

“Modelling the Microstructure of pp-MOCVD TiO₂ Thin Films”

Ethan Huang, PhD Candidate

PP-MOCVD thin films are polycrystalline materials that display a range of unique microstructures. It is evident that the promising photocatalytic and mechanical properties reported by various tests are attributed to the columnar faceted dendrite microstructure developed due to strong anisotropy. The interplay between thermodynamic and kinetic effects cannot be elucidated without the study of a model. I aim to leverage continuum models, atomistic models and modelling assisted characterisation to shed light on the development of the microstructures.

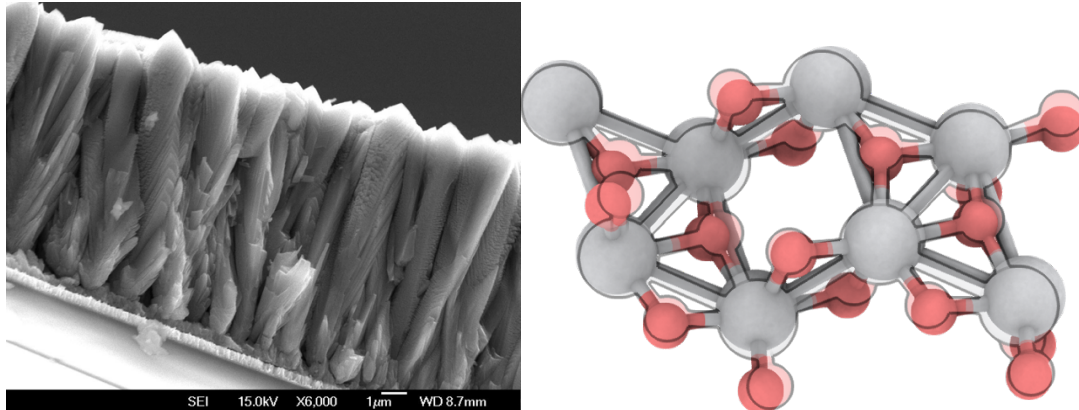


Figure 1. (left) Titania thin film grown by ppMOCVD on FTO coated glass substrate at 525 °C from liquid solution of 5 mol% TTIP in toluene and (right) anatase titania {101} (2x2) surface model showing initial and relaxed atomic positions. Titanium atoms are coloured grey and oxygen are coloured red.

Biography



Ethan joined the group in 2016 as a PhD student after obtaining his MEng in Mechanical Engineering from the University of Bristol. His master’s thesis was titled “Ultrasonic NDT of the Clifton Suspension Bridge Deck Hangers”. He is an avid and talented organist who worked briefly with the organ builder Henry Willis & Sons based in Liverpool. In his free time, he enjoys drinking tea and occasionally alcoholic drinks.

Email: yicun.huang@pg.canterbury.ac.nz