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Switching from Negative to Positive Nonlinear Absorption in Sn Doped GaSe Crystal. Ayhan Elmali[a], Mustafa Yüksek[a], Mevlüt Karabulut[b], G. M. Mamedov[b]. [a]*Department of Engineering Physics, Faculty of Engineering, Ankara University, 06100 Beşevler, Ankara, Turkey.* [b]*Department of Physics, Kafkas University, 36100 Kars, Turkey.*
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GaSe is one of the promising nonlinear crystals for middle-infrared frequency conversion, since GaSe layered crystals have low absorption coefficients in broad optical wavelengths, from near to far-infrared region (0.65- 18 μm), and they are transparent through this region [5-6]. The structure of GaSe is characterized by a strong anisotropy in the chemical bonding. Each covalently bonded layer consists of four monoatomic sheets in the order Se – Ga – Ga – Se [1,7]. The single layer is hexagonal and the c-axis is perpendicular to the layer plane. The layers are bounded together by weak van der Waals forces. In spite of its many attractive features, GaSe crystal is difficult to be cut and polished along some arbitrarily chosen directions while further improvement in the optical and mechanical properties of GaSe crystal is highly desirable for laser applications. The doping of GaSe crystal seems to be the optimal method to improve its optical and other physical properties. GaSe crystals can be both *p*- or *n*-type semiconductors, depending on growth conditions and dopant atoms.
In this study, Sn doped GaSe crystals were grown using conventional Bridgman method from a stoichiometric mixture of high purity Ga (99.9999%) and Se (99.999%) in evacuated quartz ampoules (10^{-4} Torr) whose inner walls were coated with graphite [24]. Sn doping was done by adding the 0.5 at% Sn to initial batch composition. The UV-Vis absorption spectra of the Sn doped GaSe crystal was recorded using a scanning spectrophotometer (Shimadzu UV-1800), and the bandgap of crystal determined as ~2 eV, with help of spectra. The nonlinear optical absorption of 0.5 at% Sn doped GaSe crystal was examined by open-aperture Z-scan method. Z-scan experiments were carried out with nano- and picosecond laser sources. When Z-scan experiments of GaSe crystal which have been carried out at 1064 nm wavelength exhibited two photon absorption (TPA) [3,8,9], for the first time, we observed a switching from negative nonlinear absorption (saturable absorption, SA) to positive nonlinear absorption (two photon absorption, TPA) in Sn doped GaSe crystal by increasing laser intensity.

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Keywords: nonlinear absorption; z-scan; Sn doped GaSe crystal

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Low Temperature Crystal Structure of $Li_2B_4O_7$. Anatoliy Senyshyn[a], Yaroslav Burak[b], Volodymyr Adamiv[b], Hartmut Fuess[a]. [a]*Institute of Material Science, Darmstadt University of Technology, Darmstadt, Germany.* [b]*Institute of Physical Optics, Lviv, Ukraine.*
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The crystal structure of lithium tetraborate $Li_2B_4O_7$ is known for a long time since the publication of Krogh-Moe [1]. Its structure at room temperature is tetragonal with the space group $I4_1cd$ (point group 4*mm*) and with the polar axis along the crystallographic *c*-direction. The crystal structure is formed by a boron-oxygen network throughout the crystal with metallic atoms in the interstices. The anion $B_4O_7^{2-}$ - the basic subunit of this net consists of four boron atoms, where two of them are tetrahedrally and two other are triangularly linked to oxygens**.** To our knowledge $Li_2B_4O_7$ type of structure as well as the existence of an isolated B_4O_7 unit are unique and they do not occur in nature for any materials other than $Li_2B_4O_7$.
Recently, lithium tetraborate has attracted considerable interest in nonlinear optics especially as an element of surface acoustic wave (SAW) devices, which stimulated deeper studies of its properties, especially at non-ambient conditions.
In the literature there is plenty of controversial data on $Li_2B_4O_7$ reporting either no anomalies or anomalous behaviour in the temperature range between 80 and 250 K, 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 dependencies of lattice parameters and bond lengths [4, 5], large number of phase transitions [6, 7], anomalies in sound velocities and Raman spectra [8]. The existing discrepancies between the experimental results of different authors lead us to perform systematic studies of lithium tetraborate crystals.
Due to relatively poor sensitivity of X-ray diffraction to $Li_2B_4O_7$ constituents structural studies were performed using elastic neutron scattering. For this purpose the $Li_2{}^{11}B_4O_7$ crystal (99.6% ^{11}B) has been grown using Czochralski technique. Powder diffraction examinations unambiguously indicated stability of $Li_2B_4O_7$ structure type in the temperature range 3-300 K. However, obvious anomalies in thermal dependencies of lattice parameters in *c*-direction (fully consisting with performed dilatometric studies), bond lengths and displacement parameters occurred. Crystal structure considerations yield the presence of discontinuous Li chains in *c*-direction of $Li_2B_4O_7$ structure, whilst extended bond length analysis revealed relatively high stability of B_4O_7 complex anion, thus enabling treatment of $Li_2B_4O_7$ as a diatomic solid consisting of Li^{1+} and $B_4O_7^{2-}$, as well as correlated motion of Li and B_4O_7. In the current contribution we report on complex studies of lithium tetraborate doped with ^{11}B in the broad temperature range 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

