

## **2010 DPI workshop on nanocomposites**

*By: Eddy Brinkman, Betase BV*

***On May 27, 2010, the Van der Valk hotel in Eindhoven was the scene of a DPI workshop on nanocomposites. Over 30 people gathered to discuss the science and technology of these fascinating materials. After an inspiring lecture by professor Costantino Creton, PhD students and other scientists exchanged their problems, their experience and their ideas with the aim to learn from each other, and to strengthen the field of nanocomposites.***

“Why are nanocomposites so interesting for materials research and applications?” That was the main question Costantino Creton raised at the workshop - and that was also the title of his introductory lecture. Professor Creton, active on polymer mechanical properties and interfaces at the French ESPCI ParisTech research institute, focused on the mechanical aspects of nanocomposites. According to him, nanocomposites - especially the polymeric ones - are particularly interesting due to a combination of properties. Because of the large number of interfaces between the polymer and the relatively small fraction of nanosized filler material, the manufacturing of transparent materials with improved mechanical properties is well within range. Furthermore, the size of the filler nanoparticles is comparable to - or even smaller than - the radius of gyration for polymer chains, so nanoparticles are able to influence polymer chain configurations and entanglements.

### **The road to industrial applications**

Although nanocomposites are hot in the academic world, Creton believes that ‘killer’ industrial applications of nanocomposites are still missing at the moment. Not only the relation between processing and the nanocomposite structure is tricky on an industrial scale; especially the relation between the nanocomposite structure and macroscopic properties of products made of them is still unclear to a large extent. When the way of ‘how to translate nano to macro’ has been elucidated - by having a suitable structure-property predicting model - the road to industrial applications lies open. To make such a model successful, it will not be sufficient to only look at the nano and macro scale. We also need to look at the microscopic scale, so understanding the length-scale in between is necessary.

According to Creton, polymer nanocomposites are especially useful when more than one property of ‘standard’ polymers have to be improved. Take, for example elastomers, thermoplasts or thermosets, that need to be tougher but still have to be transparent. Or polymers that have to be electrically conductive and transparent at the same time. As filler material, nanocellulose is mechanically interesting whereas carbon nanotubes are electrically interesting.

In a vivid discussion after Creton's lecture, other applications were mentioned, such as the use of nanocomposites in waterborne transparent coatings. Perhaps we can learn from these already existing nanocomposite applications: how to transfer knowledge of coatings to engineering plastics? After the introductory lecture, the people present discussed with each other in three groups on issues related to nanocomposite preparation, characterisation and properties (including modelling), and how to deal with these issues.

### **Nanocomposite preparation**

Problems issued with respect to preparation are mainly related to the dispersion of nanoparticles into the polymeric matrix. Several routes are being investigated to disperse nanoparticles made of e.g. calcium carbonate, silica, titania, carbon (nanotubes or graphene sheets) or nanoclay: by melt compounding, by solution and evaporation or precipitation, during the synthesis of the polymer itself, or by in-situ preparation of the particles. And would it even be possible to develop hierarchic composites by reactive self-organisation? It seems to be difficult during these processing steps to control the state of dispersion and to control the amount of nanoparticles within the dispersion in a reproducible way. And what would be the right dispersion technique for a given morphology? It is even a challenge to develop well-defined ‘model’ materials for understanding nanocomposite features. On this nanoscale, there is a need for a valid way to ‘measure dispersion’ - beyond the images that show dispersion.

### **Characterisation and properties**

There is a wide variety in characterisation methods for nanocomposites, ranging from surface to bulk techniques. Besides 'conventional techniques' as TEM, SEM, STEM etc. to show materials structures and morphology, it is possible to obtain chemical information via techniques as Tip Enhanced Raman Spectroscopy (TERS) and Enhanced Ellipsometry. Specific techniques are available to measure mechanical properties on this scale (stress/strain, local), and it is even possible to use conductive AFM for measuring electrical properties.

To find your way in this 'labyrinth' of characterisation techniques, it is essential to define as good as possible what you would like to know and to work in close collaboration with a characterisation expert. Often, multiple characterisation techniques are required to find your answer, on various length scales: of course on nano scale and macro scale, but also on the intermediate, connecting micro scale. And how to characterise a nanomechanical interface? For nanocomposites, knowledge from both sides - organic polymer, inorganic filler - is necessary. Related to this experimental part is the need for reliable predictive models - including models for non-linear properties - that can be validated by the experiments. Where qualitative interpretation of nanoscaled structures already offers many challenges it becomes even more so in view of the necessary quantification to connect the nanoscale effects to the macroscopic properties we experience in daily life.

### **Bring different length scales together**

A lot of questions remained unanswered in this workshop - or lead to even new questions. But also some new perceptions were gained, the other way around. For example: instead of taking the polymer matrix as a starting point, take the filler as basis. If we know how to organise the particles, we can make the polymers afterwards. Also self healing aspects are challenging. Can we go supramolecular?

As a general conclusion, this workshop has shown that it is necessary to bring different length scales together – atoms, intermediate scales and 'the real world'. Because, after all: nanocomposites are quite difficult to understand - yet - and going straight from nano-fillers and polymers to car bumpers is a giant step to take, which needs at least understanding of the intermediate length scales.

### The ins and outs of polymer nanocomposites

If you want to improve engineering plastics - for example make them mechanically stronger or electrically conducting – you can do this by incorporating filler materials into the material. Traditional fillers such as microscopically small talc, glass or carbon black particles have to be added to the polymeric ‘matrix’ in amounts of at least 15-20 volume percent to obtain a noticeable result in strength or conductivity. Unfortunately, this relatively large fraction will impair the ‘looks’ of the original material - make polymer surfaces less smooth, or make transparent polymers opaque - or make it more brittle or dense than you would like to have. To overcome these issues, it would be wise to put smaller – nanoscale – fillers into the polymer matrix. *Et voila*, a polymeric nanocomposite has been born. In fact, Mother Nature has used nanocomposites already throughout its evolution in a wide variety: in trees, in your own bones or in seashells.

A nanocomposite can be defined as a solid material, consisting of more than one phase, where for one of these phases (the nanoparticles) typical dimensions are less than 100 nanometer. These nanoparticles are for example carbon nanotubes with a diameter of a few nanometers and a length of micrometers (i.e. a high aspect ratio) or exfoliated clay platelets with a thickness of a few nanometers and much larger diameter. Especially these non-spherical nanoparticles can form a continuous network (possibly conducting when using a conductive filler) at much lower volume fractions - even down to less than one volume percent - than their traditional counterparts.

Due to the very high surface-to-volume ratio of the nanoparticles, mechanical, electrical and other properties of a nanocomposite will differ from a ‘normal’ composite. The thinner and smaller the nanotubes or platelets are, the more surface area is present for interaction with the polymer matrix. Material properties of the polymeric matrix will differ considerably in the neighbourhood of these nanoparticles. Due to the high surface-to-volume ratio, even a small fraction of nanoparticles will have a large influence on the composite properties. For an optimal improvement, the nanoparticles have to be dispersed into the polymer matrix during processing. Here are many challenges to overcome, to reach an economical viable manufacturing process.

Besides mechanical improvement of polymers, nanoparticles with a high aspect ratio that are homogeneously dispersed in polymers will act as a barrier for oxygen transport through plastic sheets (cling films), or as a flame retarding material by forming barriers between air and fuel.