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P.S.C.18

CHARACTERIZATION OF BISMUTH TITANATE CERAMIC POWDERS

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The bismuth titanate is a typical layer-structured ferroelectric material and belongs to the Aurivilius compounds family. The bismuth titanate ceramic material could be obtained by the mechanically activated synthesis after thermal treatment slightly lower then in conventional solid-state reaction. In investigated case bismuth titanate was prepared through mechanochemical synthesis starting from bismuth oxide and titanium oxide in anatas form. Mixture of oxides was milled in zirconium oxide jar in the planetary ball-mill during 1 to 12 hours. The relation between powders and zirconium oxide balls during milling was 1:20. Bismuth titanate with good crystallinity was formed after 180 min. The XRD, Raman, IR and SEM analysis were performed. Electrical and ferroelectrical properties were carried out. Very well defined hysteresis loop was obtained for bismuth titanate prepared from mechanically synthesized powders.

P.S.C.19

EXPERIMENTAL AND THEORETICAL INVESTIGATION OF HYDROGEN STORAGE IN MAGNESIUM BASED COMPOSITES

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Due to its high hydrogen storage capacity, light weight, low cost and abundance in the earth's crust, magnesium and magnesium based alloys are the most promising candidates for hydrogen storage materials. However, the hydriding/dehydriding reaction takes place at high temperature and the kinetic is relatively slow. One of the ways to improve the kinetics of magnesium based hydrogen storage materials is the addition of metals and/or metallic oxides. It has been revealed that ball milling of MgH_2 powders with small amounts of 3d-transition metals or their oxides leads to marked improvements of the hydrogen absorption/desorption kinetics. The aim of this study was to investigate the influence of Ti and Co addition on the sorption properties of MgH_2. Ball milling of MgH_2 and catalysts was performed under argon using stainless steel vial and balls in a Turbula Type T2C Mixer from WAB (Basel, Switzerland), with different weight ratios among the blend components. The powders were characterized by XRD to assess the details of the phase structure by Rietveld analysis, while microstructural studies were performed by SEM. Thermal stability and hydrogen desorption properties were also investigated by thermal analysis methods. In order to obtain deeper insight into bonding mechanisms of transition metal in MgH_2 fully relaxed structure, we have performed ab initio electronic structure calculation of MgH_2 + X (X=Ti, Co) using Full Potential Linearized Augmented Plane Wave method, implemented in WIEN2K code.