Crystal Structure and Conductivity of Ba and Y Doped LaAlO₃ Solid Electrolyte

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ABSTRACT

Doped LaGaO₃ with distorted perovskite structure exhibits higher oxygen ion conductivity than yttria stabilized zirconia. However, Ga is a very expensive element. Doped LaGaO₃ will face the challenge of higher materials cost when mass production is taken into account. LaAlO₃, which exhibits a perovskite structure, is also considered [2] as a potential candidate for a cost-effective solid electrolyte. The objectives of this work were to (1) study the solubility limit of Ba²⁺ and Y³⁺ dopants for both A- and B-site of LaAlO₃ systems and (2) to examine the dependence of dopant concentration on the ionic conductivity of LaAlO₃.

The solubility of Ba in the La-cation sublattice was found to be only 5%. In the B-site sublattice, the solubility of Y ion in Al-cation sites was only less than 10%. The reason is simply due to the 68% mismatch of ionic radius between r_{Mg} (0.90Å) and r_{Al} (0.535Å) in spite of LaYO₃ having the similar perovskite structure. With double doping of Ba²⁺ and Y³⁺ in LaAlO₃, the enhancement of Ba²⁺ solubility was also observed. These results indicate that the perovskite of LaAlO₃ can dissolve slightly higher amount of LaYO₃ and the lattice parameter was increased. Therefore, the larger Ba²⁺ was dissolved into LaAlO₃-based structure. These results indicate that the role of Y³⁺ is very important for the dissolution of Ba in LaAlO₃.

Within the solubility limit of singly doped LaAlO₃, the ionic conductivities of doped LaAlO₃ were slightly increased with the increasing dopant concentration. For La_{0.97}Ba_{0.03}AlO₃ and LaAl_{0.9}Y_{0.1}O₃ the conductivities measured were 2.68×10^{-4} S/cm and 3.41×10^{-4} S/cm at 800°C, respectively. It was quite interesting that the conductivities of the doubly doped La_{0.9}Ba_{0.1}Al_{0.9}Y_{0.1}O₃ was enhanced to 184.04x10⁻⁴ S/cm at 800°C. However, the activation energy of doubly doped La_{0.9}Ba_{0.1}Al_{0.9}Y_{0.1}O₃ (78.75KJ/mol) was slightly lower than singly doped La_{0.97}Ba_{0.03}AlO₃ (95.48KJ/mol) and LaAl_{0.9}Y_{0.1}O₃ (86.66KJ/mol).

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Reference

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Fig.1 X-ray diffraction patterns of the $La_{1-x}Ba_xAlO_3$ system prepared by sintering at 1500°C. (a) x=0.05, (b) x=0.10, (c) x=0.15, (d) x=0.20. The second phase observed is $BaAl_2O_4$ (JCPDS: 82-2001)



Fig.2 X-ray diffraction patterns of the $La_{1-x}Ba_xAl_{0.9}Y_{0.1}O_3$ system prepared by sintering at 1500°C. (a) x=0.01, (b) x=0.03, (c) x=0.05, (d) x=0.10.



Fig.3 Conductivity of doped LaAlO3 plotted as a function of 1000/T.