Origin of large electro-optic response in ferroelectrics

A. A. Demkov,[1] I. Kim,[1] T. Paolettta,[1] and S. Apte[1]

[1] *Department of Physics, The University of Texas at Austin, Austin, TX 78712, USA*

Integrated silicon photonics experiences a revolution [1]. The key element of this technology is an optical modulator (OM) playing a role similar to that of a usual transistor. OMs based on a phase shifter using a linear electro-optic (EO) effect are an attractive option for building ultra-compact, fast and low power OMs [2]. Linear EO effect can be only observed in non-centrosymmetric materials, such as ferroelectrics, which started a search for ferroelectrics that can be integrated with Si and maintain a strong EO effect in thin films [3]. Ab initio calculations became an indispensable tool in this search [4].

We will discuss our recent progress in understanding the microscopic mechanism behind the EO response in three ferroelectrics successfully integrated on Si: $BaTiO_3$ (BTO), $LiNbO_3$ (LN) and $Sr_xBa_{1-x}Nb_2O_6$ (SBN). There are three parts to the EO effect in a ferroelectric, they are ionic, piezo and electronic contributions [5,6]. In different materials, different components of the EO tensor are dominated by different contributions. This has implications for the device design, depending on the temperature and frequency range. For example, optical quantum computing occurs at cryotemperatures (when optical phonons are frozen out), and thus has rely on the electronic and piezo contributions. On the other hand, at high RF frequencies, only the ionic and electronic contributions survive. On the fundamental level, our results support the notion that P4mm BTO is a dynamic average of lower symmetry Cm structures (Fig. 1). We also discover that in SBN, surprisingly the major contribution to the EO effect comes from high frequency optical phonons (Fig. 2). And in LN, ferroelectricity and the EO response are essentially decoupled.

The work is supported by the AFOSR under Award No FA9550-18-1-0053.

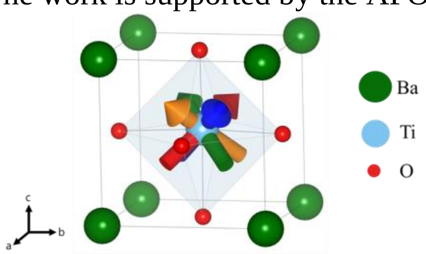

Figure 1. Ball and stick model of [111]-displacement type monoclinic *Cm* BTO, averaged in the tetragonal *P4mm* BTO.

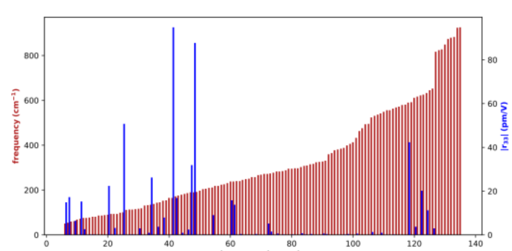

Figure 2. Phonon mode-decomposed electro-optic tensor component r_{33} in $Sr_xBa_{1-x}Nb_2O_6$. Plotted along with the mode frequencies.

[1] G. T. Reed, G. Mashanovich, F. Y. Gardes, and D. J. Thomson, Nat. Photon. **4**, 518 (2010).
[2] A. Rahim, A. Hermans, B. Wohlfeil, et al., Adv. Photonics **3**, 024003 (2021).
[3] A. A. Demkov, C. Bajaj, J. G. Ekerdt, C. J. Palmström, and S. J. B. Yoo, J. Appl. Phys. **130**, 070907 (2021); A. A. Demkov and A. B. Posadas, MRS Bulletin **47**, 485 (2022).
[4] A. K. Hamze, M. Reynaud, J. Geler-Kremer, and A. A. Demkov, Npj Comput. Mater. **6**, 130 (2020).
[5] T. Paoletta and A. A. Demkov, Phys. Rev. B **103**, 014303 (2021).
[6] I. Kim, T. Paoletta and A. A. Demkov, Phys. Rev. B **108**, 115201 520 (2023).

+ Author for correspondence: demkov@physics.utexas.edu