



# Intrinsic defect-induced tailoring of interfacial shear strength in CNT/polymer nanocomposites



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## ABSTRACT

In this study, we investigate the influence of the intrinsic defects of carbon nanotube (CNT) on the interfacial shear strength (IFSS) of the interface between CNT and a polypropylene (PP) matrix using molecular mechanics (MM) and molecular dynamics (MD) simulations. Three different inherent defects of the single void (Void) defect, adsorbed atom (Adatom) defect, and crystallographic Thrower–Stone–Wales (TSW) defect are considered. To quantitatively and qualitatively evaluate the IFSS according to the type and number of defects, quasi static CNT pull-out tests are performed through MM simulations. Among three defects, the single Void defect is found to decrease the IFSS while both the TSW and Adatom defects are found to promote interfacial shear load transfer. Moreover, self-assembly of PP molecules onto the surface of the defected CNT and resultant interfacial strength during the adsorption process are studied through MD simulations at the glassy state of the PP molecules. Consistent results on the interfacial strength between the defected CNT and PP molecules from the pull-out simulation and a defect-dependent adsorption time rate of PP in self-assembly are obtained.

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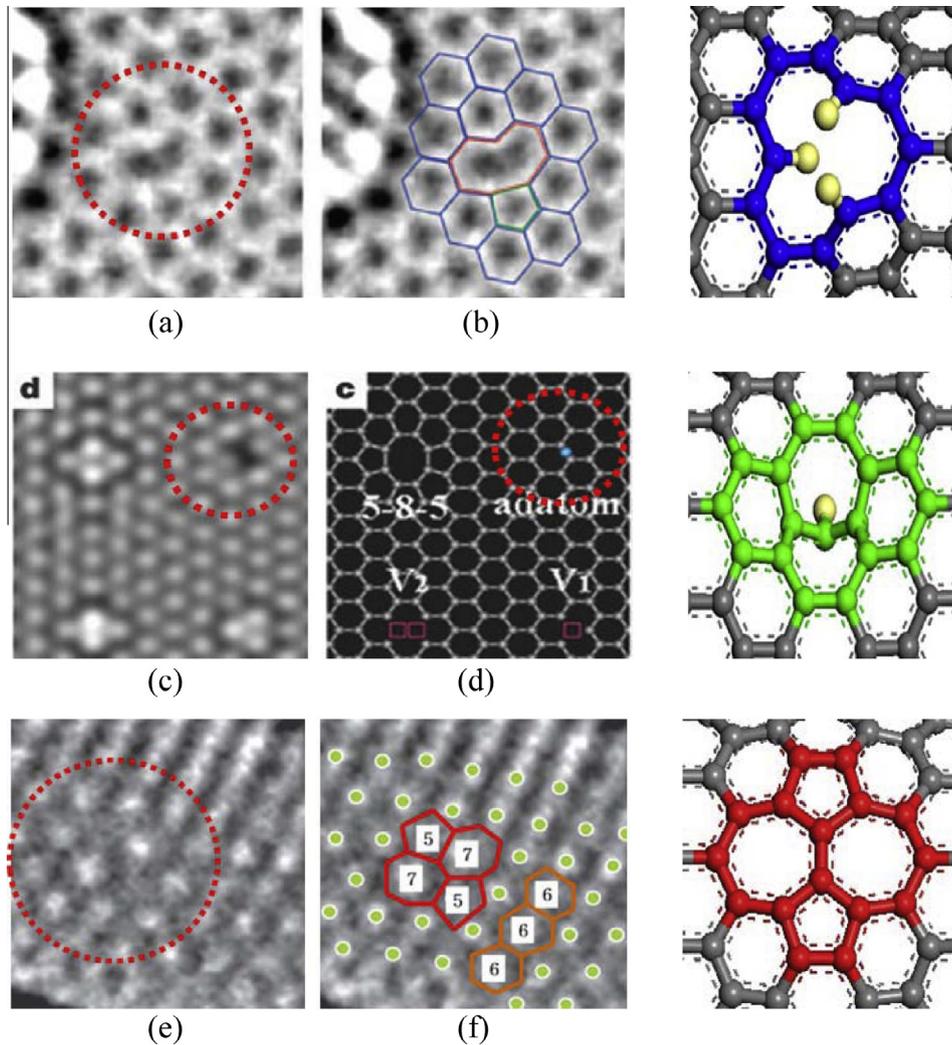
## 1. Introduction

In the design and manufacture of polymer composites reinforced with functional nanomaterials such as carbon nanotubes (CNT), graphene, and organic and inorganic nanoparticles, achievement of efficient interfacial load transfer is one of the key issues [1–5]. Since polymer adsorption in the vicinity of these nanomaterials plays an important role beyond the conventional interpretation of the reinforcing mechanism [6–12], effective load transfer at the material interface between the embedded nanofiller and the surrounding polymer is an essential design parameter to maximize the contribution of the polymer adsorption layer often referred to as the ‘interphase zone’. As has been demonstrated by experimental and computational studies, for CNT reinforced composites, the interfacial strength between CNT and the surrounding polymer is weak in nature [13–15]. Therefore, various surface functionalizations such as covalent and noncovalent grafting have been intensively studied to promote weak interfacial strength between the pristine CNT and polymer and to achieve well dispersed microstructures [16–18].

