Amino acid 2-aminopropanoic $CH_3CH(NH_2)COOH$ crystals: Materials for photo- and acoustoinduced optoelectronic applications

Abstract

Photo-induced treatment of L-alanine single crystals grown by slow evaporation method at an ambient temperature was performed using a 25 ps Nd:YAG pulsed laser in the presence of an external acoustic filed. The changes of the absorption were studied for the wavelength 265 nm near the energy band gap edge at acoustical power density varying within 4-6 W/cm^2. The observed absorption changes indicate that the external optical electric field strengths and acoustical power densities may be efficient parameters for the characterization of photo-optical and acousto-optical treatment of the samples. From the X-ray diffraction data we have optimized the atomic positions assuming that force on the atoms is around 1 mRy/au. These are used to calculate the electronic structure and the chemical bonding for the amino acid L-alanine single crystals. The calculated electronic band structure and densities of states confirms the experimental results that this compound possesses a relatively large energy band gap. The upper valence band has its maximum at the Z point of the Brillouin zone while the conduction band minimum is located at Γ point in the zone center, resulting in an indirect energy band gap. The electronic energy gap is equal to 4.19 eV within a framework of the used local density approximation and 4.54 eV with the Engel-Vosko generalized gradient approximation as the exchange correlation potential. This is in an agreement with our experimentally measured energy band gap ~4.67 eV. The existence of O-p character in the upper valence band has a significant consequence for the optical band gap. From our calculated electron charge density distribution, we obtain a space electron charge density distribution in the average unit cell of the crystal. The chemical bonding features of L-alanine amino acid were analyzed.