MOLECULAR DYNAMICS SIMULATION OF AMORPHOUS TITANIA NANOPARTICLES

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ABSTRACT

The mechanical properties of polymers could be modified by adding fillers. This combination of a polymer with a filler is called a microcomposite. The work by Selvina *et al.* [1] found that the mechanical properties of titanium dioxide-filled polystyrene microcomposites, such as Young's modulus, tensile strength, elongation at break, flexural modulus and flexural strength, increase linearly with the increase of filler concentration followed by a decrease beyond 15 wt.%. This clearly shows that titanium dioxide reinforces the polystyrene matrix effectively at lower filler content. The decrease at higher loading is due to the particle–particle interaction of the titanium dioxide leading to agglomeration. Therefore, the smaller the particles are, the more important the surface properties will be, influencing interfacial properties, agglomeration behaviour, and also physical properties of the particles [2].

In this study, molecular dynamic (MD) simulations of spherical amorphous TiO_2 cluster nanoparticles, with various sizes, were conducte, under non-periodic and periodic boundary conditions. The various models have been obtained by cooling from the melt via molecular dynamic (MD) simulations. The change in structural properties of obtained amorphous nanoparticles at 350 K were studied via partial radial distribution functions, coordinate numbers, and bond-angle distributions by comparison with the pre-simulation bulk.

The studies show that structural disorder increased after simulation and the sphericity of the nanoparticles increase from the bulk to the surface of the nanoparticles.

This research utilised resources at the Center for High Performance Computing (CHPC).

References:

[1] Selvina, T.P.; Kuruvillab, J.; Sabua, T. *Materials Letters*, **2004**, *58*, 281.
[2] Hanemann, T.; Szabó, D.V. *Materials*, **2010**, *3*, 3468.