

Micromechanics of Thermoelastic Behavior of Polypropylene/Calcite (Modified with Triton X-100) Nanocomposites

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Abstract: *The present work was to estimate thermoelastic behavior of polypropylene/calcite nanoparticulate composites. The calcite nanoparticulates were modified with Triton X-100. The RVE models were used to analyze thermo-elastic behavior. The stiffness of polypropylene/calcite nanoparticulate composites decreased with the increase of temperature.*

Keywords: Polypropylene, Calcite, Triton X-100, RVE model, thermoelastic, finite element analysis.

1. Introduction

The use of reinforcing fibers/particulates as stiffening driving force in the polymer nanocomposites has established for variety of applications. By reinforcing epoxy/carbon with fibers such as Kevlar 29 [1], E-glass [2-4] and carbon [5] the enhancement of mechanical is available in the literature. Also, reinforcing of nylon/teflon with nanoparticulates such as alumina [6], silicon carbide [7], iron oxide [8, 10] and graphite [11] were used for various applications. Calcium carbonate (CaCO_3) is one of the most commonly used inorganic fillers in polypropylene (thermoplastic polymer). Polymer/ CaCO_3 composites find applications such as sewer pipes, garden furniture and breathable films. Particulate aggregation is a major problem in CaCO_3 /polypropylene nanocomposites resulting deteriorated mechanical properties [12]. The surface of CaCO_3 nanoparticles is typically modified with sodium stearate [13], stearic acid [14] and acrylic acid [15], in order to prevent agglomeration of the particles.

The present work was intended to investigate the thermoelastic behavior of nanoparticulate calcite/polypropylene thermoplastic polymer matrix composites. The surface of calcite nanoparticles were modified with Triton X-100. Finite element analysis (FEA) was implemented to measure the local response of the material using representative volume element (RVE) reinforced by a single particle subjected to hydrostatic and isothermal loading.

2. Material and methods

In the present work, CaCO_3 was used as reinforcing filler in the form of calcite. It has elastic modulus of 70 GPa, CTE (coefficient of thermal expansion) of $13 \mu\text{m}/\text{m}^\circ\text{C}$ and surface tension of 200 mN/m. The matrix material was polypropylene (PP). It has elastic modulus of 1.4 GPa, CTE (coefficient of thermal expansion) of $160 \mu\text{m}/\text{m}^\circ\text{C}$ and surface tension of 32 mN/m. The calcite nanoparticles were modified with Triton X-100 which is a nonionic surfactant having a hydrophilic polyethylene oxide chain. Triton X-100 is a clear viscous fluid due to the hydrogen bonding of its hydrophilic polyethylene oxide parts.

The average size of calcite reinforcement nanoparticulate was 100nm. The volume fractions of calcite nanoparticles were 10% and 20%. The polypropylene/calcite nanoparticulate composites were manufactured using injection moulding process. The tensile testing was carried out on universal testing machine as per ASTM procedure at different temperatures. In this investigation, a square RVE (figure 1) was equipped to infer the thermo-elastic behavior polypropylene/calcite nanoparticulate composites. The PLANE183 element was used in the matrix and the interphase regions in the RVE models. The interphase between nanoparticle and matrix was discretized with CONTACT172 element [16]. Both uniform thermal and hydrostatic pressure loads were applied simultaneously on the RVE model.

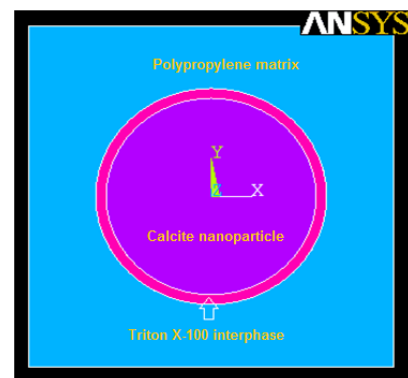


Figure 1: The RVE model.

3. Results and Discussion

The finite element analysis (FEA) was carried out at 0°C to 100°C isothermal conditions. The hydrostatic pressure load was applied RVE model to investigate micromechanics thermo-elastic tensile behavior of polypropylene/calcite nanoparticulate composites. The volume fractions of calcite nanoparticles in the PP matrix were 10% and 20%.

3.1 Micromechanics of thermo-elastic behavior

Thermo-elastic strain as a function of temperature is showed in figure 2. The increase of temperature increased the tensile

strains along the load direction. The tensile strain was higher for the composites having low volume fraction (10%) of calcite nanoparticles than those having high volume fraction (20%) of calcite nanoparticles. The matrix (PP) had experienced the large tensile strains as the temperature changed from 0°C to 100°C temperature as showed in figure 3.

