MS003.O05

Synthonic-molecular modelling of pentaerythritol and pentaerythritol tetranitrate slip systems

Siti Fatimah Ibrahim[1], Vasuki Ramachandran[2], Kevin Roberts[2]
[1]*Food Technology Engineering Section, Taboh Naning Alor Gajah, Malaysia,* [2]*School of Chemical & Process Engineering, Leeds, United Kingdom*
E-mail: sitifatimah@unikl.edu.my

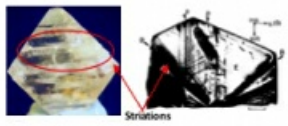
Pharmaceutical solid dosage is the most common mechanisms for drug delivery to the patient target organ. Solid dosage forms demand component particulates to blend readily by flowing well to ensure formulation uniformity. They must also be robust enough to undergo a particular manufacturing process without changing physical, chemical and mechanical properties.

A synthonic and molecular-based mechanical properties prediction model is proposed. The model has three main components. Firstly, the identification of likely dislocation Burgers vectors based on lattice geometry and dependency to line dislocation; secondly, selection of slip planes for plastic deformation using interplanar interactions, rugosity and surface energy and thirdly, characterisations of slip systems or propensity for cleavage and fracture.

Two solid forms were selected, namely pentaerythritol (PET) and pentaerythritol tetranitrate (PETN). PET and PETN are of interest because of their different mechanical properties in which when subjected to the same stress PET cleaves, but PETN slips. Additionally, PET and its derivatives are well-studied systems with experimental data available to cross check molecular computational analysis. The (001) of PET and (110) of PETN planes were characterised to have 94% and 82% of the ideal behaviour of a slip plane using the prediction model. This prediction correlates well with the observed crystals.

This study postulates the crystallographic parameters to describe the mechanical deformation are rugosity, interlock of planes, surface energy, intermolecular interactions, and dislocations. These dimensions were able to be measured using multiple molecular modelling approaches. This study, provide preliminary guidance for understanding the mechanical properties of solid forms during tabletting.

P. Halfpenny, K. Roberts, J. Sherwood (1984). Journal of Applied Crystallography. 17, 320–327



Keywords: Molecular modelling, mechanical properties, slip systems