GRAPHENE-BASED COMPOSITE MATERIALS FOR AUTOMOTIVES

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ABSTRACT

The present initiative provides a summary overview on Graphene Related materials (GRM) for automotive applications and investigates efficient ways to integrate Graphene as polymer reinforcements within composite materials for energy-efficient and safe vehicles (EESVs). An approach that starts from the nano-scale through the Graphene elaboration by experiments to meso/macro-scale by continuum mechanics modelling is discussed with respect to some limiting factors in terms of the large scale production, the interfacial behaviour, the amount of wrinkling and network structure. Finally, a strategy for modelling such a composite is elaborated in the framework of the Graphene Flagship to well understand such limitations for a full applicability of Graphene. It is anticipated that this initiative will advance innovative lightweight graphene composites and their related modelling, designing, manufacturing, and joining capabilities suitable for automotive industry which requires unique levels of affordability, mechanical performance, green environmental impact and energy efficiency. This leads to complete understanding of the new graphene composites and their applicability in high-volume production scenarios.

1 INTRODUCTION

The automotive industry is a large and critical sector within the global economy. However, the global automotive industry is currently facing great challenges, such as responsibility for increasing annual CO_2 emissions, lack of strong decarbonisation targets, and safety issues. The development and manufacture of environmentally-friendly, EESV is a great solution to these challenges (Figure 1). The most effective way to enhance fuel consumption and to decrease CO_2 emissions is producing lighter vehicles. However, vehicle safety is usually compromised due to light-weighting. Due to the trade-off between light vehicles and safety standards, new directions need to be adopted to overcome safety issues. Several attempts have been made to strengthen vehicle structure to enhance crashworthiness, however, safety issues remain the main obstacle to producing lighter and greener cars. Therefore, the need to discover a new direction for greener and safer vehicles is urgent.

Recently, Graphene has attracted both academic and industrial interest because it can produce a dramatic improvement in properties at low filler content. Graphene is expected to have plenty of potential applications and the most immediate application for Graphene-based products is to be used in composite materials. The particular example of polymer nano-composites or polymer matrix composites which incorporate nanoscale filler materials could be highlighted. Indeed, Graphene-based polymers show substantial property enhancements at much lower loadings than polymer composites with conventional micron-scale fillers (such as glass or carbon fibres), which ultimately results in lower component weight and can simplify processing. Moreover, the multifunctional property enhancements made possible with nano-composites may create new applications of polymers. It has been found that by dispersing a small amount of graphene in polymers, many properties of the resulting composites, such as tensile strength and elastic modulus, electrical and thermal conductivity, thermal stability, gas barrier, and flame retardance can be significantly improved. Based on these multifunctional properties, graphene/polymer composites are promising as both structural and functional composites that can be widely used in various important fields. The previous mentioned properties make graphene-based polymers and composites good candidate for structural materials, with integration of functionalities, within automotive sector.

This initiative aims to analyse novel Graphene-based composite materials and their potential applications in automotive industry. To this end, the utilisation of Graphene in the fabrication of nano-composites with polymer matrices is investigated. Modelling, and design strategies are explored to enhance both vehicle and occupant safety; yet remain very light.

2 GRAPHENE-BASED COMPOSITES AND TODAY AUTOMOTIVE SEGMENT

From some recent experiments and numerical simulations, it has been clarified that the impact resistance and crashworthiness optimisation studies of advanced composites components remain at an early stage. No application of graphene-based materials is currently marketed in the automotive sector. Research activities are under development for study the potentiality of these systems and all the value’s chain of automotive needs to be involved in this effort. One of most challenge aim is the economic impact of the innovative structures on the vehicle market, all the value’s chain have to address their effort to get as low as possible the final cost of the innovative products. A large amount of work remains to be done to develop a practical, reliable and capable tool to analyse and design the new Graphene-based polymer composites and study the crashworthiness optimisation for its structures and their applications in the automotive industry. The Graphene-based polymer composites are still in infancy stage with regard to high-performance structural applications. There are no theoretical studies available in the technical literature on dynamic analysis and crash behaviour, as well as the fracture and failure behaviour of Graphene composites under severe loading conditions typical for automotive applications. The reliability of determining the homogenised response of such materials depends upon the ability to accurately capture the interfacial behaviour between the Graphene and the polymer matrix. Therefore, automotive sector looks forward innovation activities on this topic to assess its potential use for different applications both for structural and functional potentialities.