While the effort to functionalize the sidewall of CNT by adding organic polymer branches to enhance the affinity of CNTs to a host matrix in synthesis focuses on efficient dispersion of CNTs and an improved local load transfer at the material interface, such a functionalization also acts as a defect of the CNTs because it alters the local bond order of the  $sp^2$  carbon. Since the properties of CNTs and other graphitic nanocarbon are sensitively dependent on the local bond order change, the above mentioned examples of the chemical processing truly involve a tradeoff. Besides the covalent functionalization, CNTs are exposed to several severe processing conditions that cause intrinsic defects in general. For example, in the filtration process of high aspect ratio CNTs, viscous and capillary forces at the nanoscale can generate plastic strain release of the CNTs to which the Thrower–Stone–Wales (TSW) defect [19,20] is applied as the primary mechanism [21]. In the acid oxidation process used to purify the CNTs, an adduct defect can be formed as a result of a rehybridization from  $sp^2$  to  $sp^3$  carbon, forming a new bond perpendicular to the side wall of CNTs [22]. Moreover, through high energy electron or neutron irradiation to the CNTs, carbon atoms can be easily dislodged and several vacancies are formed [23]. Therefore, the defects of CNTs can occur at any sequence during their sole synthesis as well as during their manufacturing process to form composites with the polymer matrix.

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**Fig. 1.** Intrinsic defects of graphitic nanocarbon. (a and b) Single vacancy (left two: High resolution transmission microscopy (HR-TEM) image [36], right: Molecular model with three dangling bonds rehybridized by hydrogen). (c and d) Single Adatom defect (left two: HR-TEM image [37], right: Molecular model with an extra rehybridized carbon dangled between two neighboring carbons). (e and f) TSW defect (left two: HR-TEM image [38], right: Molecular model made by 90° rotation of a carbon–carbon single bond).

Apart from synthesis and manufacturing, defects of the embedded CNTs into a polymer matrix are common in operating conditions as multifunctional composites.

In general, intrinsic defects of the CNTs are known to degrade the physical properties of composites [24–26]. Returning to the covalent grafting of CNTs to the polymer matrix to enhance interfacial load transfer, destruction of the conjugated system of the sidewall is a degradative feature even if the purpose of the sidewall functionalization is to promote the overall performance of CNT reinforced composites. Therefore, understanding how the intrinsic defects of the CNTs can affect the performance of the CNT reinforced composites deserves more attention. Regarding the defected CNTs, many studies have focused on revealing the degradation of the CNTs by molecular dynamics simulations and other equivalent continuum-based approaches based on empirical interatomic potentials such as reactive bond order (REBO) potentials [27]. Recalling the simple rule of mixtures, undoubtedly the defects of CNTs render them unfavorable for reinforcement in nanocomposites. However, further investigation on the effect of the defects on interfacial strength in CNTs reinforced composites should be carried out to fully understand the structure-properties relationships.

Among the three typical intrinsic defects of Void, adsorbed atom (Adatom), and TSW defects, it is well known that the TSW defect is more reactive than the perfect hexagonal structure of CNTs and graphene [28] to adsorb the surrounding species. In a recent molecular dynamics simulation study, it has been revealed that the TSW defected CNT reinforced composites can have better elastic performance in shear and transverse deformation of transversely isotropic composites than pristine CNT [29]. Even if the properties of embedded CNT have been found to decrease due to the TSW defects, the enhancement of the interfacial strength between the TSW defected CNT and polymer matrix has been found to be significantly high, overcoming the degraded elastic constants of the defected CNT in terms of the overall properties of composites. Therefore, it is of primary importance to understand how the defects of CNTs contribute to the interfacial strength in polymer composites.

Due to its chemical rigorosity and easy manipulation of CNTs and matrix molecules at the atomic and molecular levels, molecular dynamics (MD) and molecular mechanics (MM) simulations have been preferred in evaluating the interfacial shear strength (IFSS) [3,30–33] between CNT and surrounding polymeric matrices. Simple quasi-static pull-out simulations of CNTs from a

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