Making Titania in the Microwave: Efficient and Better for the Environment

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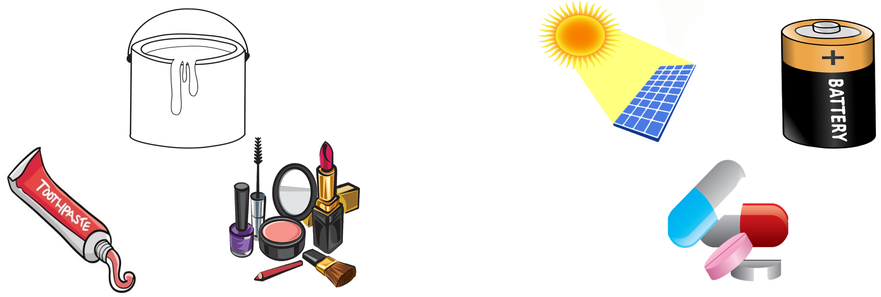
Advance Manufacturing with TiO_2

The ultimate goal is to control the structure of materials on the atomic scale. Macroscopic material properties are related to the material's atomic structure and synthesis history. Conventionally, synthesis, of ceramic oxides, is done in a furnace with the goal to reduce porosity; however, using a microwave assisted synthesis technique, we are able to achieve desirable results at lower temperatures and in less time. Microwave assisted synthesis yields an oxide with unique material properties due to the synthesis of higher crystallinity. Further investigation into these synthesis pathways is needed to better understand why higher crystallinity is achieved.

TiO2's Present and Future

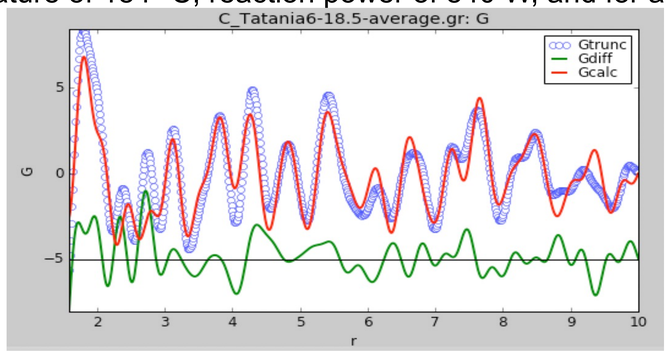
Due to desirable optical and electronic properties, and good chemical and thermal stability, TiO_2 is a safe, cheap, and attractive material for a wide variety of future applications.[3]



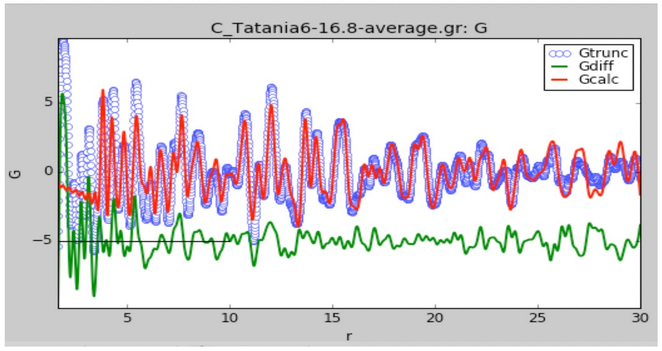
Pair Distribution Function (PDF) Analysis

Four samples of Titania were measured. Titania1 and Titania2 were synthesized at a reaction temperature of 160 °C, reaction power of 40 W, and for a reaction hold time of 60 minutes. Titania5 and Titania6 are synthesized at a reaction temperature of 184 °C, reaction power of 840 W, and for a reaction hold time of 30 minutes.[1,2]

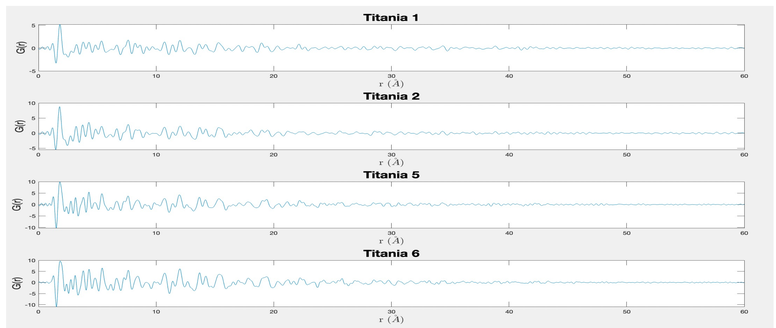
Samples are synthesized on glass slides coated with Indium-Tin-Oxide (ITO)



