

# UNDERSTANDING THE EFFECT OF THE INTERPHASE IN POLYMER NANOCOMPOSITES

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## Introduction

The interphase formed between reinforcements and matrix in polymer nanocomposites has remarkable effects on overall properties of the composites. However, the contribution of the interphase to the overall performance of the nanocomposites has not been determined [1]. This work combines 1) experimental characterization of the interphase, 2) study of conventional theoretical models with the interphase effect consideration, and 3) assessment of elastic response of nanocomposite models using computational analysis. Nanocomposites of polypropylene matrix with multi-walled carbon nanotubes (MWNT) and exfoliated graphite nanoplatelets (xGnP) at concentration of 0 to 10 wt% were fabricated using extrusion and injection molding. The tensile strength and modulus of the nanocomposites were determined as a function of the reinforcement's content. The interphase was probed and characterized using nanoindentation and atomic force microscopy (AFM). The morphology of the fractured surfaces of specimens was investigated utilizing scanning electron microscopy (SEM). Using the experimental data and treating the interphase as a third component, the tensile properties of the nanocomposites were modeled using finite element analysis (FEA). Furthermore, the addition of interphase region to the preexisting theoretical models such as the Halpin Tsai model and rule of mixtures was studied. Finally a comparison between experimental data, theoretical results predicted by micromechanical models and by numerical modeling is used to demonstrate the dominant effect of interphase in the performance of polymer nanocomposites.

## Experimental

**Materials.** The polymer used in this study is polypropylene powder (melt flow index 12 g/10 min, ASTM D1238 by Basel). Two types of nanoreinforcements were used. The exfoliated graphite nanoplatelets (xGnP) (from XG sciences) density: ~2.0g/cm<sup>3</sup>, tensile Modulus: ~1.0 TPa, tensile Strength: ~10-20 GPa. and multi-walled carbon nanotube (MWNT) (from Cheap Tubes) (OD 20-30 nm, Inside Diameter 5-10 nm, length 10-30 um, density .1 g/cm<sup>3</sup> at 20°C). In order to study the effect of aspect ratio on the results, xGnP-1 and xGnP15μm were used.

**Preparation of nanocomposites.** The xGnP and MWNT fillers were used as received. In case of xGnP-1/PP nanocomposites, the compounding was done by coating the nanofillers followed by melt mixing. Coating of the polypropylene powder with xGnP was achieved by dispersing

xGnP in isopropyl alcohol (IPA) using sonication. PP powder was added to solution and IPA was dried away, and the composite powder was fed to extruder for melt mixing.

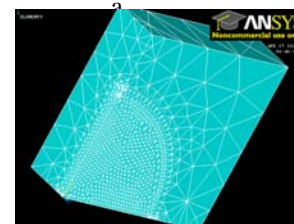
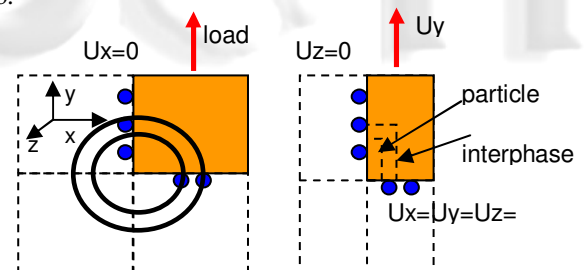
The method used for fabricating MWNT-PP nanocomposites was melt mixing using extrusion and injection molding, with processing conditions similar to those for xGnP/PP fabrication.

**Characterization.** Tensile testing was carried out according to the ASTM D638 at the ambient temperature. The nano and microscale morphology and particle dispersion of fractured surface of xGnP-1/PP and MWNT/PP specimens were studied utilizing SEM experiments.

Atomic force microscopy (AFM) studies were carried out using the tapping mode on a Veeco and Nanoscope V controller (Digital Instruments) with silicon tips (r~20 nm) to characterize the topography and compositional differences of the surface of xGnP/PP and MWNT/PP composites, and to investigate the interphase.

Nanoindentation tests were conducted to investigate the hardness and elastic modulus of the xGnP/PP and MWNT/PP nanocomposites using a triboindenter (Hysitron Inc.) with a Berkovich indenter and applying the maximum load of 200 μN with spacing between two indentations about 1μm.

Once the properties and geometry of the interphase were determined experimentally, the interphase was introduced as the a third material in numerical modeling finite element simulations using ANSYS. Fig.1.a shows the schematic used to build the model and the 1/8 symmetry employed to overcome limitations of the software. For modeling of fillers, interphase and matrix, interfaces between regions were assumed to possess a perfect contact. Optimized mesh densities for all regions were applied to meet convergent results shown in Fig.1.b.



