Nanocomposites and nanomaterials

Surface phonon studies in Cu_6PS_5X (X=I, Br) superionic nanocomposites

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Cu_6PS_5X (X=I, Br) crystals belong to the family of compounds with argyrodite structure and are characterized by high ionic conductivity. Now it is important to obtain nanostructures on the base of superionic conductors what would enable one to vary their physical properties and spheres of application. Therefore, the present work is aimed at the investigation of specific features of Raman scattering spectra of composites based on Cu_6PS_5X (X=I, Br) nanocrystals.

Cu_6PS_5X (X=I, Br) nanocrystals were obtained by ball milling, their average size was estimated from X-ray diffraction measurements. Nanocomposites were obtained by mixing with solution of such polymers as polyvinylchloride, polytrifluorethylene, copolymer of styrene with maleic anhydride (CSMA), plastificators and stabilizing agents. Structural studies by scanning electron microscopy have shown that part of nanocrystals are uniformly distributed in the polymer matrix while the rest of them are conglomerated in rather great units which are more by an order of magnitude higher than the average grain size.

In polymer nanocomposites an essential growth of Rayleigh scattering is observed, the Raman spectra contain only the A_1 band, while the one formed by the superposition of E and F_2 symmetry modes, is either revealed wery weakly, or not revealed at all. The evolution of the Raman spectra is explained predominantly by surface phonon modes whose contribution to the Raman spectrum increases due to the higher surface-to-volume ratio.

The contribution of surface phonon modes to the experimentally measured Raman band was estimated. The introduction of nanocrystals into the polymer matrices leads to an increase of the frequencies of the “bulk” and surface phonons while their halfwidths depend on the type of the polymer. The surface-to-bulk phonon integrated intensity ratio strongly varies with the type of the polymer matrix, average grain size and concentration of nanocrystals. It is shown that CSMA is a promising material as the polymer matrix for the formation of nanocomposites creation, the increase of the concentration of the nanocrystals and the decrease of their average grain size determine the increase of surface-to-bulk phonon integrated intensity ratio.