Accepted Manuscript

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PII:	S1386-1425(18)30219-1
DOI:	doi:10.1016/j.saa.2018.03.024
Reference:	SAA 15896
To appear in:	*Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*
Received date:	13 December 2017
Revised date:	28 February 2018
Accepted date:	9 March 2018

Please cite this article as: A. Garbout, M. Férid , Pyrochlore structure and spectroscopic studies of titanate ceramics. A comparative investigation on SmDyTi2O7 and YDyTi2O7 solid solutions. The address for the corresponding author was captured as affiliation for all authors. Please check if appropriate. Saa(2017), doi:10.1016/j.saa.2018.03.024

Pyrochlore structure and spectroscopic studies of titanate ceramics. A comparative investigation on $SmDyTi_2O_7$ and $YDyTi_2O_7$ solid solutions

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Abstract

Considering the features in changing the structure and properties of rare earth titanates pyrochlores, the substituted $Dy_2Ti_2O_7$ may be very attractive for various applications. Effect of Sm and Y substitution on the structural properties of $Dy_2Ti_2O_7$ ceramic was established. These ceramics were prepared by solid-state reaction and characterized by X-ray diffraction and Raman spectroscopy. Both analysis show that $YDyTi_2O_7$ with the pyrochlore structure is obtained after heating at 1400°C, but $SmDyTi_2O_7$ has already formed after sintering at 1200°C. SEM images revealed that the average grain size was increased with the increase of heating temperature, and an un-homogeneous grain growth was detected. The average size was about 37 nm and 135 nm for the $SmDyTi_2O_7$ and $YDyTi_2O_7$ particles, respectively. Structural Rietveld refinements indicate that all prepared ceramics crystallize in cubic structure with space group of Fd3m. The refined cell parameters demonstrate an almost linear correlation with the ionic radius of Ln^{3+}. The vibrational spectra revealed that the positions of bands are sensitive to the Ln^{3+}-ionic radius, and the Ti-O bond strength decreased linearly with the increase of cubic lattice parameter. Raman spectra indicate that the wavenumber of O-Ti-O bending mode is considerably shifted to lower region with increasing in mass of the Ln atom. This paper provides solid foundations for additional research of these solid solutions, which are very attractive for different fields as promising catalytic compounds for combustion applications or as frustrated magnetic pyrochlore ceramics.

Keywords: Solid state reaction; X-ray diffraction; Spectroscopy; Magnetic properties; Pyrochlore titanates

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