10th International Conference on Composite Science and Technology
ICCST/10
A.L. Araújo, J.R. Correia, C.M. Mota Soares, et al. (Editors)

NOVEL COMPOSITE MATERIALS FOR AUTOMOTIVE APPLICATIONS: CONCEPTS AND CHALLENGES FOR ENERGY-EFFICIENT AND SAFE VEHICLES

Ahmed Elmarakbi[*], Wiyao Leleng Azoti[*]

[*]Faculty of Applied Sciences, University of Sunderland, Sunderland, UK, SR6 0DD
ahmed.elmarakbi@sunderland.ac.uk, Wiyao.Azoti@sunderland.ac.uk,

Key words: Automotive applications, Composite modelling and design, Energy efficient and safe vehicles, Graphene, Graphene composites.

Summary: *The present work provides an 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). The idea is based on the Concept-oriented lightweight design aiming of combination of light structures with novel multifunctional materials. For such a purpose, GRM are addressed with respect to some challenging factors for instance the large scale production of Graphene or the non-existence of constitutive material models for high performance structural applications like crashworthiness. Therefore, accurate material models need to be developed to support simulation of structural design for these vehicles. A focus on the hierarchical modelling of GRM with an emphasis on the multiscale constitutive behaviours of each material phase is elaborated in the framework of the Graphene Flagship to well understand such limitations for a full applicability of Graphene.*

1 INTRODUCTION

The need for reducing motors engines pollution has been generalized since the carbon footprint become an important design parameter for improving the fuel economy of conventional, gasoline-powered automobiles. Electric-based vehicles, advanced combustion and fuels technologies have been developed to improve energy efficiency of cars and trucks. Lightweight materials are another important technology that can improve passenger vehicle fuel efficiency by 6–8% for each 10% reduction in weight while also making electric and alternative vehicles more competitive [1]. Therefore, the new generation of vehicles must be lighter, less polluting and more fuel-efficient. Their design should be developed aiming for individual mobility whilst also retaining safety, environmental friendliness and affordability [2]. These issues can be overcome by the design of Energy Efficient and Safe Vehicles EESVs which represents a good alternative for conventional vehicles. EESVs embed engineering research mainly focused on the area low carbon vehicles, electrical and hybrid vehicles, advanced materials and structures, vehicles safety and crashworthiness, vehicles dynamics control systems, fuel cells, advanced maintenance, digital engineering technologies, human factors and manufacturing systems. This engineering strategy known as *Concept-oriented lightweight design* results in the combination of light structures and multifunctional materials. However, significant hurdles remain with respect to improved performance, manufacturability, cost, and modelling for such materials [1]. As a consequence, considerable materials science effort and new discovery need to be developed to overcome these hurdles. The discovery Graphene with its interesting properties in terms of tensile strength and elastic modulus, electrical and thermal conductivity, thermal stability, gas barrier, and flame retardance has opened promising window for designing novel light composites while improving trade-off between lightweighting and safety issues.

In this work, it is aimed to analyse novel Graphene-based composite materials and their potential applications on EESVs. To this end, the generalised use of composite materials in automotive is presented as well as the energy efficiency processing with the trade-off with safety. The design concepts of novel Graphene/Polymer composite materials for EESVs is elaborated to enhance both vehicle and occupant safety; yet remain very light with the main issues related to technological challenges ahead of EESVs. Finally, a focus is made on the hierarchical material modelling that accounts for the constitutive behaviour of each phase within the composite by a multiscale strategy.

