Lithium tetraborate attracts considerable interest in nonlinear optics as an element of surface acoustic wave devices, a frequency-conversion material for 2nd-5th harmonic generation from a high-power Nd:YAG laser, as a high power ultraviolet light source based on SHG and SFH of the visible laser radiation *etc*. Possible applications for $Li_2B_4O_7$ require deeper understanding of its properties, especially at non-ambient conditions.

Thus in the literature there is plenty of controversial data on $Li_2B_4O_7$ reporting anomalous behaviour in the different temperature ranges, e.g. thermal scintillations have been observed in $Li_2B_4O_7$ when not excited by hard quanta [2], incommensurate structure modulation [3], anomalies in thermal expansion and thermal evolution of bond lengths [4, 5], numerous phase transitions [6, 7], anomalies in sound velocities and Raman spectra [8], strong anisotropy of ionic conductivity [9] *etc*. The existing discrepancies between the experimental results of different authors lead us to perform systematic studies of lithium tetraborate.

Structural studies were performed using coherent elastic neutron scattering on ^{11}B enriched $Li_2B_4O_7$ (99.6% ^{11}B). Powder diffraction examinations unambiguously indicated isostructurality of $Li_2B_4O_7$ structure type in the temperature range from 3 K to its melting point at ca. 1170 K. Despite this fact, an evidence for anomalies in thermal dependencies of lattice parameters, bond lengths and displacement parameters has been deduced.

In the current contribution we report on complex studies of lithium tetraborate doped with ^{11}B in the broad temperature range 3-1200 K using neutron powder/single crystal diffraction, dilatometry, specific heat, calorimetry and impedance spectroscopy together with an attempt to present our view on the nature and origin of anomalies in $Li_2B_4O_7$.

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Keywords: neutron diffraction, noncentrosymmetric oxides, boron compounds

FA2-MS14-P34

Structural, magnetic, electrical and magnetocaloric properties in $Pr_{0.6}Sr_{0.4}MnO_3/BaTiO_3$ composites.

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Composites with varying composition of ferromagnetic $Pr_{0.6}Sr_{0.4}MnO_3$ and ferroelectric $BaTiO_3$ have been prepared using a solid-state ceramic method $(1-x)(Pr_{0.6}Sr_{0.4}MnO_3)/x(BaTiO_3)$, with x is the molar ratio and x = 0.0, 0.03, 0.05, 0.10 and 0.30 using conventional ceramic double sintering process. We report the structural, magnetic electrical and magnetocalorical properties of all samples. The presence of the two phases of $Pr_{0.6}Sr_{0.4}MnO_3$ (PSMO) and $BaTiO_3$ (BTO) was confirmed by X-ray diffraction (XRD) technique and the structural analysis. Magnetic measurements of magnetization versus temperature and applied field were performed. The temperature dependence of magnetization reveals that the composite samples show paramagnetic to ferromagnetic transition when the temperature decreases at the same Curie temperature as the parent PSMO compound ($T_c \approx 273K$). The magnetic entropy change $\left|\Delta S_M\right|$ has been deduced from the M(H) data by the Maxwell relation. Close to T_c, large change in magnetic entropy has been observed in all samples. The maximum value of the magnetic entropy is $\left|\Delta S_M^{max}\right|$ decreases from 2.88 $J.kg^{-1}.K^{-1}$ for x = 0 to 1.86 $J.kg^{-1}.K^{-1}$ for x = 0.3 for an applied magnetic field of 2T. At this value of magnetic field the relative cooling power (RCP) decreases also from 63 $J.kg^{-1}$ for the parent sample to 38.3 $J.kg^{-1}$ for x = 0.3. The temperature dependence of the Landau coefficients have been deduced using the Landau expansion of the magnetic free energy, indicating the second order nature of the magnetic transition.

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Keywords: ferromagnetic, ferroelectric, magnetic entropy

FA2-MS14-P35

Twin structure and conductivity in LSGM.

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The aim of our investigations was to study the arrangement and distribution of twin boundaries during mechanical and thermal treatment in order to examine reversibility phenomena in larger ferroelastic crystal plates (5x6x0.87 mm^3) as well as the influence of the domain structure on ionic conductivity. In a selected $La_{0.95}Sr_{0.05}Ga_{0.9}Mg_{0.1}O_{3-x}$ (LSGM) - crystal plate the submicron twin structure was studied using white synchrotron radiation at the Kappa-diffractometer F1 equipped with a MAR CCD-detector (HASYLAB, DESY). Scanning of the sample under the beam (0.05x0.05mm^2) and collecting diffraction data at each step with 45 micron spatial resolution was used to map the domain pattern in the LSGM-plate after mechanical and thermal treatment. Conductivity measurements were done between ~ 70 °C and 710 °C in air. Impedance spectroscopy was applied using a HP4284 LCR-meter in the range 20 Hz – 1 MHz. Data were recorded applying AC amplitudes of 80 mV and 1V to the electrode.

