# FINAL REPORT – SUMMARY OF RESEARCH

**TITLE OF GRANT: MULTISCALE EXPERIMENTS AND MODELS FOR POLYMER NANOCOMPOSITES**

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**PRINCIPAL INVESTIGATOR: IOANNIS CHASIOTIS**

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# FINAL REPORT – SUMMARY OF RESEARCH
# MULTISCALE EXPERIMENTS AND MODELS FOR MECHANICAL ANALYSIS OF POLYMER NANOCOMPOSITES

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This report summarizes our research activities at the University of Virginia conducted under the support of this NASA research grant from March 2004 to October 2004 and provides a summary of the research to be conducted in the remaining period of the project at the University of Illinois at Urbana-Champaign (UIUC). The *original research objectives will remain the same* after our transition to UIUC. In the beginning of this program we completed the analysis on the graphite polymer micro and nanocomposites that were studied at NASA Langley and UVa in the summer of 2003. A publication summarizing this work was submitted in the fall of 2004 to the journal of Experimental Mechanics and the reviewer comments are currently addressed[1]. The research program aims at understanding the local interactions between the polymer matrix and hard reinforcement in polymer nanocomposites (PNCs). The materials selected for this study were PNCs with different fillers (14nm silica nanospheres or nanoclays) and volume fractions (0.5%, 1%, 2% and 5%). Figure 1 shows a set of Atomic Force Microscopy (AFM) images of a typical surface area from a silica sphere/epoxy composite specimen (1% volume fraction). Because of the very different mechanical properties of the silica filler compared to the epoxy matrix, the phase image resulted from phase detection microscopy seen in Figure 1(right) helped us discern the actual location of nanospheres from surface bumps that correspond to the surface roughness of the polymer matrix as seen in Figure 1(left).

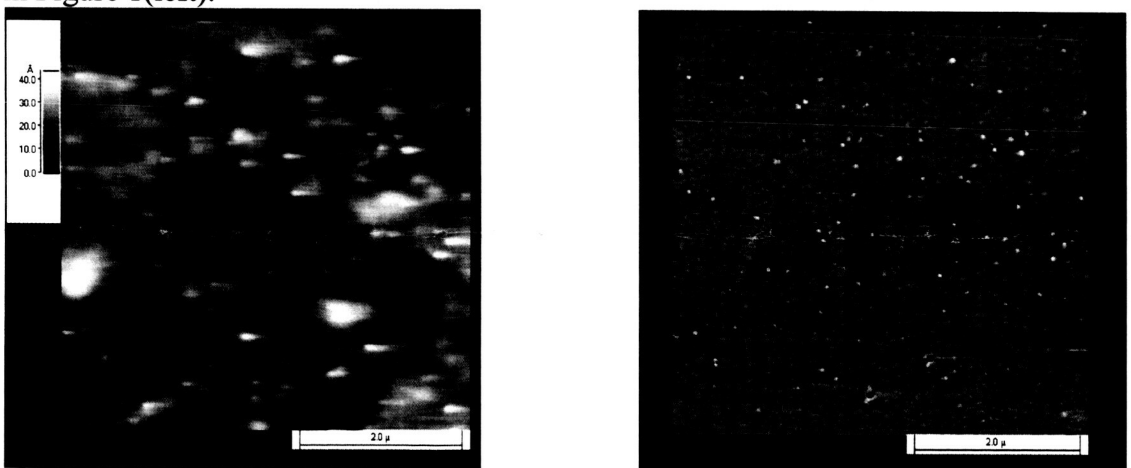



**Figure 1.** Atomic Force Microscopy topographic image (left) and the corresponding true phase image (right) of the surface of a PNC reinforced with nanospheres. The bright spots in the right figure are 50-100 nm silica spheres.

[1] I. Chasiotis, Q. Chen, G. Odegard, and T. Gates, "Structure-Properties Relationships in Graphite Micro and Nanoplatelet-Reinforced Polymer Composites", in review in *Experimental Mechanics* (2004).