2 AUTOMOTIVE AND COMPOSITE MATERIALS: CONVENTIONAL COMPOSITE MATERIALS AND THEIR USE IN AUTOMOTIVE APPLICATION IN GENERAL

The growing trend to substitute conventional steel and cast irons in vehicles for lightweight purpose leads to the development of automotive components with lighter materials. Among them, conventional materials for instance aluminium or magnesium alloy and ultra high strength steel are used in the engine block, cylinder heads as well as in transmission, cases, valves bodies and channel plates [4]. Besides these materials, others categories show most promise for instance fibre-reinforced polymer composites (including carbon and glass fibres), and advanced polymers (without fibre reinforcement) [1]. Other materials such as metal matrix composites MMC are also considered with a low-cost development processing. These latter i.e MMC cover a range of non-metallic particles/fibres based metallic matrix with a significant improvement of tensile, yield and fatigue strength over the entire range of temperature. MMCs have also enhanced physical properties such as higher modulus, lower thermal expansion coefficient, improved tribology characteristics and higher hardness versus unreinforced Aluminium [4]. An illustration of the use of MMCs in automotive is within the engine block cylinder liners. Indeed, Cole et al. [4] reported that Al MMC liners can improve engine operating efficiency by reducing knock since heat transfer from the cylinder to the water jacket is improved as the result of its increased thermal conductivity. Another application of MMC is found with the pistons. Indeed, by using low coefficient of expansion/ low thermal conductivity/high strength MMC insert at piston combustion face, Toyota produced pistons for diesel engines which could run at higher temperature leading, therefore, to reduced emissions in gasoline engines [4].

3 ENERGY EFFICIENT AND SAFE VEHICLES: GENERAL ENERGY EFFICIENCY PROCESSING/SOLUTIONS AND THEIR RELATIONS/TRADE OFF WITH SAFETY

The energy efficiency is supported by variety of technology among which the weight reduction through multifunctional materials. They are essential for boosting the fuel economy of modern automobiles while maintaining safety and performance. Because it takes less energy to accelerate a lighter object than a heavier one, lightweight materials offer great potential for increasing vehicle efficiency. Joost [1] reported that 10% reduction in vehicle weight can result in a 6%-8% fuel economy improvement when vehicle performance characteristics are maintained. A 10% weight reduction for an electric vehicle can improve electric range by 13.7% while a 5.1% improvement in fuel economy for a 10% weight reduction in a hybrid electric vehicle [1].

Replacing cast iron and traditional steel components with lightweight materials such as high-strength steel, magnesium (Mg) alloys, aluminium (Al) alloys, carbon fibre, and polymer composites can directly reduce the weight of a vehicle's body and chassis by up to 50 percent. However, significant problems exist regards to safety trade-off. They are concerned with improved performance, manufacturability, cost, and modelling. Joost [1] identify the following hurdles regards to advanced materials used in the automotive weight reduction:

- Advanced high-strength steels AHSS: No identified microstructures for meeting both strength and ductility requirements of third-generation AHSS; susceptibility to local failure during forming and crash; difficulty incorporating significant hardening/softening behaviour associated with forming and joining into processing and design models;
- Aluminium alloys: Limited formability of automotive grades at room temperature; relatively high cost of sheet material; difficulty casting complex, high-strength parts; insufficient strength and/or stiffness for certain structural applications;
- Magnesium alloys: Very low formability of sheet alloys at room temperature; challenge cost effectively preventing galvanic corrosion; insufficient strength, ductility, and stiffness for certain structural applications; difficulty incorporating unique deformation behaviour into processing and design models;
- Fibre-reinforced polymer composites: High cost of carbon fibre; limited weight reduction potential of glass fibre; long cycle times for many process; difficulty incorporating structure at many length scales into processing and design models;
- Advanced polymers: Low cure rates associated with ease of mold-filling increases cycle times; petroleum-based precursors are dependent upon the price of oil while nonpetroleum precursors are not yet mature; susceptible to deterioration during high-temperature processing such as in automotive paint ovens.

Overcoming these technical hurdles requires considerable materials science effort and new discovery. That is the case of Graphene. It has attracted both academic and industrial interest because it can produce a dramatic improvement in properties at low filler content.

