cbecimat26
26° Congresso Brasileiro de Engenharia e Ciência dos Materiais
22 a 26 de novembro de 2026
Costão do Santinho
Florianópolis-SC

Impact of Ir, Re, V, and Ta doping on the crystal structure and oxygen non-stoichiometry of $SrFe_{1-x}MxO_{3-\delta}$ perovskites for SOFC electrodes

Loreto Aguilera[1] ; Yanet Mansilla[1]; Sarabel Ordoñez[1] ; Javier Gainza[2]; Jose Antonio Alonso[3]

1.Universidad Austral de Chile ; 2. ESRF, Francia ; 3. Instituto de Ciencia de Materiales de Madrid, España

Introduction

$SrFeO_{3-\delta}$ based perovskites exhibit remarkable structural versatility due to the coexistence of different iron oxidation states (Fe^{3+}/Fe^{4+}) and the presence of oxygen vacancies. Partial substitution of Fe by transition metals can modify crystal symmetry, lattice parameters, and oxygen stoichiometry. In this work, the effect of Ir, Re, V, and Ta substitution in $SrFe_{0.9}M_{0.1}O_{3-\delta}$ perovskites was investigated using conventional and synchrotron X-ray diffraction, combined with Rietveld refinement to determine the structural modifications induced by B-site doping.

Structural characterization



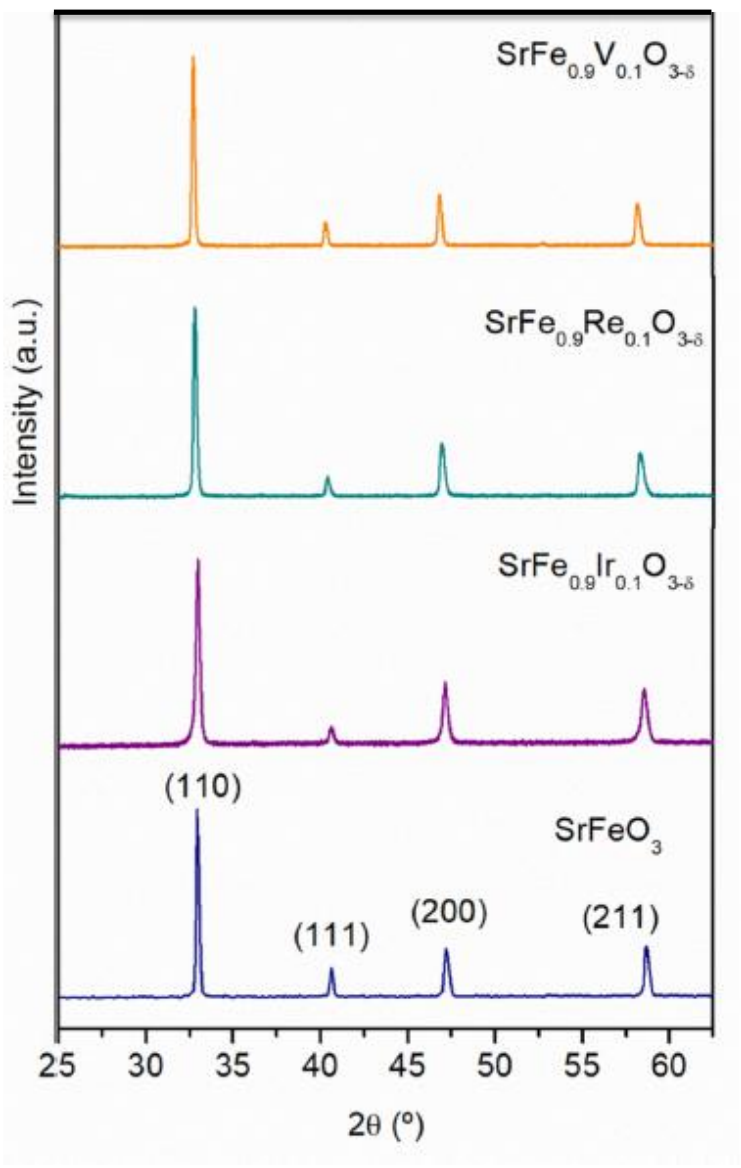
The phases were first analyzed by X-ray diffraction (XRD) using a Bruker D2 Phaser diffractometer with Cu Kα radiation (λ =1.5418 Å).

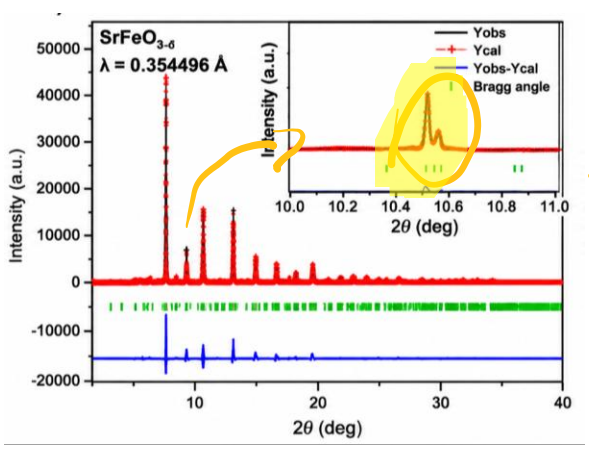


European Synchrotron Radiation Facility (ESRF, Grenoble, France). The wavelength 0.354496 Å (~35 keV).