A tensile testing apparatus, Figure 2, was designed and built for the purpose of investigating the local *vs.* effective mechanical behavior of PNCs reinforced with silica nanospheres and intercalated or exfoliated nanoclays. Figure 3 shows the implementation of this apparatus with a 200 microns thin PNC specimen attached to the grips.

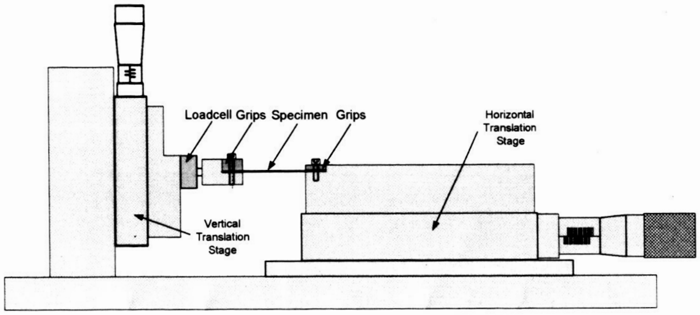



**Figure 2.** Schematic of the tensile test set-up

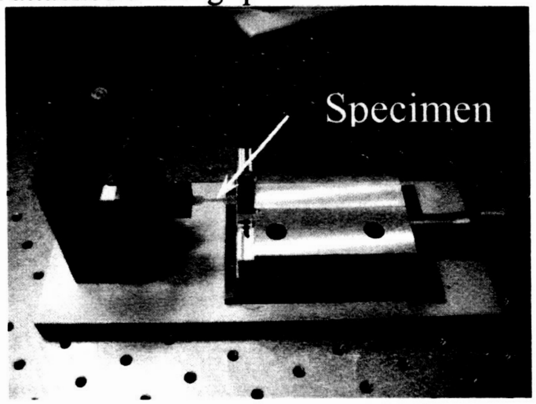



**Figure 3.** Tensile test apparatus.

The first miniature tension specimens were fabricated from silica nanocomposites based on the geometry seen in Figure 4. This task was not straightforward, as the surface roughness of these specimens should not exceed the size of the filler. As seen in Figure 1, the roughness for the prepared samples was better than 5 nm. These specimens will be tested *in situ* under Atomic Force Microscope with the tensile test system seen in Figure 5. The load capacity of the custom made tensile test apparatus is 25 $lb_f$ with accuracy within 0.05% of full scale and the horizontal linear translation stage has 0.5 $\mu$m accuracy. Upon completion of the calibration of this apparatus and the preparation of test specimens we will conduct experiments with application of the AFM/DIC method.