4 NOVEL COMPOSITES SOLUTIONS: GRAPHENE-BASED COMPOSITES

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. However, to take full advantage of its properties for applications, integration of individual Graphene in polymer matrices is prime important. Many challenges, in terms of mechanical and interfacial properties can affect the final properties and applications of Graphene-based polymer composites

4.1 Concepts

They are based on the *Concept-oriented lightweight design* that results in the combination of light structures with novel multifunctional materials. The ***Graphene Flagship*** through one of its comprehensive tasks, the **i**nnovative **G**raphene-based Polymer **C**omposite materials for **Auto**motive ***iGCAuto*** applications, proposes to combine novel materials concepts with the latest safety design approaches through the development and optimization of advanced ultra-light Graphene-based polymer materials, efficient fabrication and manufacturing processes, and life-cycle analysis to reduce the environmental impact of future vehicles. It allows the utilisation of Graphene-based materials in the fabrication of nanocomposites with different polymer matrices to be investigated, modelled, and designed, as candidate for structural applications, to enhance both vehicle and occupant safety; yet remain very light (Figure 1). This material will provide benefits such as improved strength, dimensional stability and better thermal behaviour, better flame behaviour (active as flame retardant and for reducing the emission of smoke), and superior durability.

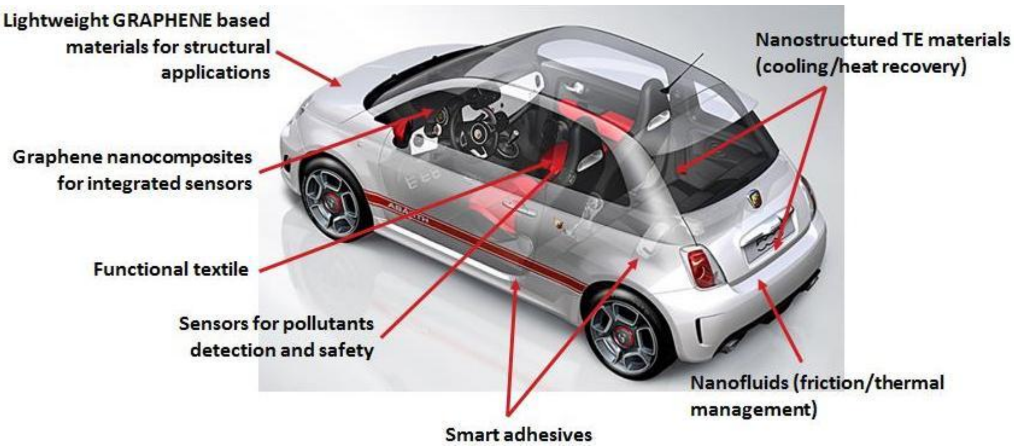

Figure 1: Potential applications of Graphene-based composite in automotive

The initiative also focuses on the development of advanced Graphene-based materials for vehicles, contributing to an accelerated market introduction of new energy-efficient and safe vehicles (Figure 2). This initiative is complex and multidisciplinary by nature. In order to successfully reach the technical objectives of the work, a holistic approach is adapted to include a wide range of activities spanning from material development and new synthesis to final products and new joining and fabrication technologies as shown in Figure 3.

