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Anisotropic Optical Behavior of Ferroelectric Bismuth Titanate: A Comparison of Experiment and Theory AMRITENDU ROY, Mat. and Met. Engg., IIT Kanpur, RAJENDRA PRASAD, SUSHIL AULUCK, Physics Department, IIT Kanpur, ASHISH GARG, Mat. and Met. Engg., IIT Kanpur — Optical properties of bismuth titanate (Bi4Ti3O12 or BiT) are of technological interest as its band gap lies in the visible region. Here we compare the results of theoretical and experimental studies conducted on pure bismuth titanate single crystals. Highly oriented BiT single crystals were synthesized using flux growth method. Spectroscopic ellipsometry measurements were made between 300 to 800 nm for different sample orientations. To obtain the absorption coefficient near the band edge, optical transmission measurements were also made. The refractive index data was fitted to a two-term Sellmeier formula. We also calculated the optical constants for both ferroelectric and paraelectric phases of bismuth titanate using density functional theory as implemented in the Vienna ab-initio simulation package (VASP) in conjunction with projector augmented wave method (PAW). Our calculations show the anisotropy of the optical properties for the electric field parallel and perpendicular to the c-axis of the crystal. Our calculations are in good agreement with the experimental data.

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