VIBRATIONAL SPECTRA OF TRIGLICINE SULFATE

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Abstract

The polydomain structure of ferroelectric materials, the mobility of their orientation, the possibility of fixing it, ensures the existence of ways to control their macropolarization. Polydomain materials of this type predetermine the defectiveness of their crystal structure. These are, perhaps, orientation defects, whose existence for molecular crystals is very likely at room temperature

The stability of the properties of the ferroelectric phase of these materials also depends on the properties of elementary excitations: phonons and internal vibrations of molecular ions. Since the interpretation of the Raman spectra of triglycine sulfate (TGS) in the literature does not reflect the defectiveness of the crystal structure, and it has a significant effect on its properties, to determine the relationship between the macro and microproperties of such materials, it is necessary to determine the effect of defectiveness on their vibrational spectra. Therefore, the Raman spectra are recorded from the splitting of plates of triglycine sulfate monocrystals obtained by splitting. The registration of the Raman spectra was carried out with the Confotec NR500 microscope. For the excitation of Raman scattering, laser radiation with generation wavelengths of 532 and 632.8 nm was used. The power of the radiation focused on the sample was 3 mW. The optical signal was recorded from a site approximately 0.5 μm in diameter from the depth of the sample at a distance of 4 μm from the surface of the single crystal. All recorded spectra for the separation of overlapping bands were processed using the software package Origin 8.1. From the clarification of the existing interpretation of the Raman spectra, the presence of position-group splitting of the bands of degenerate sulphate-ion oscillations is determined, the absence of dynamic resonant interaction of the vibrations of ions of a primitive crystalline cell. The existing idea of the location of chromium ions implanted in the TGS was confirmed. Changes in the phonon bands of TGS as a result of doping: an increase in the area of higher-frequency bands, an increase in their half-width, and shifts to the low-frequency region are explained by a change in the distribution and properties of the electron density of the TGS structure bonds.

The simulation of the bands of non-degenerate vibrations by the sum of two Lorentz contours is explained by the presence of orientational structural defectiveness, and the change in the area of model contours in the spectra of doped samples is due to an increase in the unipolar properties of the samples: the dominance of one orientation of the domains. The appearance of oscillation bands in the region of overtones and composite oscillations for doped TGS samples is explained by the presence of other types of defects that fix the unipolar structure of macro samples. The increase in the relative intensity, half-width, and the decrease in the frequencies of the maxima of the phonon bands in doped samples probably determine the change in the conditions for the transformation of the ferroelectric phase into the paraphase of TGS.

Keywords — defects of the crystal structure, ferroelectric materials, Lorentz contours, Raman spectra

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Khamchukov Yu.D. graduated from the Belarusian state university, an optics and spectroscopy in physical faculty. It has degree of the candidate of physical and mathematical sciences (PhD) in a chemical physics (N.N.Semenov Institute of Chemical Physics, Moscow, 1990) He was Head Laboratory Physical methods of research, Senior Researcher laboratory informational technologies and non-linear materials. He has published more than 56 papers in reputed journals, coauthor of three books monographs.

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