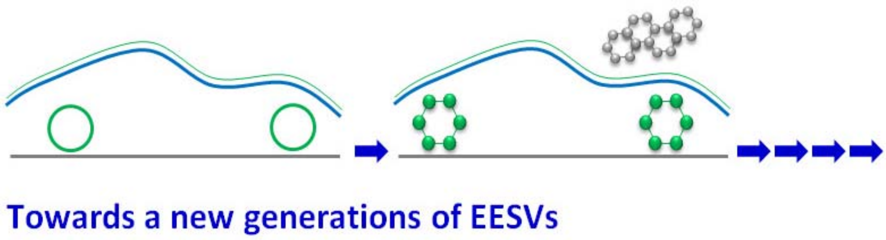

Figure 2: Moving towards Graphene-based composite Car

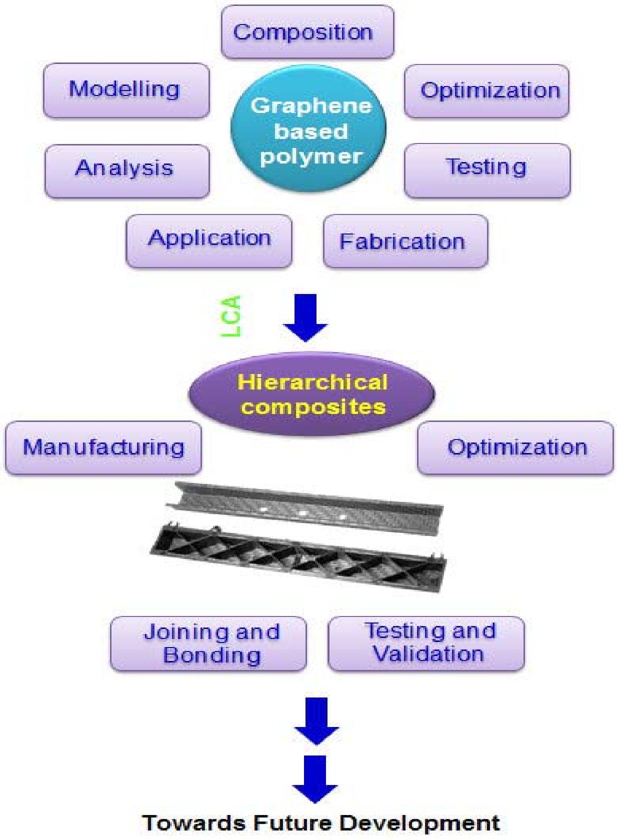

Figure 3: Approach for Automotive Graphene Composites

4.2 Technological challenges ahead of Graphene-based composites

Though, several technologies are embedded in the next generations of multifunctional Graphene-based composites, there are still a lot of technological challenges to overcome, particularly in the area of 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 [5]. Hence, the present challenges for researchers are in the development of lightweight, high-performance, cost-effective and multi-material solutions:

- Lack of new methods of large scale production of Graphene based products - mechanical exfoliation is not scalable to an industrial process;
- Lack of new methods of functionalization;

- Investigation of the exfoliation process of Graphene based material during the process;
- Expected low ductility of Graphene-based composites structure. Considering implementation on several vehicle components (i.e. front end), this will lead to high vehicles' deceleration, which minimising the vehicle safety;
- Insufficient knowledge on attainable strength/stiffness of Graphene thermosets/ thermoplastic polymer composites;
- No existed materials model on commercial explicit finite element software to model Graphene based composite materials for high performance structural applications;
- Graphene-based composite material characterisation and modelling still not fully investigated especially with regard to automotive applications and different loading conditions;
- Lack of knowledge on Graphene composites for high performance structural applications and interface properties between the Graphene and polymer matrix under severe loading condition (i.e. fragmentation and crash);
- Preparation of automotive composites-Lack of knowledge on how to design in Graphene composites automotive structures that can offer high stiffness, strength and predictable and safe failure modes;
- Nowadays vehicle and body architectures do not usually take advantage of the essential qualities of new composite materials;
- Some approaches to joining and bonding of Graphene-based composites parts insufficiently covered by simulation and modelling tools; no automotive experience available;
- The joining of dissimilar materials is not covered by an appropriate know-how and several critical points are not yet solved by the scientific community and researcher;
- Great attentions focused on embedded CO_2 in overall LCA within lightweighting process; however, no solid info on how to evaluate pro's and con's inside design process.

Besides, 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.

