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The crystal structure of $Ba(Ce_{0.8}Zr_{0.2})O_3$

Jong Sung Bae[a], Woong Kil Choo[a] and Chang Hee Lee[b]

[a]*Department of Materials Science and Engineering, Korea Advanced Institute of Science and Technology, 373-1 Gusong-Dong, Yusong-Gu, Taejon, Korea*

[b]*Neutron Physics Department, HANARO Center, Korea Atomic Energy Research Institute, Taejon 305-600, KOREA*

Trivalent rare earth-doped $BaCeO_6$ has been investigated extensively due to its high ionic conduction property for electrolyte in solid oxide fuel cell (SOFC) application. However, its application has been restricted to oxygen atmosphere, instead of reformer gas under ambient atmosphere, because its chemical stability deteriorates on contact with CO_2 and H_2O. Recent studies have reported that the chemical stability can be increased by zirconium substitution, in spite of the unavoidable reduction in ionic mobility. But, 20% Zr substitution is considered to be enough for the structural stability, not sacrificing conductivity too much.

The crystal structure of $Ba(Ce_{80}Zr_{20})O_3$ has not been studied by neutron and x-ray diffractometry yet. A raman study just suggested that phase transition occurs in Zr substituted $BaCeO_3$. The purpose of this work is to investigate the crystal structure of 20% Zr substituted $BaCeO_3$ which is reported to be structurally stable and which may provide the fundamental information about ionic transport phenomena. Crystal structure study by neutron and x-ray were performed. Then, the space group has been established by Rietveld refinement.