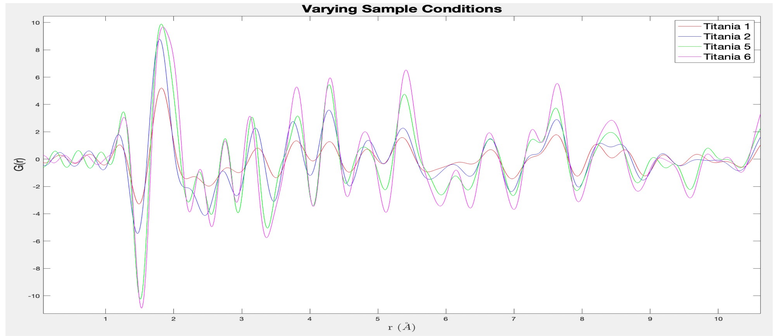
Single phase fitting with Anatase



Two phase fitting with Anatase and Rutile



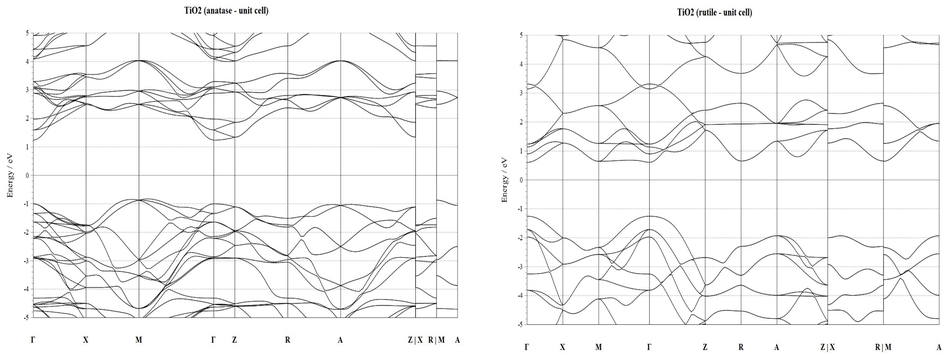
Stack plot shows how atomic distances vary with respect to synthesis conditions



Direct comparison of peak widths for all samples to illustrate how well defined the structure is

Density Functional Theory (DFT+U) Calculations

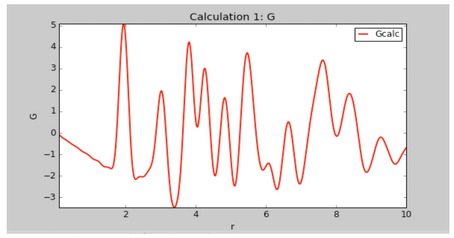
Approximated calculated band gaps using the Hubbard Factor:
Anatase: 2.08 eV
Rutile: 1.86 eV



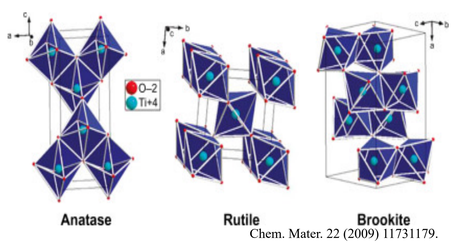
Anatase is more active than Rutile due to more charge carriers participating in surface reactions.

TiO_2 Polymorphs

All TiO_2 polymorphs consist of Titania tetrahedra. We expect the first peak in the PDF to be the same for all phases, since it models the distance between the nearest neighbors (Titanium and Oxygen).



Theoretical calculation of the Anatase Structure



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The three common Titania Polymorphs: Anatase, Rutile, and Brookite. Both Anatase and Rutile belong to the tetragonal crystal system and Brookite belongs to the orthorhombic crystal system.

Acknowledgements

The Billinge Group

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