

tungsten atoms by titanium atoms in the published literature has not enough for understanding of laws of formation properties of system "WC-Ti". Therefore in the given work the electronic structure and character of chemical bonding in carbide systems WC,  $W_{1-x}Ti_xC$  is theoretically investigated. Recently presence lattice as C-, and W-vacancies in WC is shown. At mechanical activation in ball mill of powders WC and Ti, the size of a grain of which makes size about 1...5 micron, it is possible to expect solid-solid of reaction. Our estimations, carried out on basis of quantum-mechanical accounts of their electronic structure, show, that the mechanical properties of the given system can grow. The samples are investigated XRD by a method, analysis of areas coherent dispersion is carried out which are called to supervise changes of structure and properties during mechanical activation. Complex research of crystal and electronic structures of the given system allows to understand the laws of formation of physical properties of new materials.

**Keywords:** structure-physical properties relationships, tungsten compounds, X-ray powder diffractometry

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#### Search for Polarons in $Li_{1-5x}Nb_{1-4x}O_{3-y}$ . Structural Investigation of the Defect Structure in Thermally Reduced Single Crystals

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In the search for new complex materials for optical data storage, a main effect to understand is the refraction index. A bigger refraction index separates the holograms more in space, therefore allowing a higher hologram density in the material. Interesting materials for both, application and basic understanding, are for example  $LiNbO_3$ ,  $LiTaO_3$  [1] and sodiumnitroprusside,  $Na_2[Fe(CN)_5NO] \cdot 2H_2O$  [2].

$Li_{1-5x}Nb_{1-4x}O_{3-y}$  is a widely used material. We are introducing polarons by removing oxygen in order to tune the refraction index. Neutron single crystal diffraction (TriCS, SINQ) has been used in order to determine the structural changes, mostly the determination of the removed oxygen. The results are needed in order to calculate the polaron density. We report on the defect structure of single crystals exposed to vacuum for 24h at 800°C.

[1] Strehlow W.H., et al., *J. Opt. Soc.*, 1974, **64**, 543. [2] Schaniel D., Schefer J., Delley B., Imlau M., Woike Th., *Phys. Rev. B*, 2002, **68**, 104108.

**Keywords:** optical materials, neutron diffraction, polarons

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#### Structural Origin of the low Superconducting Anisotropy of Bi,Pb-2212 Crystals

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Systematic investigations were performed with the aim to improve the properties of  $Bi_2Sr_2CaCu_2O_8$ . The structure of Bi-2212 is modulated, the atom arrangement in the BiO layers changing from square meshes (rocksalt-type) to chains with a given periodicity. Due to the insertion of additional O atoms, the actual composition of these layers is  $Bi_9O_{10}$  ( $Bi_2O_{2.22}$  per formula unit, leading to a total oxygen content per formula unit 8.22). This deviation from electroneutrality, which is partially compensated for by the presence of  $Bi^{3+}$  in the Ca layers, is a crucial parameter for the existence of the superconducting phase. By replacing part of the cations in Bi-2212 by chemically similar cations in a lower oxidation state it is possible to keep the same electron concentration, while removing the additional O atoms, thus suppressing the structural modulation. This was achieved by substituting ~22% of  $Bi^{3+}$  by  $Pb^{2+}$ . The arrangement of atoms in the BiO layers in modulation-free Bi,Pb-2212 can be considered as distorted rocksalt-type. The cell parameter along the stacking direction is slightly larger for Bi,Pb-2212 than for the Pb-free phase. However,

the distance between the two Bi layers is decreased by 0.13 Å, which is in agreement with the fact that these layers are no longer corrugated but planar. The superconducting anisotropy of the Pb-doped crystals was found to be reduced with respect to undoped ones. Consequently, modulation-free Bi,Pb-2212 has an enhanced irreversibility field and a lower relaxation rate than in modulated Bi-2212.

**Keywords:** high- $T_c$  superconductor, modulated structure, structure-property relationship

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#### Structure Investigation of Pure and Cr Doped $Li_3VO_4$

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$Li_3VO_4$  finds applications in the fields of optics, electrochemistry (ionic conduction) and electronics. The RT  $\beta$ II form is orthorhombic (S.G. Pmn2<sub>1</sub>) with  $LiO_4$  tetrahedra larger and more distorted than  $VO_4$  ones; empty sites exist allowing the  $Li^+$  cation migration. Other polymorphs were revealed by increasing temperature up to the melting point. Our study deals with the effect of chromium doping (up to 10% of the V-cationic fraction) on the structure of  $Li_3VO_4$ . The structural investigation was carried out by means of XRD,  $\mu$ -Raman, EPR and  $^7Li$  and  $^{51}V$  MAS-NMR. To study the thermal stability of the solid solutions also HT XRD measurements were performed. XRD and  $\mu$ -Raman analyses point out that Cr ions can easily substitute on the cationic sites of  $Li_3VO_4$  without evidence of impurity phases. The host crystal structure does not depend on Cr-doping, neither at RT nor at HT. The EPR spectra put into evidence the presence of  $Cr^{3+}$  and  $Cr^{5+}$ . The combined analysis of EPR and  $^7Li$  and  $^{51}V$  MAS-NMR signals allows us to detect that  $Cr^{5+}$  and  $Cr^{3+}$  substitute on  $V^{5+}$  and  $Li^+$  site respectively. The  $Cr^{3+}$  presence on Li site is also compatible with Rietveld refinements and Raman results: such substitution requires vacancies formation on Li sublattice, so increasing the ionic conductivity of the material as demonstrated also by our impedance spectroscopy and thermoelectric power measurements.

**Keywords:** ionic materials, vanadium compounds, occupancy

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#### Structures of *C.perfringens* $\alpha$ -toxin mutant, T74I, that Affects its Activity

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The  $\alpha$ -toxin of *Clostridium perfringens* is the major virulence determinant produced by the bacterium associated with gas gangrene in man. The toxin is a  $Zn^{+2}$  dependent,  $Ca^{+2}$  activated phospholipase C (PLC), is haemolytic and able to interact with membrane-packed phospholipids. The ability to interact with eukaryotic cell membranes distinguishes the  $\alpha$ -toxin from related enzymes, such as *C. bifermentans* and *B. cereus* PLC.

Several crystal structures of this enzyme from different Clostridial strains and sources have showed the structure is composed of two, an  $\alpha$ -helical (N-terminal) and a  $\beta$ -sandwich (C-terminal) domains.

A site directed mutagenesis study revealed that the substitution of a single residue, Thr74 with Ile (T74I), resulted in the loss of haemolytic, phospholipase C and the sphingomyelinase activities by 1/250 fold to that of wild enzyme. We have determined the crystal structure of T74I mutant in two different crystal forms, C222<sub>1</sub> and P4<sub>3</sub>2<sub>1</sub> to 1.9Å and 3.2Å resolution respectively. The crystal contains a monomer, in C222<sub>1</sub> structure, and a trimer in P4<sub>3</sub>2<sub>1</sub> structure, in the asymmetric unit of their unit cell. The overall topologies of the mutant structures are very similar, but have conformational differences in the mutant containing 60-90 loop, which is one of the proposed membrane interacting loops. We will compare the structures of T74I mutant with other  $\alpha$ -toxin structures and relate the differences to the