Contribution ID: **272** Type: **Poster Presentation**

Structural and optical properties of natural single crystalline TiO2

Titanium dioxide (TiO2) is a promising material for applications in photocatalysis and photo-electrochemical water splitting. However, very few studies have been reported on the properties of bulk, single crystalline material. As a consequence, there is a substantial lack of understanding of some of the basic fundamental properties of this important compound, including its accepted band gap energy (3.2 eV, at room temperature) and the origin of near band edge emission (from 2.9 to 3.4 eV) sometimes reported in literature. Optical properties of semiconductor materials are intrinsically linked to their crystal structures. Therefore, a high-resolution X-ray diffractometer is employed to examine the crystalline phase, in order to link the unique luminescent properties observed for bulk single crystalline anatase TiO2 to existing knowledge of the band structure and phonon dispersion relations. The structural properties of natural single crystal anatase TiO2 is studied under different modes of measurement namely: rocking curve (ω) scans, ω - ϕ scans and θ–2θ scans. The standard θ–2θ scans show an extremely sharp diffraction peak with a full-width at half-maximum (FWHM) of ~0.025. However, the rocking curve revealed multiple peaks which is unusual of a single crystalline material. The rocking curve peak positions are also found to depend on the azimuthal angle ϕ. This study seeks to identify the primary impurities present in the natural crystals through the application of secondary ion mass spectroscopy. Additionally, it aims to ascertain whether they can be correlated with specific near band edge photoluminescence lines observed at low temperatures (~5 K).

Apply for student award at which level:

PhD

Consent on use of personal information: Abstract Submission

Yes, I ACCEPT

Primary authors: Mr MUTUBUKI, Arnold (Nelson Mandela University); Dr TALLA, Assane (Nelson Mandela University); Dr URGESSA, Zelalem (Nelson Mandela University); Prof. BOTHA, Johannes R. (Nelson Mandela University)

Presenter: Mr MUTUBUKI, Arnold (Nelson Mandela University)

Session Classification: Poster Session

Track Classification: Track A - Physics of Condensed Matter and Materials