Ab initio calculation of dynamic and elastic properties of $Sn_2P_2S_6$ ferroelectric crystals

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Chalcogenide semiconductor ferroelectrics of the $Sn_2P_2S_6$ family show a variety of important physical properties that makes them the objects of intense research, both for practical applications and fundamental studies.

In this work, dynamic and elastic properties of $Sn_2P_2S_6$ crystals were calculated from first principles. We performed our calculations using the plane wave density functional theory (DFT), program ABINIT [1], within local density approximation (LDA). All calculation were performed by using the resources of the cluster at the V.M. Glushkov Institute of Cybernetics of the National Academy of Science of Ukraine. The Troullier-Martins norm-conserving pseudopotential was used with a plane wave kinetic energy cutoff of 30 Ha. Brillouin zone integration for charge density and total energy is performed with a 6x6x6 Monkhorst-Pack grid. We optimized the lattice geometry by the Broyden-Fletcher-Goldfarb-Shanno method and obtained values, which is only slightly different (<2%) from the experimental values at atmospheric pressure. Phonon spectra and elastic properties for $Sn_2P_2S_6$ crystals were calculated by using the density functional perturbation theory (DFPT).

Here we present *ab initio* calculation results of phonon spectra, the complete matrices of elastic stiffness and compliance coefficients as well as piezoelectric constants for ferroelectric state of $Sn_2P_2S_6$ crystals based on the DFPT method. Calculated frequencies and phonon modes symmetry in the center of the Brillouin zone are in good agreements with available theoretical and experimental data obtained from Raman and infrared spectra. From the compliance tensor Young's modulus as a function of direction were calculated, that are in good agreement with results of our experimental nanoindentation study. Elastic stiffness and compliance tensors are compared with existing experimental results for $Sn_2P_2S_6$ crystals at room temperature.

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References

[1] Gonze et al: Firstprinciples computation of material properties: the ABINIT software project. *Comput. Mater. Sci.*, 25(3): 478-492, 2002.