

CO oxidation activity of the Ba-Fe-O system

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Abstract

The substitution of so-called critical elements, among which Noble Metals (NM) and some Rare Earths (RE) are included, has become a question of major concern to reach the goal of sustainable development. ABO₃ perovskite related oxides have been essayed as catalysts in a number of reactions, most of them redox processes. The high flexibility of the perovskite structure offers much more opportunities to tailor the oxidation state and the characteristics of the oxygen environment of the catalytically active B element, while preserving a high thermal stability. Lanthanide based Fe, Mn and Co perovskites, LnBO₃ (Ln=lanthanide, B=Fe, Co, Mn), have been extensively studied systems, particularly as catalysts in the CO oxidation reaction. Total substitution of La by Ba fits perfectly with the actual demands to replace critical RE since we have investigated the Ba-Fe-O system as catalyst in the CO oxidation process. BaFeO_{3-δ} (0.2 < δ < 0.4) depicts a 6H perovskite hexagonal structural type with Fe both in III and IV oxidation states and oxygen nonstoichiometry accommodated by random distribution of anionic vacancies [1]. Nano - BaFeO_{2.78} proved to be more active than the above-mentioned LnFeO₃ (Ln=La, Sm, Nd) phases. The BaFeO_{3-δ} catalyst was prepared by a sol-gel method. BaFeO_{2.78} nanoparticles of around 100 nm were obtained. The decrease of the particle size dramatically decreases the temperature of the reduction process of the sample and, under soft conditions (T ≈ 200 °C/H₂), nano-BaFeO_{2.78} suffers an easy and reversible reduction process that occurs by a different pathway than that described for BaFeO_{3-δ} bulk material. The temperature dependence of the redox process has been followed by in situ X-ray, Neutron and selected area electron diffraction. Besides, atomically resolved images and chemical maps obtained using different Aberration-Corrected Scanning Transmission Electron Microscopy techniques, have provided a clear picture of the accommodation of oxygen- non-stoichiometry in these materials.

[1] J.M. González-Calbet et al., J. Solid State Chem. 1990, 86, 149-59.

Biography

Full professor attached to the Department of Inorganic Chemistry I of the Faculty of Chemistry of the UCM, and member of the research group "Functional Inorganic Materials". Research in Solid State Chemistry focused on the synthesis of mixed functional oxides and oxihalides as well as their structural and morphological characterization (diffractometric techniques and high resolution electron microscopy) in order to establish the relation particle size-structure-properties in materials with possible magnetic, electrical, superconducting and catalytic properties. Co-author of more than 100 publications in international journals related to Inorganic and Solid State Chemistry and Materials Science. Assistance to 90 International Congresses.



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