Crystals of langasite structure (La$_2$Ga$_5$SiO$_{14}$ - La$_3$Ga(1)Ga$_3$(2) (GaSi)$_3$(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 decagonal, octahedral, tetrahedral and trigonal-pyramidal sites, respectively.

In this work we demonstrate an analysis of the structure refinements of the langasite family compounds La$_2$Ga$_3$Ga$_5$Si$_3$O$_{14}$, La$_2$Ga$_5$(GaSi,Ge)$_3$O$_{14}$, La$_2$Ga$_3$M$_{0.4}$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: $s_{ij} = 4 \exp ([R_{ij} - d_{ij}]/b)$;
- method of Brown and Wu: $s_{ij} = (R_{ij} - d_{ij})^{-n}$

The calculation of $s_{ij}$ values for cation and anion sites was fulfilled by Pyatenko method: $s_{ij} = k_{ij}/d_{ij}^{-n}$; $k_{ij}=\gamma_{ij}/Z_{d_{ij}}^{-n}$ ($d_{ij}$ –cation-anion distance).

With these results, it is possible to confirm the occupancy of the Ga(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(3)), respectively.

Keywords: langasite, point defects, bond valence method

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 photocatalytic activities, a series of new compounds, LiBi$_4$Ta$_3$O$_{14}$ and LiBi$_4$Nb$_5$O$_{14}$ in the Li$_2$O-Bi$_2$O$_3$-(Nb/Ta)$_2$O$_5$ 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, $\beta = 101.477(3)^\circ$, $V = 1182.6(5)$ Å$^3$ and $Z = 4$; $a = 13.035(3)$ Å, $b = 7.647(2)$ Å, $c = 12.217(3)$ Å, $\beta = 101.512(4)^\circ$, $V = 1193.4(5)$ Å$^3$ and $Z = 4$ for LiBi$_4$Ta$_3$O$_{14}$ and LiBi$_4$Nb$_5$O$_{14}$ respectively. The structures were solved by direct methods and refined to $R$ of 0.025, 0.10) and (Na,La,Ce,Er)$_3$MoO$_4$ with $x=0.0$, 0.10, 0.125, 0.15, 0.175, 0.20 belonging to scheelite family have been grown by Czochralski technique in a different atmosphere, treated by

Keywords: structure, point defects, bond valence method.

The Bond Valence Model and Point Defects in Langasite Family

The Bond Valence Model and Point Defects in Langasite Family

These complexes show 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 pursued 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 an 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

Piezoelectric Materials

Piezoelectric Materials

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 homotypic 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

Unusual Structural Properties of (Na,Gd,Yb)WO$_4$ and (Na,La,Ce,Er)MoO$_4$

Unusual Structural Properties of (Na,Gd,Yb)WO$_4$ and (Na,La,Ce,Er)MoO$_4$

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 show 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.
a different conditions and studied by X-ray diffraction. The
(Na8Ga2O3)MoO3 with \(\Delta r_{\text{MoO}}=2\times10^{-5}\) Å has the scheelite structure (sp. gr. I41/a) in contrast to the
(Na8Ga2O3)WO4 (\(\Delta r_{\text{GaO}}=0.13\) Å) and (Na8Gd2O3)Y2O3 (\(\Delta r_{\text{GaO}}=2\times10^{-1}\)
\(\Delta r_{\text{GaO}}=2\times10^{-1}\) Å) with the pseudo-tetragonal superstructure unit cell with double
parameters. The non-annealed (growth in Ar) and annealed by 1000º
for 4 days in air crystals of (Na8Gd2O3)Ce1.0Er0.05MoO3 nominal
composition have “enantimorphic” structures. The annealed
for Ar in air have the scheelite structure. A statistical distribution of oxygen on two sites of
structure of non-annealed (growth in 99%N 2+1%O2) and annealed by 700º
for 100 h in air of these crystals was found.

Keywords: scheelite, structure, properties

P.08.14.19

Lattice Parameters Measurements of YBa2Cu3O7-
Superconductors Prepared under Various Forming Pressures

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The effect of pressure on the critical temperature \(T_c\) is studied for
YBa2Cu3O7 compounds prepared under various forming pressures.
A systematic decrease in lattice parameters is observed with forming
pressure. Resistivity measurements show an increase of the onset
for 100 h in air of these crystals was found.

Keywords: superslattice, structure, parameters

P.08.14.20

On a New Wave Type Generated in Deforming Metal Crystals
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Quasi-static deformation was studied on tensile fcc, bcc and hcp
single crystals by holographic technique. It has been found that slow
wave processes are generated in the deforming material. These
involve concerted motion and temporal evolution of local flow nuclei
whose nature is defined by micro-scale self-organization mechanisms.

