Multiscale Modelling of ABS – Montmorillonite System

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In this paper, we present a hierarchical procedure for bridging the gap between atomistic and macroscopic (FEM) modelling passing through mesoscopic simulations. In particular, we will discuss the concept of multiscale (or many scale) modelling, and present an example of applications of multiscale procedures for ABS - organoclay nanocomposites of industrial interest.

Extended Abstract

Many industrial scraps cannot be reused in an advantageous way, mainly because of their degradation. When possible, rejects of industrial scraps are added to the virgin material for new moulding, although the amount of recycled block co-polymer cannot exceed 15% of mouldable material to obtain good final performances. For this reason, post industrial rejects constitute a major problem both from the standpoint of the European legislation and policy and from the economic side where enterprises are concerned. Moreover, in the last decade nanotechnologies have opened spaces and possibilities which are not yet fully explored. Those are related with the techniques of embedding nanostructures in polymer matrix, such as montmorillonite layers (MMT), which offer a considerable improvement of physical and mechanical properties, increasing life cycles and versatility of such materials.

The role of modelling and computer simulation in the design of new multifunctional materials is crucial to avoid long and expensive experimental work thus reducing the time to market of the new product. Modelling is performed at molecular level. Atomistic – based simulations such as molecular mechanics (MM), molecular dynamics (MD), and Monte Carlo-based methods (MC) have come into wide use for materials design [1-5]. Although a possible molecular structure can be simulated by the atom-based simulations, it is less realistic to predict the mesoscopic structure defined on the scale of 10 -100 nm. For the morphology on these scales, mesoscopic simulation methods are available as alternatives to atomistic simulations [6-8]. Furthermore, it is possible to transfer the simulated mesoscopic structure to finite elements modelling tools (FEM) for calculating macroscopic properties for the systems of interest [9]. If all these methods are tightly integrated we obtain the multi scale molecular modelling. This is discussed and applied here to the simulation of the nanostructured equilibrium morphology of blends consisting of mainly recycled acrylonitrile – butadiene – styrene (ABS) block co-polymers of special interest in the automotive industry. Our matrix was composed of a blend of

acrylonitrile – styrene (SAN) block copolymer and a branched copolymer of acrylonitrile – styrene and butadiene (polyB – SAN).
Blends are employed as matrixes for embedding MMT layers, which undergo intercalation and exfoliation. Intercalation is due to the modification of MMT layers via the use of compatibilizers, typically quaternary ammonium salts (quats). Quats have a polar hydrophilic head, which is able to substitute Na+ cations over the MMT surface by ionic exchange, and a hydrophobic tail, which favourably interacts with polymer structures. Partial or total exfoliation consists in a wider separation and de-orientation of the MMT and is due to the mixing and shear effect during the nanocomposite preparation. Multiscale investigations have been carried on with the aim of investigating several aspects of this complex phenomenon:

1. model and describe single monomer structures at quantum – mechanics level;
2. polymer and copolymer chains behaviour: free chains, inclusion in MMT, interaction between MMT – quat – polymers at molecular mechanics and molecular dynamics level;
3. polymer blend morphology at mesoscale level;
4. mechanical properties of the blend at finite element level;
5. mechanical properties of the nanocomposites, which includes the bulk (polymer blend) and the MMT layers at finite elements level.

The first two aspects enable the choice of the best quat in terms of binding energies and MMT basal spacing, and generate the necessary input information for the simulations at the upper scale, such as Flory – Huggins interaction parameters χ, characteristic ratios C_∞, self diffusion coefficients D.
The third one gives important indications on the mesoscale behaviour (dimensions of 10 – 100 nm) of the pure blend in terms of density profiles and, in a sort of 'message passing' multiscale simulation, provides information for subsequent finite element simulations (issue n. 4) where polymer blend mean and local mechanical properties (Young modulus) are calculated. Mean mechanical properties of the ABS blend will also be used in input for estimating the mechanical properties of the bulk, necessary for the calculations of point 5. Finally, in the fifth point (length scale approximately 100 – 1000 nm), the mechanical properties of the entire nanocomposite is calculated.
Simulated data at each single scale will be compared with experimental information to validate the methodology and to be supported in the final design.

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