectangles are the unit cells. "Plane 1" and "Plane 2" are two planes, the top views of which are shown in Figure 3. Magnified area on the right shows distances calculated from STEM images (error is 0.1 Å). (f) The profiles of Lu L <sub>$\beta$</sub>  and Fe K <sub>$\alpha$</sub>  intensities perpendicular to the interface, where each peak correlates well with atomic planes in the interface area (dotted lines).



**Figure 3** | Top view of the reconstructed surfaces of (a) LuFeO<sub>3</sub> and (b) Fe<sub>3</sub>O<sub>4</sub> at the interface (respectively, "Plane 1" and "Plane 2" in Figure 2(e); colors of atoms are the same). Orange lines represent the unit cell of the main crystal and red lines mark the "unit cell" of the reconstructed surface. The arrows show unit vectors of the structures. The structures were drawn using VESTA software<sup>22</sup>.

ature-pressure diagram of Fe-O system<sup>15</sup>, under the conditions used in our MOCVD process Fe<sub>2</sub>O<sub>3</sub> is the thermodynamically stable phase. The partial oxygen pressure was at least 10<sup>3</sup> times higher than needed for the equilibrium phase formation of the magnetite phase. In pulsed-laser deposition experiments carried out by Liu *et al.*, it was shown that magnetite phase appears in the thin films of the Lu-Fe-O system only in the temperature range of 700–900 °C and under extremely low pressure of 10<sup>-10</sup> atm<sup>16</sup>. It suggests that in our case (T=900 °C, p(O<sub>2</sub>)≈10<sup>-3</sup> atm) a more complex mechanism rather than epitaxial stabilization alone took place during the film growth.

Similar phenomena have been described in the literature. Nanoinclusions of metallic iron (Fe<sup>0</sup>) were found both at the interface and within the film of (111) Fe<sub>3</sub>O<sub>4</sub> epitaxial films grown on the polar surface of (111) MgO substrates<sup>7</sup>. Analogously, Fe<sup>0</sup> and FeO inclusions formed in (111) Fe<sub>3</sub>O<sub>4</sub> films grown on (0001) Al<sub>2</sub>O<sub>3</sub> substrates<sup>17</sup>. Such an unusual phase behavior was observed neither in (001) Fe<sub>3</sub>O<sub>4</sub> films on (001) MgO, nor in (111) Fe<sub>3</sub>O<sub>4</sub> films on (111) Pt substrates<sup>18,19</sup>. Recently, Lazarov *et al* reported the formation of a single Fe<sub>3</sub>O<sub>4</sub> nanolayer on a surface of reconstruction-stabilized (111) MgO substrates in thin films of the hematite phase ( $\alpha$ -Fe<sub>2</sub>O<sub>3</sub>)<sup>6</sup>. On the contrary, when the unreconstructed (111) surface of MgO was hydrogen-stabilized, the magnetite phase was not detected in Fe<sub>2</sub>O<sub>3</sub> thin films<sup>6</sup>. Thus, the polarity of the oxide surface and its reconstruction may play a crucial role in the process of phase stabilization. In this study we did not find magnetite nanolayers grown directly on the non-polar (111) surface of the ZrO<sub>2</sub>(Y<sub>2</sub>O<sub>3</sub>) substrate. To explore the distribution of cations at the oxide interface we performed a detailed HAADF STEM imaging and atomically

resolved mapping of chemical elements by energy-dispersive x-ray spectroscopy.

