Crystal-structure and Mössbauer studies of Sr3Fe2+xMo1-xO9-3x/2 (0.3 ≤ x ≤ 1)

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Résumé

Perovskites-type oxides Sr3Fe2+xMo1-xO9-3x/2 (x= 0.30, 0.45, 0.60, 0.75, and 1.00) (1) were synthesized in polycrystalline form using solid-state reaction route, in air. These oxides have been studied at room temperature using of XRD, Mössbauer and UV-Vis spectroscopy. The crystal structures were refined by Rietveld's method, and revealed that this series adopts two phase transitions from a tetragonal $I4/mcm$ (x= 0.30, 0.45, and 0.60) to a simple cubic Pm-$3m$ (x= 0.75) to another tetragonal $P4/mmm$ (x= 1.00) phase. The values of the isomer shift and quadrupole splitting confirm that the formal oxidation state of iron containing our compounds consist of the mixed valence of the Fe3+ and Fe4+ cations for octahedral environment. The Mössbauer spectrum of the sample (x= 0.75) SrFe0.917Mo0.083O3-δ is consistent with Fe in a cubic lattice site.

Spectral dependence of optical parameters such as; absorption coefficient, refractive index, extinction coefficient, optical conductivity, real and imaginary parts of the complex dielectric function, complex electric modulus and complex impedance were performed in the range 1.54 -4.94 eV using UV- spectroscopy experiments. The direct bandgap energy increases from 1.70 to 2.25 eV with increasing x.

Figure 1: Final Rietveld refinement plot.

References

(1) El Hachmi, A., Manoun, B., Sajieddine, M., Tamraoui, Y., El Ouahbi, S., 'Synthesis, structural and optical properties of perovskites-type: Sr3Fe2+xMo1-xO9-3x/2 (x = 0.30, 0.45, 0.60, 0.75 and 1.00)'. Polyhedron, 200 (2021) 115133, https://doi.org/10.1016/j.poly.2021.115133

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