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Spectroscopic Study and Third-order Nonlinear Optical Behavior of N-(2-Hydroxy-4-methoxybenzylidene)-3-nitroaniline.

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N-(2-hydroxy-4-methoxybenzylidene)-3-nitroaniline (1) has been synthesized and characterized by X-ray diffraction analysis, FTIR and 1H NMR spectroscopy. The maximum one-photon absorption (OPA) wavelengths recorded by quantum mechanical computations using a configuration interaction (CI) method are estimated in the UV region to be shorter than 450 nm, showing good optical transparency to the visible light. We have computed both dispersion-free (static) and also frequency-dependent (dynamic) linear polarizabilities and second hyperpolarizabilities by using the time-dependent Hartree-Fock (TDHF) method to provide an insight into the microscopic third-order nonlinear optical (NLO) behavior of the title compound. The ab initio calculation results with non-zero values on (hyper) polarizabilities indicate that the synthesized molecule might possess microscopic third order NLO phenomena.

Keywords: hyperpolarizability; nonlinear optical behavior; spectroscopy

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The Peculiarities of Angular Width of Diffracted X-Rays at The Presence of Temperature Gradient.

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As it is known ref. [1] under the external influences (temperature gradient, ultrasound excitations) in the result of X-ray reflection from (10-11) plain sets of SiO2 single crystal in Laue geometry at certain values of influences it is observed the full pumping from the transmitting direction into the reflection direction.

To study the noted phenomena and to discover the peculiarities numerous theoretical and experimental works by different authors have been done. The angular width and energetic dispersions of full pumped X-rays have been studied. Particularly in ref. [2] it is shown that the angular width of the beam reflected from the transmitting direction into the reflected direction is strongly depends on the width of the pumping single crystal.

The submitted investigation is linked to the study of the dependence of the full pumped monochromatic X-ray angular width from the transmitting direction depending on the distance between source-pumping single crystal (sample).

To carry out the noted investigations it has been used MoK monochromatic radiation obtained of the Brag reflection from SiO_2 single crystal (10-11) plain sets. As a sample it has been selected the parallel samples of SiO_2 single crystal of different width in order to obtain to observe reflections from plain sets in Laue geometry.

To study the influence of X-ray full pumping angular width from the transmitting beam from the source-sample distance the sample was placed on distances of L_1=27cm and L_2=110cm and the section topograms of the transmitting beam have been obtained in the full pumping mode.

The investigations of the section topograms of the transmitting beam from the samples of L_1 and L_2 distances show that the X-ray angular width full pumped from the transmitting beam is decreased with increasing of the source-sample distance.

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Effect of Cobalt Doping on the Gahnite Structure.

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Zinc aluminate ($ZnAl_2O_4$) is known by mineral name gahnite. It is a semiconductor with a wide energy band gap of ~3.8 eV, transparent for wavelengths greater than 320 nm which makes it useful in ultraviolet photoelectronic devices [1,2]. When doped with Co^{2+}, Mn^{3+} or rare-earth cations, it exhibits luminescence and can be used as a cathodoluminescent material [3]. Gahnite is cubic with the normal spinel structure, space group *Fd*-3*m*. Powder