Electro-optic Effects of Borate Crystals Studied by First Principles Method

Li RK[1,2,*]
*lead presenter: rkli@mail.ipc.ac.cn
1 Beijing Centre for Crystal Research and Development, Key Laboratory of Functional Crystals and Laser Technology, Technical Institute of Physics and Chemistry, Chinese Academy of Sciences. Beijing 100190, China
2 Center of Materials Science and Optoelectronics Engineering, University of Chinese Academy of Sciences. Beijing 100049, China.

Electro-optic (EO) crystals play vital roles in long range tele-communication, sensing, laser modulation and quantum technologies. Fully characterization of the EO properties experimentally needs to grow high quality single crystal at least in center meter sizes and may take years of efforts. High accuracy first principles theoretical methods can help to provide a full set of material properties and to evaluate whether a newly found crystal is worth to pursuing further development when only structure determination from sub-millimeter crystallites is available.

The electro-optic effect has three main origins: the second order electronic polarizability equivalent to the nonlinear optical (NLO) effect, the vibrational contributions and the lattice deformation under electric filed. Recent development of the first principles quantum chemical calculation methods lead to the possibility to obtain each of the three contributions reliably. I will present their applications to the borate crystals including β-BaB_2O_4 (BBO), $Li_2B_4O_7$ (LB4), plus newly developed $KB_6O_{10}Br$ (KBB), $KB_6O_{10}Cl$ (KBC) and other borate crystals.

These studies not only present the complete sets of material characteristics including dielectric and elastic constants, piezo-electric and NLO coefficients and elastic-optic or AO coefficients but also can provide each parts of the contribution origins. For example, it is found that for the BBO crystal, the vibrational contributions to the major EO coefficient γ_{11} dominates with ratio of about 60:40 to the electronic contributions, whereas for LB4 crystal both electronic and vibrational contributions are insignificant and the dominate contributions are found to come from the lattice deformation induced by the applied electric field-a cooperative piezo-electric and acoustic-optic effect. Further analysis of the results may lead to the proposals of developing new practical EO or AO materials for applications in laser and communication systems.