Graphene Nanoribbon - Polymer Composites: The Critical Role of Edge Functionalization

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Abstract

The extraordinary mechanical properties of graphene prompt its incorporation into a wide range of polymeric nanocomposite materials (NCMs). However, similar to other nanomaterials (NMs), the reinforcement efficiency of graphene and its derivatives is hindered by their agglomeration and poor compatibility with the polymer matrix. In this paper, edge-functionalized graphene nanoribbons (EF-GNR) are incorporated in brittle epoxy polymer matrix. The functionalization process by polyvinylamine (PVAM) chains occurs only at the edges (Figure 1), preserving the in-plane sp^2 of the graphene; thereby the PVAM EF-GNRs are both compatible and strong. The produced NCMs exhibit a wide range of enhanced mechanical properties including fracture toughness, flexural strength and shear strength. A critical concentration in which optimal mechanical properties enhancements was observed (0.15 wt%). Above this concentration, the mechanical property degraded dramatically due to re-agglomeration and elevated viscosity (rheological percolation threshold). The elevated viscosity results in air voids which are points of weakness in the resulting NCM. The effect of the edge functionalization is indeed critical, demonstrating superior mechanical properties by the EF-GNR loaded NCMs compared to pristine-GNR loaded composites. A Fractography study shows that the GNRs toughen the epoxy matrix by bifurcating the crack propagation path. Finally, by improving the interfacial adhesion, the edge-functionalization of GNRs alters the failure mechanism from pullout to fracture.

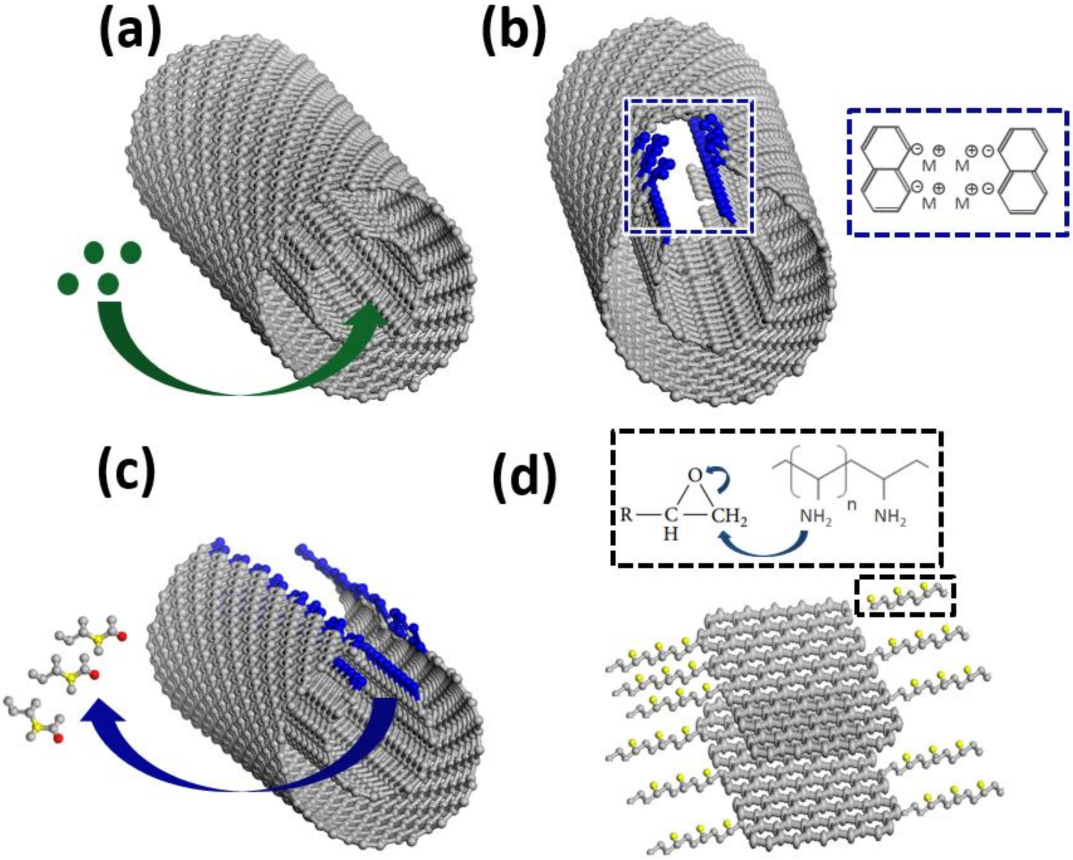

Figure 1. Schematics of EF-GNRs synthesis: (a) intercalation of CNT by Na\K alloy (green dots), (b) longitudinal unzipping and formation of carbanions (blue dots), stabilized by cation ($M=Na^+$ or K^+), (c) in-situ functionalization of unzipped CNT by n-vinyl formamide, (d) EF-GNR formation upon n-vinyl formamide groups hydrolysis. The polymerization reaction between the PVAM and the epoxide groups is marked by dashed box. Nitrogen and oxygen atoms are indicated by yellow and red dots, respectively. [1]

[1] Roey Nadiv, Michael Shtein, Matat Buzaglo, Sivan Peretz-Damari ,Anton Kovalchuk, Tuo Wang, James M. Tour and Oren Regev. Graphene Nanoribbons - Polymer Composites: The Critical Role of Edge Functionalization. Carbon- *Accepted, in press* (2015).