According to the mapping results (Figure 2(b–c)), no noticeable doping of Fe<sub>3</sub>O<sub>4</sub> by lutetium was observed, and the interface was chemically abrupt in most cases. The most intriguing result is the interface reconstruction along the entire interface that is designated by Lu atoms belonging to both Fe<sub>3</sub>O<sub>4</sub> and LuFeO<sub>3</sub> structures at the interface. In Figure 2(a) yellow arrows point at the Lu sites occupied by Fe atoms and green circles mark similar sites in LuFeO<sub>3</sub>, which are occupied by Lu atoms. The atoms at the interface form the Fe<sub>3</sub>O<sub>4</sub> motif, yet with a periodic substitution of Fe by Lu (the in-plane period is 2Lu+1Fe atoms). The top layer of the alternating two Lu and one Fe atoms appears to be isostructural to Fe<sub>3</sub>O<sub>4</sub> and becomes the first atomic layer of the magnetite phase grown on LuFeO<sub>3</sub> (Figure 2(a–d)). A model interface between LuFeO<sub>3</sub> and Fe<sub>3</sub>O<sub>4</sub> and the sequence of ions perpendicular to the substrate are shown in Figure 2(e). The shift of some of Lu ions along the *c* axis is characteristic of hexagonal LuMO<sub>3</sub> (M=Fe, Mn) with the P6<sub>3</sub>cm space group (in paraelectric state hexagonal RMO<sub>3</sub> belongs to the centrosymmetric P6<sub>3</sub>/mmc space group). One would expect the Lu atoms to be shifted along the [001] direction to be present at the reconstructed interface, because in this case the shifted Lu<sup>3+</sup> ions would find perfectly matched sites within the Fe<sub>3</sub>O<sub>4</sub> crystal structure. However, this scenario does not take place at the interface between Fe<sub>3</sub>O<sub>4</sub> grown *on top* of LuFeO<sub>3</sub>, where the interface reconstruction is accomplished by the downward shift of Lu<sup>3+</sup> ions (Lu4 and Lu5 in Figure 2(e)). Only when the Fe<sub>3</sub>O<sub>4</sub> layer thickness reaches ~5 nm does hexagonal LuFeO<sub>3</sub> grow on top of it in a manner expected from our speculation above: Lu ions that are shifted downward (Lu3 in Figure 2(e)) participate in the formation of the reconstructed interface, and the growth of LuFeO<sub>3</sub> proceeds.

Using the distribution of atoms along the [010] direction of LuFeO<sub>3</sub>, schemes of the individual reconstructed surfaces of Fe<sub>3</sub>O<sub>4</sub> and hexagonal LuFeO<sub>3</sub> at the interface were created (Figure 3). The reconstruction of the Fe<sub>3</sub>O<sub>4</sub> surface is described as Fe<sub>3</sub>O<sub>4</sub>–(111) ( $\frac{\sqrt{3}}{2} \times \frac{\sqrt{3}}{2}$ )R30–Lu. On the contrary, LuFeO<sub>3</sub> has a (1×1) surface reconstruction without the rotation of the "surface" unit cell relative to the "bulk" crystal structure. Based on a high-resolution HAADF STEM imaging, the distances between atomic planes/columns were calculated (red-framed zoomed structure in Figure 2(e)). The Fe1–Fe2 distance is 1.8 Å, being identical to that in bulk Fe<sub>3</sub>O<sub>4</sub>. The Lu1–Lu2 distance is very close to the Fe1–Fe2 distance (1.9 Å), yet the distance between Lu1 and Fe2 is rather elongated (2.3 Å). The Lu1 atom is shifted towards Fe3, shortening the Lu1–Fe3 distance to 3.0 Å (the bulk value is 3.2 Å) and noticeably increasing the Fe2–Lu1 distance. Figure 2(f) shows the profiles of Lu and Fe distribution perpendicular to the interface, from which one can easily deduce the sequence of different atomic planes. Intriguing is the fact that Lu<sup>3+</sup> ions (labeled "Lu2") take the position of Fe<sup>2+/3+</sup> in Fe<sub>3</sub>O<sub>4</sub>, which suggests an electron doping may occur in the interface area (if it is not compensated by oxygen vacancies). The possibility of the surface-reconstruction-induced carrier doping at the interface requires further studies.

## Discussion

We suppose that, despite the perfect lattice match of the (111) Fe<sub>3</sub>O<sub>4</sub> and (001) LuFeO<sub>3</sub> crystal planes, the reconstruction that takes place at the interface between these surfaces is driven by their polarity. To underpin our assumptions, we should take into account the following facts. First, based on a complete structural similarity of hexagonal orthoferrites to hexagonal manganites one can expect the presence of spontaneous polarization along the *c* axis in hexagonal RFeO<sub>3</sub>, which has recently been proved in<sup>13</sup>. Second, the sequence of atomic layers in LuFeO<sub>3</sub> along the [001] direction includes a polar fragment O- $\frac{2}{3}$ Lu- $\frac{1}{3}$ Lu-O that makes the (001) surface of the hexagonal phase to