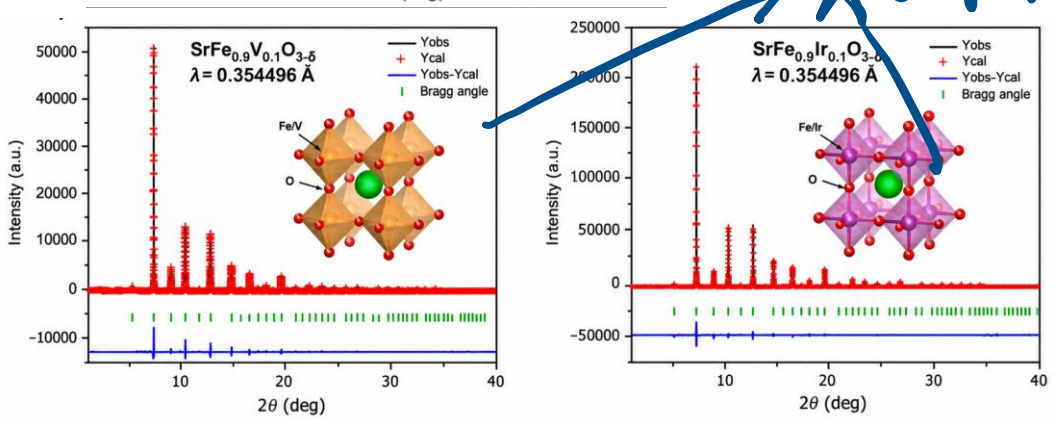
Results and discussion

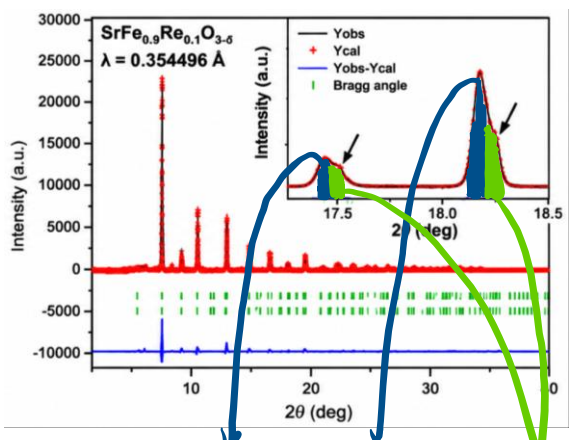
XRD patterns obtained at room temperature. The (hkl) indicates planes of the cubic phase.





tetragonal structure!
I4/mmm
Pm3̄m was confirmed





Composition	Space group	Oxygen content
$SrFeO_{3-}\delta$	I4/mmm	2.95
$SrFe_{0.9}Re_{0.1}O_{3-}\delta$	Pm-3m	2.92
$SrFe_{0.9}Re_{0.1}O_{3-}\delta$	Pm-3m	2.89
$SrFe_{0.9}V_{0.1}O_{3-}\delta$	Pm-3m	2.56
$SrFe_{0.9}Ir_{0.1}O_{3-}\delta$	Pm-3m	2.56

$SrFe_{0.9}Re_{0.1}O_3$ Phase 1

$SrFe_{0.9}Re_{0.1}O_3$ Phase 2

Conclusions

The undoped composition crystallized as a single tetragonal phase (I4/mmm), whereas Ir, V, and Re substitution stabilized the cubic perovskite structure (Pm-3m) at room temperature. Notably, the Re-doped composition showed two coexisting cubic phases with slightly different lattice parameters, potentially arising from an inhomogeneous Re distribution and/or local variations in the Fe oxidation state. The stabilization of the highly symmetric cubic structure, with reduced lattice distortion, is particularly beneficial for SOFC cathode applications, as it favors oxide-ion (O^{2-}) mobility.

References

[1]X. Yu, W. Long, F. Jin, T. He, Cobalt-free perovskite cathode materials SrFe1-xTi xO3-δ and performance optimization for intermediate-temperature solid oxide fuel cells, Electrochim. Acta
[2] P. Kaur, K. Singh, Perovskite-structured cobalt-free cathode materials for solid oxide fuel cells, Recent Adv. Renew. Energy Technol. 2 (2022) 357–373, https:// doi.org/10.1016/B978-0-12-823532-4.00009-4. Elsevier.
[3]Y. Li, A.L. Larralde, J. Cai, S. Du, L. Troncoso, M.T. Fernandez-Díaz, J.A. Alonso, Novel cobalt-free family of SrFe1-xScxO3-δ perovskite materials for cathode applications in solid oxide fuel cells, Int. J. Energy Res. 44 (2020) 11702–11710, https://doi.org/10.1002/er.5797.

Acknowledgments: Fondecyt 1260447 and MIGA (ICN2021_023) by ANID