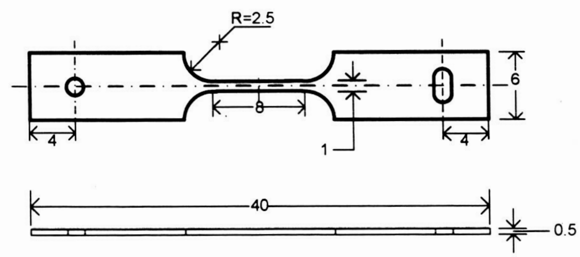



**Figure 4.** Miniature tensile specimen (units in mm)

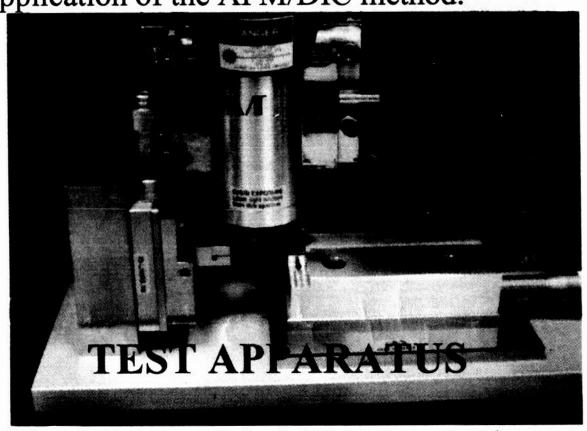
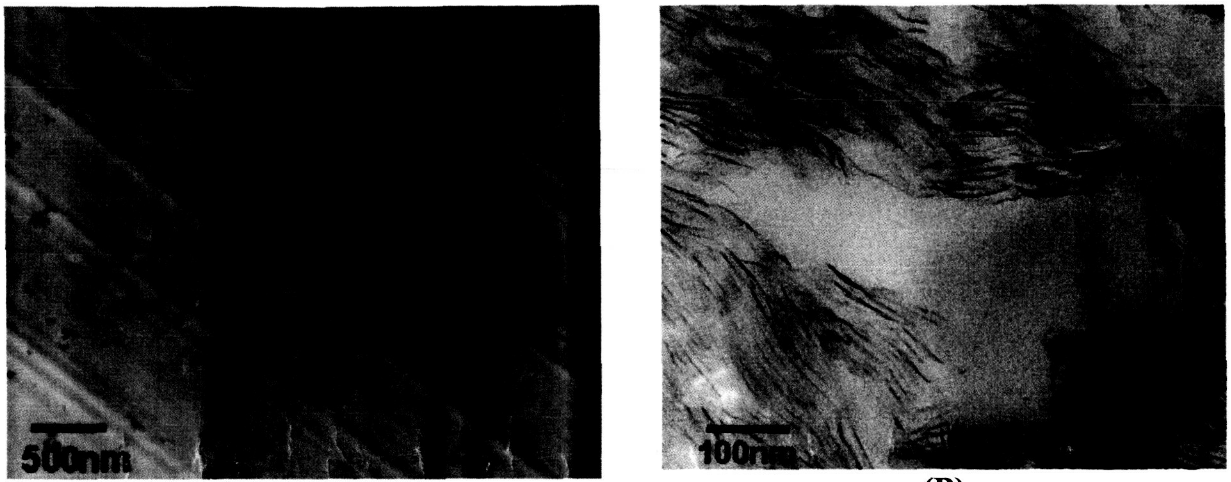



**Figure 5.** *In situ* uniaxial tension test under AFM

The goal of these experiments is to derive the structure-properties relationships by assessing the influence of filler distribution, dimensions, and volume fractions on the local deformation fields. These experiments are expected to be challenging as the scale of the reinforcement is on the same order of magnitude as the probe diameter. Figures 6(A) and 6(b) show TEM images of the nanoparticles. The particles shown in Figure 6(A) are clusters of nanospheres. Figure 6(B) shows a clay nanocomposite. The latter has been more difficult to work with using the AFM to selectively identify the hard phase on the surface of the specimens.




(A) (B)

**Figure 6.** **(A)** Silica nanospheres PNC, **(B)** Clay PNC. Images are courtesy of C. Chen (WPAFB).

***The work to be conducted at UIUC will follow the original objectives of this program.*** The graduate student who has worked on this project at UVa will transfer to UIUC, which will ensure the smooth continuation of this research. Specifically, we will pursue the

- Characterization of the nanometer level deformation properties of PNCs that incorporate nanoparticles of different dimensions and geometry (nanospheres, clays, or CNTs).

- Establish structure-properties relationships based on local strains and assist the development of two or three phase micromechanics constitutive models to describe the mechanics of PNCs.

- Study of the viscoelastic behavior of PNCs and the effects of ambient conditions and loading rates on pre-treated PNCs in connection with particle density and geometry.

- Identify damage mechanisms occurring during loading in connection with particle size and geometry. Obtain understanding of the damage mechanisms (microcracking, debonding, and particle fracture) and the connections between microstructural details of damage evolution and macroscopic failure (fracture).

These objectives will be coordinated with the activities of the Computational Materials Group at NASA LaRC so that our results will be of direct relevance and benefit to NASA's research mission.