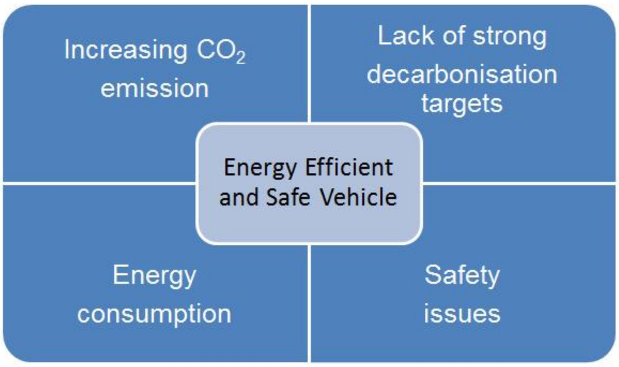

Figure 1: EESV and its compromising targets.

3 MATERIAL CHALLENGES

To take full advantage of its properties for applications, integration of individual Graphene in polymer matrices is prime important. Many factors, including the type of Graphene used and its intrinsic properties, the dispersion state of Graphene in the polymer matrix and its interfacial interactions, the amount of wrinkling in the Graphene, and its network structure in the matrix can affect the final properties and applications of Graphene-based polymer composites [1].

3.1 Large scale dispersion techniques

A key consideration when targeting the large scale production of Graphene nano-composites is the extent to which we can extrapolate the laboratory scale results in order to predict the properties of Graphene-reinforced polymers produced on a large-scale. Often the laboratory scale composites are produced using "ideal" Graphene i.e. known to contain only one or two layers. In reality, as we look to scale the Graphene production process, the likelihood is that we will produce material with a distribution of layer thicknesses. The question then is: what effect does the number of layers have upon the properties of the composite? This has been studied recently by Gong et al [2], who used Raman spectroscopy to firstly characterise the Graphene (in terms of number of layers) and also to monitor its subsequent deformation during atomic force microscopy (AFM) nano-indentation experiments on polymer composites, by utilising stress-induced shifts in the Raman bands.

This method has previously shown that individual flakes of Graphene have the capability to reinforce a polymer matrix but, interestingly, the recent work by Gong et al [2] has shown that bi-layer Graphene would be equally as good as monolayer Graphene, whilst tri-layer Graphene would only show a 15% reduction in reinforcing efficiency. Furthermore, it is only when the number of layers is >7 that the reinforcing efficiency of Graphene falls to less than half that of monolayer Graphene. If we consider the Graphene interlayer spacing in relation to the dimension of the polymer coils (which would separate the layers in a polymer composite), however, it can be shown that higher volume fractions of Graphene can be obtained for the multi-layer material than for monolayer Graphene. Therefore there is a balance to be struck between the ability to achieve higher loadings and the reduction in reinforcing efficiency as the number of Graphene layers is increased.

In addition, the best method of producing Graphene to be introduced in composites for industrial applications is the reduction of graphite oxide in controlled conditions. The chemical or thermal reduction of Graphene oxide can produce Graphene with a large number of defects, reducing the quality of the final product and worsening the expected properties. Without introducing functional groups, reduction of graphite oxide produces Graphene with different percentages of oxygen, a good quality Graphene need to have less than 2.5% of oxygen and preferable less than 1% of oxygen. However, the presence of oxygen helps to introduce new functional groups through chemical reaction such as covalent reactions (nucleophilic substitution, electrophilic substitution, and condensation and addition reactions) and non-covalent reactions [3]. The direct chemical reaction in pristine Graphene involves the use of powerful chemical reactions like radical reactions or the use of dienophiles to react with the C-C bond [4].

