CORRELATION BETWEEN PHASE TRANSITION BEHAVIOR AND STRUCTURAL PROPERTIES IN Ba^{2+} -SUBSTITUTED La_2 Mo_2O_9

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Lanthanum molybdate ($La_2Mo_2O_9$) is a well-established oxide-ion conducting material that has been extensively investigated due to its potential application in intermediate-temperature solid oxide fuel cells, oxygen separation membranes, and gas sensors [1]. Its functional properties are strongly influenced by a reversible first-order phase transition from a low-temperature monoclinic α-phase to a high-temperature cubic β-phase, which is accompanied by significant changes in crystal symmetry, lattice structure, and ionic transport behavior [2]. While the cubic phase exhibits higher oxide-ion conductivity, its stabilization over a broader temperature range remains a key challenge for practical applications.

Chemical substitution at the La^{3+} site has been widely recognized as an effective strategy to control the structural stability and phase transition characteristics of $La_2Mo_2O_9$-based materials [3]. In particular, alkaline earth cation substitution has attracted increasing attention due to its ability to induce lattice distortions, affect point defect distribution, and influence the thermodynamic characteristics of the phase transition. Recent studies have demonstrated that the size and valence mismatch between the host and substituent cations play a critical role in determining phase stability and transition temperature [4]. Despite growing interest, the influence of Ba^{2+} substitution on the crystal structure and phase transition in the $La_2Mo_2O_9$ system remains insufficiently explored, especially for materials synthesized via low-temperature chemical routes.

The aim of this study was to investigate the correlation between Ba^{2+} substitution, structural properties, and phase transition behavior in $La_2Mo_2O_9$. Ba^{2+}-substituted $La_2Mo_2O_9$ samples were prepared using an aqueous sol-gel synthesis route, ensuring homogeneous cation distribution at the molecular level. Structural and phase analysis was carried out by X-ray diffraction (XRD), while microstructural features were examined using scanning electron microscopy (SEM). Differential scanning calorimetry (DSC) was employed to evaluate the phase transition behavior.

XRD analysis indicated that the sol-gel synthesis method is suitable for the preparation of a single-phase compound without detectable secondary phases. SEM analysis revealed a relatively dense ceramic microstructure with the presence of a limited number of pores. Differential scanning calorimetry results suggested that partial substitution of lanthanum with barium contributed to the stabilization of the cubic β-phase at room temperature.

Keywords: LAMOX, phase transition, SOFC, sol-gel

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