Modulation of the microstructure and electrical properties of $LaAlO_3$ ceramics induced by doping with rare earth elements (Eu, Gd, Ho, and Tm)

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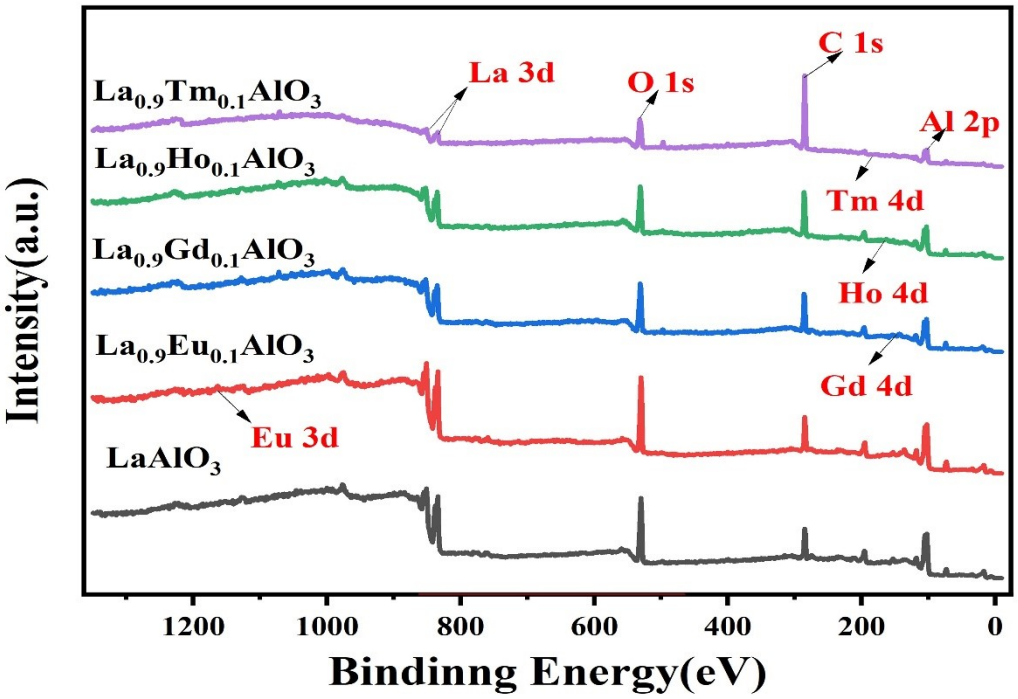

Figure S1. XPS full spectra

Table 1. Cell parameters of the $La_{0.9}X_{0.1}AlO_3$ (X = Eu, Gd, Ho, Tm) and $LaAlO_3$ ceramics

	Lattice constants (Å)	Lattice constants (Å)	Cell volume (Å3)
$LaAlO_3$	a = b = 5.34739	c = 13.04416	323.02
$La_{0.9}Eu_{0.1}AlO_3$	a = b = 5.33692	c = 13.03766	321.6
$La_{0.9}Gd_{0.1}AlO_3$	a = b = 5.33495	c = 13.02154	320.96
$La_{0.9}Ho_{0.1}AlO_3$	a = b = 5.33686	c = 13.02857	321.37
$La_{0.9}Tm_{0.1}AlO_3$	a = b = 5.37488	c = 13.03974	326.24

Table 2. Cell refinement factors obtained by Rietveld refinement $La_{0.9}X_{0.1}AlO_3$and $LaAlO_3$ samples.

Refinement factors	$LaAlO_3$	$La_{0.9}Eu_{0.1}AlO_3$	$La_{0.9}Gd_{0.1}AlO_3$	$La_{0.9}Ho_{0.1}AlO_3$	$La_{0.9}Tm_{0.1}AlO_3$
Rp (%)	6.16	6.61	5.41	6.58	7.91
Rwp(%)	9.317	8.569	8.282	8.572	9.564
$\chi 2$ (%)	2.48	2.48	2.32	2.57	2.81

Table 3. Binding energy and vacancy oxygen concentration of lattice oxygen (O lattice) and vacancy oxygen (O vacancy) in $La_{0.9}X_{0.1}AlO_3$ (X=Eu, Gd, Ho, Tm) and $LaAlO_3$ ceramics

	O 1s O lattice (eV)	O1s O vacancy (eV)	O vacancy concentration
$LaAlO_3$	529.79	531.98	0.3578
$L_{a0.9}Eu_{0.1}AlO_3$	529.59	531.50	0.3895
$La_{0.9}Gd_{0.1}AlO_3$	529.90	532.04	0.3038
$La_{0.9}Ho_{0.1}AlO_3$	529.67	531.77	0.4154
$La_{0.9}Tm_{0.1}AlO_3$	529.62	531.64	0.7243

Computational details

The calculations of density functional theory are done with the projector augmented plane-wave basis, which is implemented in Vienna ab-initio simulation package. And the plane-waves are cut-off at 550 eV. The exchange-correlations of electrons are described by the generalized gradient approximations with the form proposed by Perdew, Burke, and Ernzerhof. To improve the descriptions on the correlation interactions, the Hubbard U scheme is employed with Ueff = 5.0 eV applied on the f-shell of Eu, Gd, Ho and Tm. The energy converge criterion for solving self-consistent Kohn-Sham equations is 10^{-6} eV. The Brillouin zone is sampled with resolution of 0.03 $Å^{-1}$, using the scheme of Monk horst-Pack. All the structures in this study are fully relaxed until the Hellman-Feynman smaller than 0.05 eV/Å. [1-5]

References

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