The wave pattern type is determined for a given flow stage by
work hardening law \(\theta(\varepsilon)\), where \(\theta=G\cdot d\varepsilon/\varepsilon\) is the work hardening
coefficient; \(G\), the shear modulus; \(\varepsilon\), the plastic flow stress and \(\varepsilon\), the
deformation. The waves are characterized by wavelengths \(552<\lambda<1.8\)
propagation rate \(10^{-9}<v<10^{-1}\) m/s and frequency \(10^{-3}<\omega<10^{2}\) Hz. The
waves are found to exhibit the following regular features: wave rate
\(v=\varepsilon/\theta\), where \(\varepsilon=\varepsilon_{\text{constr}}=10^8\) m/s; quadratic dispersion law \(\omega(k)=1+k^2\)
and a concurrent decreases in the entropy of material by wave
generation \(\Delta S<0\).

These can be likened to quasi-particles whose mass as calculated from the de Broglie equation for all the monocrystals tested
\(m=n/1.5\mu\) and dimensionless mass \(\mu=m/\mu_0\) (\(A\) is the respective metal’s atomic mass) are found to grow with the number of electrons
\(n\) per metal unit cell as \(\mu\propto n\times k n\).

Thus it is confirmed that by plastic flow slow waves would be
generated spontaneously in a single metallic crystal, which is regarded as
a complex thermodynamically open system. The nature of these
wave processes and their role on plastic deformation are discussed.

Keywords: plasticity, wavelength, entropy

P.08.14.21

Structure and Magnetic Properties of 3-substituted-5-(2-pyridyl)
Pyrazole Metal(II) Complexes

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Five substituted pyridyl-pyrazole metal(II) complexes, [Fe(Hpp-
Buty)(OH2)X3], \(X^2\text{ClO}_4\) (I), \(X^2\text{ClO}_4\) (II), [Co(Hpp-Buty)(OH2)X3] (3), cis-
[Fe(Hpp-phen)(NCS)2] (4) and trans-[Fe(Hpp-phen)(NCS)2] (5), were synthesized. Molecular and crystal structures of these complexes were investigated by single crystal structure analysis. The comparison in molecular structures between these complexes will be presented. The magnetic properties were studied by SQUID magnetometer.

Complex (I) and (2), with t-Butyl substituted group, are spin-
crossover compounds. Complex (I) is a gradual but completed spin
transition from RT to 200K. The Fe L2,3-edge of iron(II) of (I) and (2)
absorption spectroscopy are studied using synchrotron radiation. The apparent change due to HS-LS transition will be
presented in coordination geometry around Fe and in Fe core electron excitation. However, compound (4) and (5), with substituted phenyl group, show no spin transition phenomenon within the temperature range studied. The relationship between structure and magnetic properties will be discussed.

Keywords: structure-magnetism relationships, spin crossover, magnetism

P.08.14.22

X-ray Absorption Studies of Fe-btr Spin Crossover Complexes
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The aim of this work is to take the advantage of the X-ray absorption spectroscopy to get insight into the evolution of electronic configuration in HS and LS states of the specific absorption atoms at various temperatures and also in the LIESST state. Three Fe spin
crossover complexes, (1) Fe(btr)(NCS)2H2O (11) (2) Fe(btr)(ClO4)2
and a Co doped Fe2O3(btr)(NCS)2H2O (3) were chosen to be studied. With temperature changing 1 shows an abrupt spin transition with a hysteresis of 25K (T1/2 = 119.8K) and T1/2 = 145.1K) while 2 was found to behave as a two-step spin crossover complex.

K-edge absorption spectra of 1 and 3 were collected in both RT
and 16K (LS) and also after irradiating by a laser light of 532
nm. The existence of the HS-2 after irradiation in both 1 and 3 is
verified by Fe K-edge spectra. However, spin transition only occurs at Fe site not at Co site, though they should be situated on the same site.

Fe L-edge spectra of 2 illustrate a two-step spin transition; one is
abrupt and the other one is gradual, which is consistent with the
results reported earlier.


Keywords: spin-crossover, X-ray absorption, Fe(II) complexes

P.08.14.23

Change of Structure and Properties of System WC-Ti at
Mechanical Activation

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Tungsten carbide is one of the most interesting representatives of carbides transition of metals of maximum groups, which can have as cubic, and hexagonal crystallographic modification. In particular, cubic WC with structure as NaCl has rather wide area homogeneity on carbon and has high temperature melting, hardness and durability, and also propensity to formation double carbides with transitive 3d-metals. The data about peculiarities of the chemical bonding and changes in thin electronic structure of the cubic WC at partial replacement of