(b)

**Fig.1** (a) FEM symmetric RVE model with rigid body boundary conditions for embedded xGnP1 in matrix, and (b) ANSYS meshing model for embedded particle and interphase

## Results and discussion

The hardness and modulus of PP control, 1wt% xGnP-1/PP and 1wt% MWNT/PP nanocomposites obtained from the nanoindentation tests with appropriate indent spacing are shown in Fig.2.

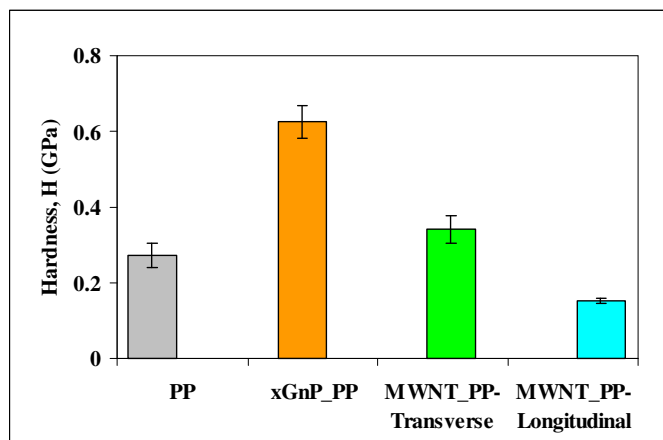


Fig.2 Hardness of polymer matrix and nanocomposites using nanoindentation

In case of xGnP-1/PP nanocomposites, the width of the interphase found to be about 30 nm based on the AFM studies. It should be noted that due to the imperfect attachment of polymer chains to the particles, and hence lower effective particles' surface area and a discontinuous interface, the regions closer to the fillers possessed higher stiffness and those near to the matrix showed lower stiffness with respect to that of the matrix.

FEA solutions helped to determine the Young's modulus of the nanocomposites with and without considering the interphase by attributing distinct properties to it. As shown in Fig.3, the computational and conventional composites theoretical models overpredicted the tensile modulus of the nanocomposites respect to the experimental values with and without consideration of the interphase effects due to simplifications such as assuming the presence of well bonded contacts and perfect surface attachments in oriented particle models. However, both computational and theoretical models predicted lower values of tensile modulus when the interphase properties were attributed to them due to the negative interaction of the fillers and matrix at the same particle loadings. Based on the theoretical and FEM models, the interphase produced a greater deviation to the experimental results in higher filler loadings of xGnP1 and MWNT particles. This effect can be thought of the higher interphase concentrations generated around the particles[2].

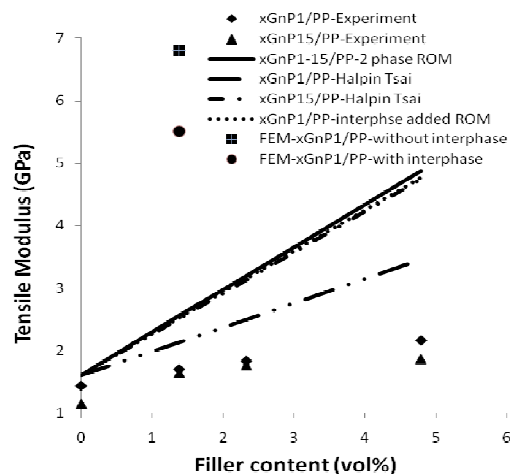


Fig.3 Effect of Vol% of fillers on tensile Young's modulus of xGnP/PP nanocomposites: Comparison between theoretical, computational and experimental data

## Conclusion

Nanoindentation tests and AFM quantitative analyses were carried out to characterize the interphase in xGnP1 and MWNT/PP nanocomposites in nanoscale level. SEM was used to study the particles' dispersion and their bonding conditions in the polymer matrix. FEA computations as well as conventional composite theoretical models were employed with and without considering the interphase to investigate the effect of interphase on the tensile Young's modulus of nanocomposites. This study showed the results predicted by the models overestimated the Young's modulus respect to the experimental tensile values. However, by considering the interphase, as the characterized third region surrounding the particles, the models predicted lower values for the modulus closer to the tensile experimental results. This work showed the interphase region has its own properties and size distinct from those of reinforcing phases and matrix. It is expected that this study can help in a better understanding of the significant influence of interphase on overall properties in the field of nanoreinforced composites.

## References

- Gao, S.-L. and E. Mäder, Characterisation of interphase nanoscale property variations in glass fibre reinforced polypropylene and epoxy resin composites. *Composites Part A: Applied Science and Manufacturing*, 2002. 33(4): p. 559-576.
- Liu, H. and L.C. Brinson, Reinforcing efficiency of nanoparticles: A simple comparison for polymer nanocomposites. *Composites Science and Technology*, 2008. 68(6): p. 1502-1512.