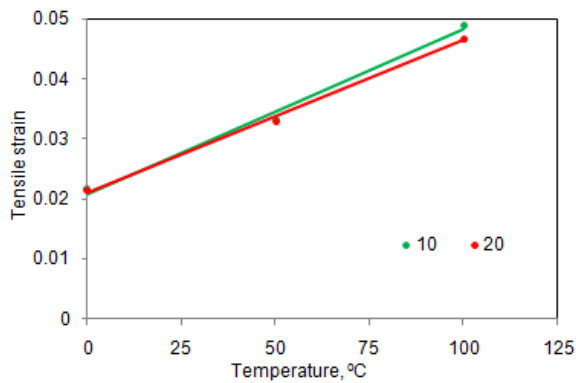


Figure 2: Influence of temperature on thermoelastic strain.

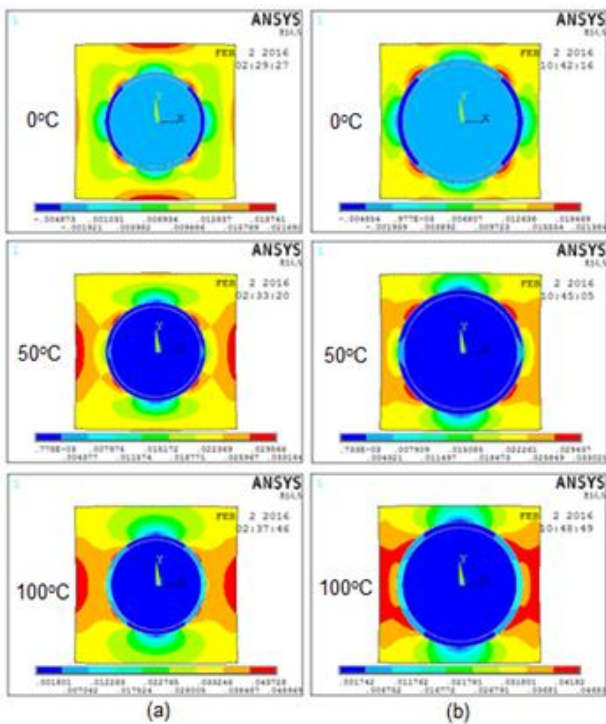


Figure 3: Raster images of tensile strains of PP/Calcite nanocomposites: (a) 10% Calcite and (b) 20% Calcite.

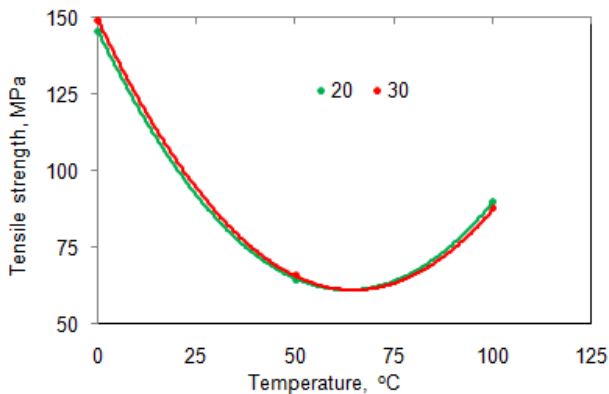


Figure 4: Influence of temperature on strength.

Tensile strengths as a function of temperature is depicted in

figure 4. The tensile strength decreased with the increase of temperature from 0°C to 50°C and it increased from 50°C to 100°C. Figure 5 shows raster images of stresses induced in the composites having 10% calcite and 20% calcite nanoparticles, respectively. The transfer of stresses increased with the increase of temperature from the matrix to the nanoparticle as seen from the order of colors. As the temperature increased the interphase experienced high compressive stress. The tensile elastic modulus decreased with the increase of temperature as showed in figure 6. The calcite nanoparticles are very stiffer to undergo deformation under tensile loading. The elastic modulus was higher for nanocomposites having high volume fraction (20%) of calcite nanoparticles.

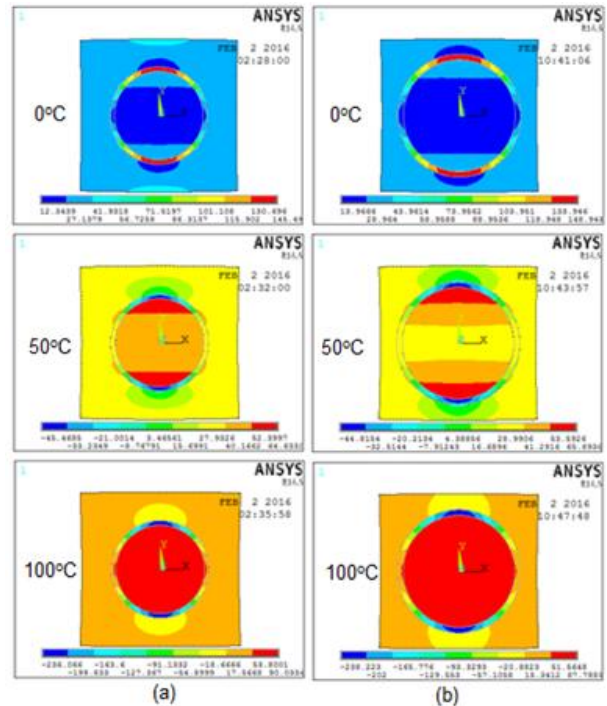


Figure 5: Raster images of tensile stresses of AA2024/20% MgO composites.

