Mechanical Properties of Graphene with Defects and Its Application in Nanocomposites – Brief Overview.

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Abstract. Graphene, monolayers of two-dimensional (2D) carbon atoms arranged in a honeycomb lattice structure have distinct properties in the field of materials especially in Nano composites. Graphene is also a potential nanofiller compared to other materials with better mechanical and thermal properties. However, synthesis of nanomaterial in its pristine form is challenging and defects are unavoidable during the synthesis through various techniques. Even though defects such as point and line defects may retard some physical properties, these are also intentionally created in specific applications such as nanocomposites, nanosensors and others. In this article various mechanical properties of nanofillers such as graphene with defects are compared in the application of composites.

1. Introduction

Extensive research is carried out on one atom thick carbon day by day due to its remarkable physical properties [1]. Unique 2D honeycomb lattice structure in graphene has outstanding physical properties such as modulus of elasticity (1100 GPa), High thermal conductivity and Fracture strength [2] and so on. Because of its unique properties it is found in many engineering applications such as memory devices, nanosensors, nanoactuators, graphene-based gas/bio sensors, solar cells and water purification [3]. It is also a top potential nanofiller in the field of nanocomposites. During the synthesis of nanomaterial defects are inevitable and bound to happen. Some of the defects are Vacancy, Grain boundary and Stone wales Defect (Figure 1). These defects are tailored in order to attain certain properties. For example, modulus of elasticity of graphene is reduced with increase in vacancy defect and flat declination in StoneWales [4] whereas defect concentration plays a major role in thermal conductivity.

Figure 1 - Defects in Graphene (a) single vacancy (SV), (b) double vacancy (DV) and (c) Stone Wales (SW) [12].
2. Effects of Nano fillers in composites

Guoson Shao found that mechanical properties of graphene nanoplatelet (GNPs) and copper (Cu) are increased and then decreased with increase in GNPs content [2]. Highest mechanical properties are achieved at 0.2 wt% volume of GNPs. Fadavi [5] found the agglomeration of SiC nanoparticles can be decreased with graphene encapsulating process. With thermally activated dislocation the strength of aluminium metal matrix composites can also be improved and pinning the SiC nanoparticles helps in increasing tensile ductility. Adding a slight volume of GNP managed to a major improvement in strength and stiffness of GNP/Al composites, also the elasticity and strength is relational with the dimension of GNPs [6]. Mohammad A. Rafiee and his team members stated that with less nanofiller graphene platelets is better than carbon nanotubes in terms of mechanical properties such as tensile strength, fracture toughness, Young’s modulus, fracture energy, and arresting fatigue crack growth[7].

3. Effects of defective Graphene in Nanocomposite

3.1. Thermal properties

Saeed et al., and his teammates stated that thermal conductivity of graphene is decreased with increase in concentration of defects and in amorphous graphene it is reduced drastically [8]. Also, thermal conductivity reduces when applied strain rate is increased. Addition of nitrogen and boron atoms in pure graphene decreases the thermal conductivity about 10 times of the defect concentration [9]. It is also proved that relation between thermal conductivity of polycrystalline graphene and strain falls by reducing the grain size. Ghasemi [3] in his work reported that thermal conductivity is directly proportional to porosity and nonlinear with respect to pore orientation. It is also found that the normalized heat capacity inversely proportional to porosity. Mortazavi [10] found that free standing graphitic carbon nitride (SgCN) is having 12% higher thermal conductivity along the armchair direction than zigzag. Through molecular dynamics simulations it was found that GNM with triangle and square nano holes having the same porosity have the lowest and highest thermal conductivities respectively [11]. Maoyuan Li [12] reported that STW and Multi vacancy defects are noticeably enhancing the Interfacial thermal conductance (ITC) of graphene and epoxy matrix when defect concentration is increased also the thermal conductivity with defective graphene is better compared to pristine graphene due to the improvement of ITC.

3.2. Mechanical properties

In Gr/polymer Nano composites, single and double vacancy are reducing cohesive and shear strength of the composite when the defect concentration is enlarged from 0%-13%[13] also shear strength is more sensitive to defects than the cohesive strength and with Stone Wales (SW) defect cohesive strength and shear strength are found to improve. Mechanical properties of graphene like modulus of elasticity, fracture strain and fracture strength are decreasing with the increase in temperature, with defects these properties are reducing particularly with singe vacancy at same concentration [14]. It is also proved that longitudinal modulus of elasticity and in-plane shear modulus are slightly decresing with the presence of Stone Wales defect. Whereas, the transverse shear modulus is improving with the increase of Stone Wales defect concentration [15]. Shaoping Xiao and Wenyi Hou found that single vacancy defect can extremely decrease the strain and failure stress of carbon nanotubes and in defected carbon nanotubes with a lesser volume fraction cannot reinforce but deteriorate the nanocomposites [16]. In radiation induced defects in carbon Nano tubes/ polymer derived ceramic (PDC) matrix composite increasing in the interfacial shear strength (IFSS) was observed and shorter pull-out lengths with higher defect levels is creating high bonding at the nano tube and PDC interface [17]. Jaemin cha proved that strong interfacial bonding between Melamine-CNTs and epoxy matrix increases the fracture toughness and presence of crack bridging mechanisms affecting the fracture toughness [18]. Graphene defect engineering with plasma treatment is enhancing the mechanical properties of graphene/metal composites [19]. Yogeeswaran et.al., found that multi wall carbon nanotubes (MWNT) synthesized through nitrogen doping is having certain degree of ductility at room
temperature\cite{20}. The wrinkles of Graphene and poly (methyl methacrylate) (PMMA) composite results in improvement of interfacial mechanical properties \cite{21} compared to flat graphene. Graphene and polymer composites with STW defects can critically increase the shear load bearing capability in longitudinal shearing \cite{22}. Another result shows that modulus of elasticity, tensile strength and fracture strain of the functionalized graphene weakens because of H-coverage up to 30% in hydrogen functionalized graphene \cite{23}. In grain boundary defects (GB) it can support or weaken graphene based on the position of these defects and arrangement, not by the density of defects \cite{24}. Seunghwa Yang \cite{25} stated that the longitudinal shear modulus is enhanced with the oxygen functional groups in nano composites comparing with the pristine graphene in oxygen functionalized graphene/polymer nanocomposites. Another research proved radiation damage in composite can be tailor-made by selecting the suitable component materials \cite{26}.

4. Conclusion
Various literature has been reviewed and the effects of defective graphene in numerous nanocomposite are examined. Based on the findings, defect concentration is important in the property of thermal conductivity. The defect concentration reduces the thermal conductivity of graphene. The mechanical properties of graphene such as modulus of elasticity, tensile strain and fracture toughness depends on the nature of defects and its geometry. Thus, by engineering the defects in nanofillers such as graphene can have numerous applications in mechanical as well as thermal application. I addition to that Nano composites is also a wide area in which monolayer of graphene with defects can be applied.

5. References
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