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The Bond Valence Model and Point Defects in Langasite Family

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Crystals of langasite structure ($La_3Ga_5SiO_{14}$ - $La_3Ga(1)Ga_3(2)(GaSi)(3)O_{14}$) belong to the sp.gr. P321 and have four kinds of cation sites. The La, Ga(1), Ga(2) and (GaSi)(3) ions are located on a decahedral, octahedral, tetrahedral and trigonal-pyramidal sites, respectively.

In this work we demonstrate an analysis of the structure refinements of the langasite family compounds $La_3Ga_4(Ga_xSi_{2-x})O_{14}$, $La_3Ga_4[Ga(Si,Ge)]O_{14}$, $La_3Ga_{5.5}M_{0.5}O_{14}$ c M=Ta, Nb with the bond valence models. The calculation of bond valence (s_{ij}) for cation sites was made by the two methods:

- method of Brese and O'Keeffe: $s_{ij}=\exp[(R_{ij} - d_{ij})/b]$;
- method of Brown and Wu: $s_{ij}=(R_i/d_{ij})^{-N}$

The calculation of s_{ij} valus for cation and anion sites was fulfiled by Pyatenko method: $s_{ij} = k_i/d_{ij}^n$; $k_i=\upsilon_{kj}/\Sigma d_{ij}^{-n}$ (d_{ij} –cation-anion distance).

With these results, it is possible to confirm the occupancy of the (GaSi)(3) sites by some cations and their correlation, to suppose a presence of cation vacancies in La and Ga(1) sites, to prove a distribution of the Ta and Nb ions into two sites (Ga(1) and (GaSi)(3)) and one site (Ga(1)), respectively.

Keywords: langasite, point defects, bond valence method

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Synthesis, Structure and Photocatalysis in $LiBi_4Ta_3O_{14}$ and $LiBi_4Nb_3O_{14}$

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The application of photocatalytic materials in wastewater treatment, control of toxic air contaminants and remediation of hazardous wastes has been of interest. Several materials like TiO_2, pyrochlores and bismuth tantalates have been extensively studied. In search of novel structural types with enhanced photo-catalytic activities, a series of new compounds, $LiBi_4Ta_3O_{14}$ and $LiBi_4Nb_3O_{14}$ in the Li_2O-Bi_2O_3-$(Nb/Ta)_2O_5$ system have been isolated for the first time in the hitherto unknown lithium bismuth niobates and tantalates. Both the compounds crystallize in the monoclinic space group, C2/c with a = 13.115(2) Å, b = 7.583(1) Å, c = 12.226(2) Å, β = 101.477(3)°, V = 1182.6(5) $Å^3$ and Z = 4; a = 13.035(3) Å, b = 7.647(2) Å, c = 12.217(3) Å, β = 101.512(4)°, V = 1193.4(5) $Å^3$ and Z = 4 for $LiBi_4Ta_3O_{14}$ and $LiBi_4Nb_3O_{14}$ respectively. The structures were solved by direct methods and refined to R of 0.057 and 0.078. The crystal structure consists of layers of $[Bi_2O_2]^{2+}$ units separated by layers of LiO_4 tetrahedra and $(Nb/Ta)O_6$ octahedra hence depicting a new structural type.

The UV-Visible diffuse reflectance spectra suggest a band gap of 3.4eV and 3.2eV for $LiBi_4Ta_3O_{14}$ and $LiBi_4Nb_3O_{14}$ respectively. Photo-catalytic degradation of a wide range of dyes was studied.

Keywords: crystal structures, photocatalysis, dyes

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Peculiarities of the Electronic Structure and Dynamics in the Nanosystems

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From the experimental results with Electron Spin Resonance in combination with other methods, numerous special complexes of odd electrons in many different materials and biomedical nanosystems and the concerning unique effects have been revealed. The behaviour of these complexes shows some unusual characteristics very distinct from the ones in the normal crystalline systems. It is especially notable that these new effects stand in close connection with the fundamental properties of the materials such as the conformation, the conductivity, the biomedical activity.

Over a long period of time we have carefully persued these phenomena and come to the conclusion that they only can be adequately explained through a new consideration on the ground of the Structure and Dynamics of the Quasi-Free Electrons in the Short-Range Order of the nanosystems. On the basis of this elaborated model there is the possibility of a profound interpreting the molecular electronic mechanisms of the particular features and technological factors of the materials and biomedical nanosystems.

As illustration examples, the effect of strong crystal field, the effect of sudden change of the conductivity, the effect of radiation emission in some materials and biomedical systems, the molecular electronic mechanism of the toxicity of Dioxin, the superconducting nanomechanism in YBCO compounds, and other phenomena are briefly exposed and discussed.

Keywords: structure and dynamics in nanosystems, electron dynamics in nanostructures, electron dynamics in nanosystems

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High-temperature Structural Disorder in α-Quartz-Type Piezoelectric Materials

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Piezoelectric materials are used at high temperature in important technological applications such as microbalances, pressure sensors and field-test viscometers. At room temperature in the α-quartz group of materials, the piezoelectric coupling coefficient can be related to the structural distortion with respect to the β-quartz structure type. Piezoelectric properties of α-quartz resonators, however, begin to degrade well below the α-β phase transition temperature at 846 K. In order to identify new higher performance materials, it is essential to develop structure-property relationships *in situ* at high temperature.

Quartz and the promising homeotypic material $GaPO_4$ were studied at high temperature by total neutron scattering and by piezoelectric measurements. In contrast to the results of Rietveld refinements of the average structure, reverse Monte-Carlo refinements using total neutron scattering data indicate that structural disorder in quartz significantly increases well below the α-β transition. In the case of $GaPO_4$, an increase in disorder is observed beginning above 1023 K. Piezoelectric measurements indicate that the quality factor of $GaPO_4$ resonators begins to degrade at this temperature. This degradation can be correlated to the increase in structural disorder. Gallium phosphate is thus a promising material for applications at temperatures up to 1000 K.

Keywords: structure-property relationships, quartz, high-temperature structures

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Unusual Structural Properties of $(Na,Gd,Yb)WO_4$ and $(Na,La,Ce,Er)MoO_4$

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Single crystals of general formula $(Na^{+1},R^{3+})T^{6+}O_4$ (R^{3+}=Gd,La; T^{6+}=Mo и W), doped by Yb^{3+}, Ce^{3+}, Er^{3+} meet very high interest of different scientific groups as active media for solid-state lasers.

Crystals of $(Na_{0.5}Gd_{0.5-x}Yb_x)WO_4$ with x=0.0, 0.0025, 0.0075, 0.025, 0.10) and $(Na_{0.500}La_{0.495-x}Ce_xEr_{0.005})MoO_4$ with x=0.0, 0.10, 0.125, 0.15, 0.175, 0.20) belonging to sheelite family have been grown by Czochralski technique in a different atmosphere, treated by