Integration of graphene sheets and carbon nanotubes as fillers in polymer matrices, and their implementation.

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The unique properties and growing availability of nanoscale fillers (NF) such as graphene sheets (GS) or carbon nanotubes (CNT) have driven research aimed at large-scale production and commercialization of NF-based polymer composite materials (NPC) with enhanced thermal, mechanical or electrical properties at low filler loading. The major hindrances in successful utilization of NPC are shortage of effective methods for dispersion of individual NFs in polymeric matrices and NF concentration determination in multicomponent solutions. To address these issues we developed a thermogravimetric-spectroscopy approach to accurately determine the NF concentration in dispersion [1]. Consequently, a conventional spectroscopy-based concentration calibration plot is constructed for simple and swift use in further concentration measurements (Figure 1). Such true concentration analysis is crucial for studying the concentration–property relationship.

High GS (0.7 mg/mL) and CNT (5mg/mL) concentrations in water were prepared by optimizing the nature of dispersant and the type of ultrasonic generator [2]. These NF were further employed to fabricate NPC with enhanced properties:

**Electrical conductivity**: A hybrid of GS-CNT was employed to fabricate conductive transparent electrodes for a molecularly-controlled solar-cell with an open-circuit voltage of 0.53V [2].

**Mechanical properties**: Upon loading of individual CNTs in the polymer matrix using a novel dispersion method, we achieved a record fracture toughness enhancement (150%, Figure 2) at very low (0.1 vol.%) filler concentration. For the first time, we showed a coherent quantitative correlation between the fracture toughness and the surface roughness. The failure mechanism (pullout or fracture) is predicted by the slope of the surface roughness vs. fracture toughness curve [3].

**Thermal properties**: We demonstrated that beyond GS concentration, its size and surface treatment affect the thermal properties of GS-epoxy NPC. An excellent NF distribution is achieved by non-covalent modification of the NFs surface and a new dispersion approach. The structural parameters of the NF, i.e., lateral size and thickness strongly affect the thermal conductivity of the composites. When optimized, they result in a record thermal conductivity, (6.5W/mK, 3750% enhancement) of the NPC (Figure 3). Finally, optimized GS/nano Boron-nitride/epoxy hybrid composites with synergistic effect and tunable electrical properties, suitable for different thermal management applications, were demonstrated.

**References**

Figure 1: Calibration curve of GS concentration: a UV-vis absorption intensity vs TGA-determined GS concentration. The extracted extinction coefficient is the slope. Circles and triangles correspond to two different stock solutions.

Figure 2: Fracture toughness as a function of nanotubes' volume percent.

Figure 3: Thermal conductivity (k) of the composites as a function of filler type and volume fraction *(same units as fig 2 abscissa/ BN in red and larger symbols).