Multiphonon Absorption as a Test of Lattice Vibration Model: ZnO Case

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The lattice vibrations dispersion models are usually compared with experimental data of phonon energies measured along high symmetry directions in Brillouin zone or of one-phonon density of states (DOS), both determined by an inelastic scattering of neutrons or X-rays (INS and IXS, respectively). However, there exist also other demanding test – comparison of theoretical two-phonon DOS with absorption curves obtained in the infrared.

The wurtzite-type zinc oxide (ZnO) is a very promising candidate for any potential applications in transparent electronics and UV optoelectronic. Since phonon interaction with the free carriers has a great impact on optoelectronic devices performance, detailed knowledge of the vibrational properties of ZnO is essential. The phonon dispersion along selected, high-symmetry directions in the ZnO Brillouin zone was calculated using various models and also was determined by INS (see [1, 2] and references). However, the insights concerning the multiphonon processes taking part in the middle-infrared (MIR) part of spectrum are still very limited.

The main goal of this work is the attempt to understand the optical properties of ZnO in MIR region. The transmission measurements were performed with the use of FTIR Bruker 113v spectrometer at temperatures from 15 K to 295 K. Several absorption bands were observed and identified for the wavenumbers ranging from 650 cm^{-1} to 1200 cm^{-1}. The energy and temperature dependence of absorption suggested that the two phonon processes could be responsible for the structure. Therefore, the spectra were compared with two-phonon DOS calculated in [1]. Obviously, this theoretical model does not adequately take into account the phonons from selected optic branches between Γ and A points (along the [00α] direction). The GaN is very similar to ZnO semiconducting compound that is also crystallizing in the wurtzite structure. Contrary to the ZnO case, there is a good agreement when one analyze the analogous comparison in GaN [3].

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