11th World Congress on Computational Mechanics (WCCM XI)
5th European Conference on Computational Mechanics (ECCM V)
6th European Conference on Computational Fluid Dynamics (ECFD VI)
July 20 - 25, 2014, Barcelona, Spain

INTERPHASE EFFECTS ON POLYMER NANOCOMPOSITE PROCESSING: PHYSICALLY-BASED MULTISCALE MODELLING

Łukasz Figiel [1,2]

[1] Centre of Molecular and Macromolecular Studies, Polish Academy of Sciences, Sienkiewicza 112, 90-363 Łódź, Poland; lfigiel@cbmm.lodz.pl
[2] School of Engineering, University of Portsmouth, PO1 3DJ, UK; lukasz.figiel@port.ac.uk

Key Words: *Polymer-clay nanocomposites, Quasi-solid state processing, Elastoviscoplasticity, Interphase effect, Physically-based multiscale modelling.*

Polymer-clay nanocomposites offer cost-effective material solutions for physical and mechanical property improvements of thermoplastic polymers. Quasi-solid state manufacturing techniques such as injection-stretch blow moulding [1], originally developed for product forming from unfilled thermoplastic polymers, can directly be used for manufacturing nanomposite products. Additionally, those manufacturing techniques, which typically operate at temperatures near the glass transition, can also assist in further improvement of nanocomposite morphology during product forming [2]. However, their application requires careful selection of process parameters such as deformation, deformation rate and temperature. Optimum choice of those parameters can prove tedious and costly. Therefore, the development of advanced computational material models can assist experiments in finding the optimum processing window for thermoplastic polymer-clay nanocomposites to exploit fully their potential.

Modelling of large, temperature- and rate-dependent nonlinear deformations of thermoplastic nanocomposites in the temperature, strain and strain rate window typical of quasi-solid state manufacturing is complex and computationally demanding. Thus, it still remains in its infancy. Few papers have addressed this industrially important problem [3-5]. However, all the aforementioned contributions did not consider the effect of the interphase polymer region, which is now widely accepted to be present in nanocomposites.

Therefore, a finite-strain, physically-based multiscale computational model was developed in this work for predicting the morphology evolution and macroscopic response of polymer nanocomposites during semi-solid state processing [6]. The nanocomposite model consisted of three basic components: linear elastic nanoparticles, nonlinear bulk polymer and nonlinear interphase polymer. The behaviour of nanoparticles was adopted from molecular mechanics simulations, while the response of polymer matrix and polymer interphase was developed based on experiments. The nonlinear mechanical response of the interphase was described by a physically-based nonlinear stress-strain relationship with relaxation behaviour different from the bulk polymer. Relaxation characteristics and viscosity of the interphase were defined by the reference temperature correlated to the viscoelastic experimental data to capture the observed shift in the loss tangent. The model was then implemented into the finite strain, nonlinear finite element (FE) framework, and combined with the RVE concept and numerical homogenisation. The computational model was then used to assess the effects of the interphase region on the macroscopic response and morphological changes in polymer-clay nanocomposites during their semi-solid processing near the glass transition.

ACKNOWLEDGEMENTS

Financial support from the National Science Centre Poland through the OPUS programme (Grant No. 2011/01/B/ST8/06492) is gratefully acknowledged.

REFERENCES

[1] Salomeia Y.M., Menary G.H., Armstrong C.G. Experimental Investigation of Stretch Blow Molding, Part 1: Instrumentation in an Industrial Environment, *Advances in Polymer Technology* 32, S1: E771-E783, 2013.

[2] Y. Shen, E. Harkin-Jones, P. Hornsby, T. McNally, R. Abu-Zurayk. The effect of temperature and strain rate on the deformation behaviour, structure development and properties of biaxially stretched PET-clay nanocomposites. *Composites Science and Technology* 71: 758-764, 2011.

[3] Spencer P.E., Spares R., Sweeney J., Coates P. Modelling the large strain solid phase deformation behaviour of polymer nanoclay composites. *Mechanics of Time-Dependent Materials* 12: 313-327, 2008.

[4] Figiel Ł., Dunne F.P.E., Buckley C.P. Computational modelling of large deformations in layered-silicate/PET nanocomposites near the glass transition. *Modelling and Simulation in Materials Science and Engineering* 18: 015001 (21pp), 2010.

[5] Pisano C., Figiel Ł. Modelling of morphology evolution and macroscopic behaviour of intercalated PET-clay nanocomposites during semi-solid state processing. *Composites Science and Technology* 75: 35-41, 2013.

[6] Figiel Ł. Effect of the interphase on large deformation behaviour of polymer-clay nanocomposites near the glass transition: 2D RVE computational modelling. *Computational Materials Science* 84: 244-254, 2014.