3.2 Modelling of Graphene-based composite materials

The number of theoretical/numerical works published on Graphene-based composites has so far been limited. A variety of techniques could be used in modelling the Graphene-based composite materials; however, the clear integrations between these techniques are still not clear for some applications (i.e. high performance structural applications). Much of the previous works has focused on modelling the elastic modulus at a set temperature. Since temperatures vary widely in space, a temperature-dependent model is required for the elastic modulus. There are two main approaches taken when modelling Graphene composites. The first focuses on the molecular level interactions. Molecular models use simulations to determine local interactions among atoms or chemical reactions between the matrix and nanotubes [5]. Molecular models are limited to very small systems due to their high computational cost. The second is continuum modelling which considers overall deformations. Continuum models include the Mori-Tanaka model, rule of mixtures, and the Halpin-Tsai model [6]. Multi-scale models, which combine molecular and continuum models, have also been developed [7].

Examples of existing works in this field are, for example, the molecular dynamics-based simulation techniques employed by Awasthi et al [8], who studied the load transfer mechanisms between polyethylene and a Graphene sheet. Cho et al. [9] employed a Mori-Tanaka approach to study the elastic constants of nano-composites with randomly distributed Graphene sheets. Most recently, Montazeri and Tabar [10] developed a multi-scale finite element model to study the elastic constants of a Graphene-based polymer nano-composite. Parashar and Mertiny [11] also proposed a multi-scale model using finite elements to characterise the buckling phenomenon in Graphene-based polymer composites.

4 GRAPHENE FLAGSHIP INITIAVE FOR A BETTER UNDERSTANDING

The Graphene flagship initiative through the **i**nnovative graphene-based polymer composite materials for automotive applications task proposes to investigate the Graphene-based polymer composites properties as candidate for structural applications. With the developed unique synthesis of the Graphene/polymer campsites, appropriate constitutive models are sought to predict their macro-scale behaviour. Great efforts will be given to establish and develop a reliable material models and constitutive laws to investigate the energy absorption characteristics of new developed Graphene-based polymer composites. New combination of several modelling techniques will be considered including Molecular Models (i.e. Monte Carlo Simulations); Continuum Models (i.e. Eshelby Model, Mori-Tanaka, representative volume elements (RVE), and Halpin-Tsai Model); and then using smooth transition analysis considering combination of both meso-scale and multi-scale modelling.

The proposed constitutive law will be implemented in LS-DYNA finite element code as a user defined material subroutine (UMAT). The explicit nonlinear finite element code LS-DYNA will be used as an effective tool to numerically simulate the problem and to predict the effect of the crash load on the proposed composite materials and its components. The software has the ability to simulate dynamic structural response in several ways, including pure Lagrangian, and coupled Lagrange–Eulerian methods. This accurate and reliable numerical simulation does not exist in the market for initial design concept for automotive applications for such novel Graphene-based composite materials.

This initiative will also optimise the proposed material models to enhance the energy absorbing capability to improve the vehicle safety.

5 CONCLUSIONS

The applicability of Graphene-based polymer composite materials is discussed during this work. Open challenges regarding Graphene reinforcements need to be addressed from experimental aspects to modelling viewpoints. They are related for instance to interfacial behaviour in the overall response, crashworthiness optimisation, large-scale applications. From modelling view point, this initiative presents strategies to overcome the above limitations by developing appropriate constitutive models to integrate the macro-scale behaviour. These strategies bind combination of several techniques form Molecular mechanics to Continuum mechanics. Finally, the developed constitutive law will be coupled with a finite element code for instance LS-DYNA.

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