Public Abstract

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Graduation Term:SP 2009
Department:Physics
Degree:PhD

Title:Neutron Diffraction Studies on ABO3 (A=La, Sr; B=Fe, Co, Ni, Cu, Mn, Ti) Perovskite Used in Solid Oxide Fuel Cell (SOFC) and Double Perovskite Ba2YRu0.85Cu0.15O6 Superconductor

ABO3(A=La, Sr, B=Fe, Co, Ni, Cu, Mn, Ti) perovskites are of great interest due to their mixed electronic and oxygen ion conductivity. They are candidates for the electrodes of SOFCs. The mixed conductivity can be enhanced through the substitution of La3+ by Sr2+ at A sites, and the substitution of Fe3+ by other transition metal ions at B sites. The charge imbalance and overall charge neutrality can be maintained by the presence of charged oxygen vacancies and mixed valence state ions at the B sites. These point defects are the origin of the mixed electronic and oxygen ion conductivity. This study investigates the effects of substitutions at A sites and/or B sites on the crystal and magnetic structure, oxygen vacancies, and the thermal expansion coefficients at different temperatures and gaseous environment. The oxygen vacancy concentration can relax the perovskite distortion and has a close relationship with the magnetic properties. La0.6Sr0.4FeO3, La0.6Sr0.4Fe0.8Co0.2O3, and La0.8Sr0.2Fe0.8Co0.2O3 can be good candidates for the cathodes of SOFCs at intermediate temperature.
The double perovskite Ba2YRu0.85Cu0.15O6 superconductor and a mixture of 5wt% YBa2Cu3O7 and undoped Ba2YRuO6 were investigated with the aid of neutron diffraction. The 1:1 B site ordering is observed and long range antiferromagnetic ordering of the Ru sublattice with a type I magnetic structure appears when the temperature is below 38K. The decomposition of Cu-doped Ba2YRuO6 into undoped Ba2YRuO6 and YBa2Cu3O7 is not seen. YBa2Cu3O7 is not stable at the temperature used to prepare the Cu-doped Ba2YRuO6 superconductor. These results confirm the presence of superconductivity without CuO2 planes.