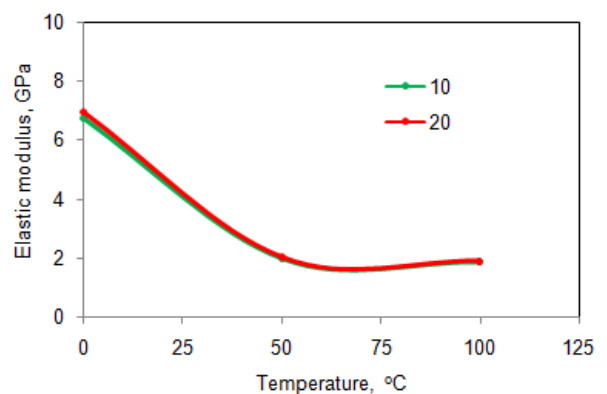


Figure 6: Influence of temperature on elastic modulus.

3.2 Fracture behavior

Figure 7 describes the von Mises stress induced in the composites. The von Mises stress decreased with the increase of temperature from 0°C to 50°C and later it increased with the increase of temperature. The von Mises stress was nearly same in the nanocomposites having 10% and 20% calcite nanoparticles. In all the cases the calcite nanoparticles were

debonded from the PP matrix (figure 8). The Triton X-100 interphase is seen around the calcite nanoparticle (figure 9a). Figure 9b reveals the scanning electron microscope image of particle debonding and interphase fracture. The stress levels at the interphase indicate the interphase fracture and particle debonding as obtained from the finite element analysis (figure 9c).

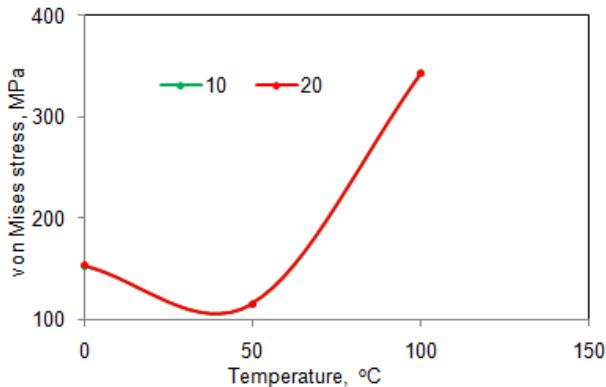


Figure 7: Influence of temperature on von Mises stress.

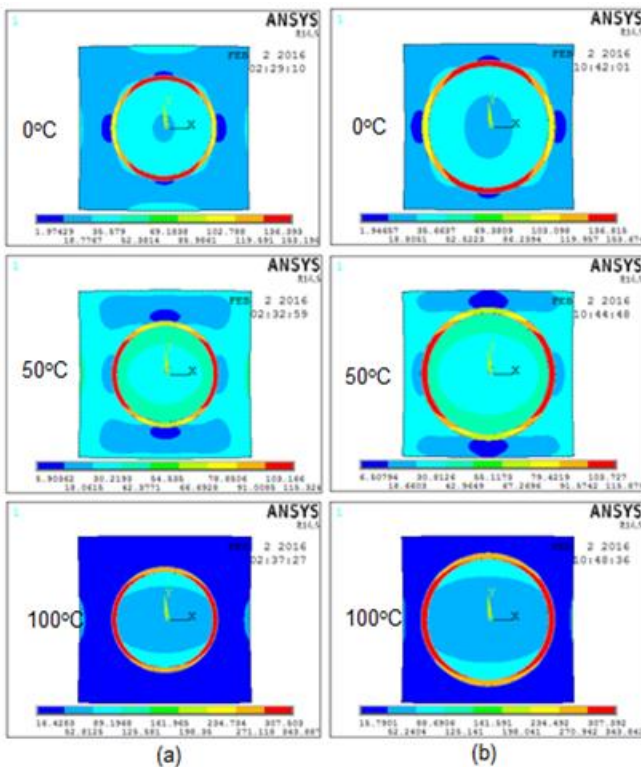


Figure 8: Raster images of von Mises stress of PP/calcite nanocomposites: (a) 10% calcite and (b) 20% calcite.

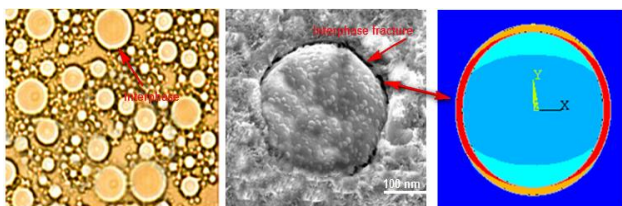


Figure 9: Interphase around calcite nanoparticle (a); interphase fracture (b); and finite element analysis showing the possibility of interphase fracture (c).

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