be of the type 3 according to Tasker's notation<sup>20</sup>. Third, the growth of magnetite was observed only for the (001) surface of LuFeO<sub>3</sub>, and not for the non-polar (111) surface of ZrO<sub>2</sub>(Y<sub>2</sub>O<sub>3</sub>). As a result, in our scenario after the reconstruction of the oxide interface a following formation of magnetite layers was driven by epitaxial stabilization up to the thickness when the polar catastrophe of (111) Fe<sub>3</sub>O<sub>4</sub> made it impossible for magnetite to grow any further under the deposition conditions used. Hence, in such a layered composite both its components form *in situ* and assist each other via the process that occurs in two stages - compensation of surface polarity of the (001) LuFeO<sub>3</sub> sublayer and epitaxial stabilization of the (111) Fe<sub>3</sub>O<sub>4</sub> nanolayer (and vice versa). Our results are important for the growing field of interface engineering, where magnetite, which has already found various technological applications, can be used as a spintronic material with a high tunneling magnetoresistance<sup>21</sup>. Also, it is worth noting that in our films the ferroelectric hexagonal LuFeO<sub>3</sub> is combined with ferromagnetic Fe<sub>3</sub>O<sub>4</sub>, thus forming a layered multiferroic composite *in situ* (no layer-by-layer deposition is required) with both phases perfectly tailored through the reconstructed interface. Moreover, in layer-by-layer deposition (using, for example, pulse laser deposition) one can obtain a multiferroic superlattice with the same perfect epitaxial growth of each layer.

In conclusion, the *in situ* formation of Fe<sub>3</sub>O<sub>4</sub> in the hexagonal LuFeO<sub>3</sub> thin films in the form of continuous layers (~5 nm thick) that preserved the stability of the epitaxial hexagonal phase, simultaneously changing its in-plane orientation, was observed in MOCVD process. The formation of magnetite occurred only on the polar (001) surface of LuFeO<sub>3</sub> under the conditions, under which Fe<sub>2</sub>O<sub>3</sub> phase is thermodynamically stable. A peculiar structural reconstruction along the interface between the (111) Fe<sub>3</sub>O<sub>4</sub> and (001) LuFeO<sub>3</sub> surfaces is found and analyzed. Most likely, the polarity of the (001) surface of ferroelectric hexagonal LuFeO<sub>3</sub> induces the interface reconstruction during growth and the subsequent epitaxial stabilization of nanolayered magnetite, which is consistent with other recent studies. The interface reconstruction turns out to be one of the universal mechanisms of the stabilization of polar surfaces.

## Methods

Thin films of hexagonal LuFeO<sub>3</sub> were grown on single-crystalline (111) ZrO<sub>2</sub>(Y<sub>2</sub>O<sub>3</sub>) substrates at 900 °C using MOCVD with a flash evaporation at 250 °C of a mixture of Lu(thd)<sub>3</sub> and Fe(thd)<sub>3</sub> (thd = 2,2,6,6-tetramethylheptane-3,5-dionate) precursors. The total pressure was 5 mbar, the oxygen partial pressure was 1–2 mbar. The growth rate was 5 nm/min, which was small enough to ensure the surface-diffusion-driven growth. After the deposition the same oxygen partial pressure was used for the *in-situ* post-deposition annealing carried out for 20–30 min at 900 °C and the subsequent cooling process. More information regarding the chemical equilibrium achieved in MOCVD process can be found in Supplementary material. X-ray diffraction (XRD) study of thin films was performed using Rigaku SmartLab 5-circle X-ray diffractometer. Scanning transmission electron microscopy (STEM) study was performed using probe-corrected FEI Titan 80–300 S/TEM operating at 300 kV. Atomic-resolution maps of chemical elements were obtained by energy-dispersive x-ray spectroscopy (AR EDS) using a high-sensitivity Super-X EDX detector system in a probe-corrected FEI Titan G2 60–200 S/TEM with X-FEG source (ChemiSTEM technology). The Lu L<sub>α</sub> and Fe K<sub>α</sub> lines were identified on the spectra and used in the mapping procedure.

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## Author contribution

A.A. planned and performed the deposition of thin films. V.A. measured XRD. A.V. and V.R. performed preliminary HRTEM experiments and S.L. carried out the atomic-resolution EDX measurements. A.A. interpreted the data and with the help of A.K. proposed the model describing the results. The manuscript was written by A.A. and A.K. with critical comments made by all co-authors.

## Additional information

Supplementary information accompanies this paper at <http://www.nature.com/scientificreports>

**Competing financial interests:** The authors declare no competing financial interests.

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