Pockels Effect in Single-Domain a-Oriented BaTiO₃ on vicinal Si (001)

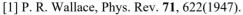
<u>Jason P Tischler</u>¹, Agham B. Posadas², D. J. Smith³, Kamyar Barakati⁴, Sergei V. Kalinin⁴ and Alexander A. Demkov¹⁺

¹ Department of Physics, The University of Texas at Austin, Austin, TX 78712, USA ² La Luce Cristallina, Inc., Austin, TX 78759, USA

Silicon (Si) integrated photonics is an emerging technology developed for the communications industry with emerging applications in quantum and neuromorphic computing [2, 3]. These devices provide advantages in data transmission rates by modulating optical signals in Si waveguides. However, Si by itself is a poor modulator of light as it has no intrinsic electro-optic effect. Barium titanate (BTO) demonstrates a large electro-optic response known as the Pockels effect due to it being a non-centrosymmetric medium. The Pockels effect is the change in refractive index of the material due to an external electric field. This response is described by a tensor and the largest component for BTO is r₄₂, which is reported to be 1,300 pm/V in bulk [4], and 923 pm/V in thin films [5,6]. To access this large value in a waveguide phase-shifter, one uses thin BTO films with the so-called a-axis orientation [7]. When BTO is epitaxially grown on Si (001) in the a-axis orientation, meaning the long c-axis is in-plane, two orthogonal in-plane crystallographic domains form. This creates problems in the form of Rayleigh scattering at the domain boundaries and not being able to fully utilize the high r₄₂ coefficient.

In this talk we demonstrate the use of a 4° miscut vicinal Si (001) substrate to stabilize a single in-plane orientation growth of a-axis BTO on strontium titanate (STO) buffered Si by

molecular beam epitaxy (MBE). In this study, utilizing x-ray diffraction (XRD) techniques and scanning transmission electron microscopy (STEM), we detail the crystalline microstructure confirming a single in-plane BTO orientation; The ferroelectric domain structure is characterized using piezo-force microscopy (PFM) and the electro-optic response is probed via transmission geometry Pockels measurements.



^[2] S. Shekhar et al., Nat Commun 15, 751 (2024).

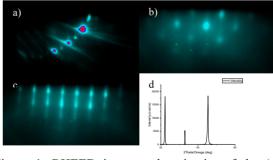


Figure 1. RHEED images taken in-situ of the (a) substrate after Sr desorption of SiO2, (b) 12uc STO buffer layer, and (c) 250uc BTO epilayer. (d) XRD $2\theta/\omega$ scan from 20° to 60° showing the 001 and 002 BTO peak

Department of Physics, Arizona State University, Tempe, AZ 85287, USA
Department of Materials Science and Engineering, University of Tennessee, Knoxville, TN 37920, USA

^[3] D. Brunner *et al.*, Journal of Applied Physics **124**, (2018).

^[4] M. Zgonik et al., Phys. Rev. B 50, 5941 (1994).

^[5] S. Abel et al., Nature Mater 18, 42 (2019).

^[6] I. Kim, T. Paoletta, and A. A. Demkov, Phys. Rev. B 108, 115201 (2023).

^[7] M. Reynaud et al., Phys. Rev. Materials 6, 095201 (2022).

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