It was shown that before mechanical treatment mainly twin walls normal to the largest surface of the plate occurred. The observed domain structure was partially switched to another twin configuration with domain walls parallel to the surface or to certain domain states during polishing. After annealing the domain configuration with prevalent domain walls normal to the largest plate surface was fully restored.

Impedance plots show two semicircular arcs. The first high frequency arc corresponds to the bulk conductivity while the second low frequency one corresponds to the conductivity on domain boundaries.

Our results show that strain can relax completely by forming

phase-specific domain wall configurations [1], and hence, reorientations occur during thermal cycling. This feature may be of practical use as the preparation of electrolyte and electrode ceramics for SOFC includes compaction during one of the synthesis stages. Ceramics of LSGM can be approximated by an ensemble of small crystallites. Mechanical pressure imposed to such an electrolyte pellet causes the rearrangement of the twin structure of "chevron cells" in ceramic grains along the direction parallel or nearly parallel to the imposed pressure. Hence, such pressure will cause memory texturing of twin "chevrons" in electrolyte layers along the direction of oxygen diffusion in the SOFC structure. Keeping in mind the influence of twin walls on the conductivity and the high density of twin walls in LSGM solid solutions, it is supposed that texturing of the twins, e.g. reorientation of "chevron cells" increases the conductivity of the perovskite-type electrolyte LSGM along the cathode-anode direction.

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Keywords: twin structure, ionic conductivity, electrolytes

FA2-MS14-P36

A new model of localized plastic flow and failure of solids.

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Plastic flow localization was investigated on the micro- and macro-scale levels. Localization behavior was examined for a range of metals and alloys that differ in chemical bond and crystal lattice type (BCC, FCC, HCP, tetragonal and monoclinic), in structural state (single- or polycrystal, nanostructure, amorphous) and in deformation mechanism type (dislocation glide, twinning, martensitic transformation) [1]. It was established that deformation localization has the following regular features.

- Macro-scale plastic deformation tends to localize from microplasticity to viscous fracture stage.

- Four types of macrolocalization patterns are observed for yield plateau, linear and parabolic work hardening and prefracture stages.

- These patterns are regarded as different versions of self-excited wave generation.

- Significant variations in material structure and microstructure entail certain quantitative changes in localization patterns; however, their distinctive features remain intact.

- A correspondence rule is formulated, which holds that pattern type is determined by work hardening law acting at a given flow stage.

General regularities are discussed for plastic flow processes. On the base of this evidence a new plastic flow model is proposed the main assumption of which is that the regular features exhibited by the deformation behavior of a crystal are due to the interaction between its dislocation subsystem and acoustic emission pulses caused by dislocation shears.

It is shown that during material form changing, the deforming system would spontaneously separate into deforming volumes that alternate with those remaining undeformed at a given instant of time. Localization nuclei distributions tend to evolve in space and with time. Their evolution can be treated as self-organization manifested in terms of self-excited waves of different types generated in open systems. The separation of a medium into individual volumes and its self-organization involving interaction of its dislocation subsystem with acoustic emission impulses are of equivalent status. Moreover, the emergence of localized plasticity patterns is found to entail a decrease in the entropy of the deforming system. It is thus maintained that plastic flow macrolocalization can be addressed in the context of self-organization approach.

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Keywords: plasticity, wavelength, localisation

FA2-MS14-P37

TEM-based electron energy loss spectroscopy of (In,Ga)N/GaN heterostructure nanowires: influence of strain and composition.

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Wide-band gap materials basing on GaN are already commercially exploited for light emitting devices. (In,Ga)N/GaN heterostructures are fabricated as quantum wells or quantum dots. Up to now, axial heterostructure nanowires (NWs) were generated mostly via lithographic approach starting from quantum wells. We report on axial (In,Ga)N/GaN heterostructure NWs grown catalyst-free by plasma assisted molecular beam epitaxy on (111) silicon.
In addition to optical characterizations, transmission electron microscopy (TEM) investigations were performed. Cross-section samples were elucidated in a TEM/STEM JEOL 2200FS operated at 200 kV. Analytical TEM and in particular electron energy loss spectroscopy (EELS) was applied to characterize the (In,Ga)N nanodisks embedded in GaN NWs.