A compositionally and disorderedly doped, Bi-based pyrochlore phase found in a range of ternary Bi$_2$O$_3$-M$^3$O-$\text{Nb}_2$O$_5$ systems has been the subject of much recent interest as a result of its relatively low sintering temperatures and often excellent dielectric properties, including electric field tuneability. In this study, two such A$_2$B$_2$O$_6$(O$_1$O$_2$)$_2$ pyrochlore type phases of stoichiometry (Bi$_{0.825}$Ni$_{0.125}$)$_{3+2}$O$_{1.000}$[(Ni$_{0.235}$Nb$_{0.765}$)$_{3.000}$]O$_{1.000}$ (BNN) and (Bi$_{0.825}$Mg$_{0.125}$)$_{3+2}$O$_{1.000}$ (BMN) have been synthesized via solid-state reaction. Their average as well as their local structure have been investigated by means of Rietveld refinement of neutron powder diffraction data combined with an study of structured diffuse intensity via electron diffraction. The refined average structures of both phases show large amplitude Atomic Displacement Parameters (ADP’s) for the atoms occupying the A and O(2) sites of the ideal pyrochlore structure. A disordered model, involving splitting of the Bi$^{3+}$/M$^3+$ atoms on the A-site from the 16d to the 96h and of the O(1) atoms from the 8b on to the 32c positions was found to significantly improve the average structure refinements as well as substantially reduce the refined A-site ADP’s. A highly structured characteristic diffuse intensity distribution was found in electron diffraction patterns of both phases and was partially interpreted in terms of large amplitude rotations of the O(2)A$_2$ tetrahedral framework, β-cristobalite sub-structure of the ideal pyrochlore structure. The BMN and BNN show relatively high dielectric permittivities at room temperature and at 1MHz, 116 and 151 respectively. Their dielectric loss tangents under the same conditions were also very good i.e. as low as 0.00065 and 0.00042.

Keywords: bismuth compounds, local structure, dielectric properties

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**Structural study of Co-doped zinc aluminate**

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Zinc aluminate, Zn$_2$Al$_2$O$_4$, is a wide-band-gap semiconductor transparent for light wavelengths greater than 320 nm [1]. When doped with Co$^{3+}$, Mn$^{3+}$ or rare-earth ions it exhibits luminescence and can be used as a cathodoluminescent material [2]. Zinc aluminate, Zn$_2$Al$_2$O$_4$, possesses a spinel structure, the space group Fd-3m. Its unit cell contains 32 atoms from the 8A site and 32 atoms from the 16A site from the 16A-type sub-structure of the ideal pyrochlore structure. Recently, a detailed structural study of ITO has been reported [3]. Powder ITO samples with Sn doping level up to 28 at% were prepared by a solid-gel technique from In$_2$O$_3$ and SnCl$_2$. The samples were examined by XRD and TEM. Diffraction lines were broadened. The line broadening increased with Sn content. Analysis of line broadening was performed in the Rietveld structure refinement by the PANalytical XPert HighScore Plus program. Silicon powder was used as a size-standard. Crystallite sizes decreased from 25.5 to 16.8 nm, while strain increased from 0.112 to 0.369 %, as Sn level increased from 0 to 28 at %. The interplanar distances, d, in the samples determined by the selected area electron diffraction (SAED) agreed with XRD data. SAED showed that the observed regions appear to be nanocrystalline with a bixbyite-type structure, giving a strong evidence on incorporation of Sn in the starting structure of In$_2$O$_3$. TEM studies proved that ITO samples contained nanosized particles/grains. The grains had nearly spherical shape at lower size level, while at higher level (>8 at %) they were elongated. The crystallite sizes determined by TEM well agreed with those obtained from XRd. HRTEM gave an additional insight into ITO microstructure.

Keywords: Sn-doped In$_2$O$_3$, X-ray diffraction, transmission electron microscopy

**P11.16.117**


**Crystal structure and site occupancy of boron in synthetic high-pressure spinel MgAl$_2$B$_2$O$_6$**

Shunsuke Sakai$^1$, Kazumasa Sugiyama$^1$, Akira Yoshiasa$^2$

A compositionally and disorderedly doped, Bi-based pyrochlore phase found in a range of ternary Bi$_2$O$_3$-M$^3$O-$\text{Nb}_2$O$_5$ systems has been the subject of much recent interest as a result of its relatively low sintering temperatures and often excellent dielectric properties, including electric field tuneability. In this study, two such A$_2$B$_2$O$_6$(O$_1$O$_2$)$_2$ pyrochlore type phases of stoichiometry (Bi$_{0.825}$Ni$_{0.125}$)$_{3+2}$O$_{1.000}$[(Ni$_{0.235}$Nb$_{0.765}$)$_{3.000}$]O$_{1.000}$ (BNN) and (Bi$_{0.825}$Mg$_{0.125}$)$_{3+2}$O$_{1.000}$ (BMN) have been synthesized via solid-state reaction. Their average as well as their local structure have been investigated by means of Rietveld refinement of neutron powder diffraction data combined with an study of structured diffuse intensity via electron diffraction. The refined average structures of both phases show large amplitude Atomic Displacement Parameters (ADP’s) for the atoms occupying the A and O(2) sites of the ideal pyrochlore structure. A disordered model, involving splitting of the Bi$^{3+}$/M$^3+$ atoms on the A-site from the 16d to the 96h and of the O(1) atoms from the 8b on to the 32c positions was found to significantly improve the average structure refinements as well as substantially reduce the refined A-site ADP’s. A highly structured characteristic diffuse intensity distribution was found in electron diffraction patterns of both phases and was partially interpreted in terms of large amplitude rotations of the O(2)A$_2$ tetrahedral framework, β-cristobalite sub-structure of the ideal pyrochlore structure. The BMN and BNN show relatively high dielectric permittivities at room temperature and at 1MHz, 116 and 151 respectively. Their dielectric loss tangents under the same conditions were also very good i.e. as low as 0.00065 and 0.00042.

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