5 APPLICATION EXAMPLE ON THE MODELLING OF GRAPHENE COMPOSITE MATERIALS FOR AUTOMOTIVE APPLICATION

A working modelling example is depicted by Figure 4. It deals with a multiscale modelling of Graphene/polymer composites for automotive lightweighting or crashworthiness purposes. The constitutive law of each phase in the composite is accounted for by a comprehension derivation of the mechanical properties. Indeed, a starting point of such modelling is the derivation of Graphene Sheets mechanical properties. At the atomistic scale, the Graphene sheet is considered undergoing non-linear deformations. Therefore, a Taylor series expansion in powers of strains [6], establishes the expressions of its second order linear elastic modulus ***E*** and third order non-linear elastic modulus ***D***. This enables the derivation of a non-linear constitutive behaviour and thus based on the Modified Morse potential [7, 8]. For the polymer matrix, a rate-dependent elasto-plastic behaviour is selected to account for the crashworthiness. Also, it is assumed that the matrix undergoes ductile damage behaviours with either isotropic or kinematic hardening. The modelling strategy developed in [9] is used to express the consistent tangent operator of the polymer matrix.

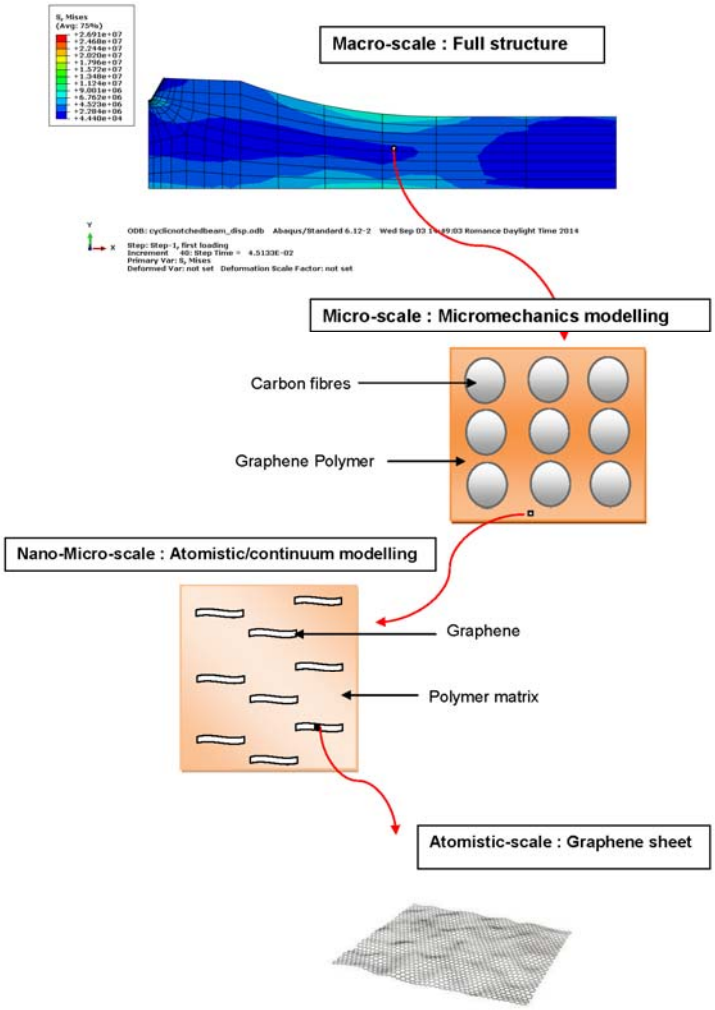

Figure 4: Multiscale modelling of Graphene/polymer composites

The homogenized properties of the Graphene Polymer Composites are derived by combining atomistic continuum approaches with micromechanics methods. To this end, a RVE is selected such as Graphene sheet represents the inclusion phase that will be embedded in the polymer matrix phase. To resolve the heterogeneous material problem, the kinematic integral equation of Dederichs and Zeller [10] is used as formal solution of micromechanics problem leading to the derivation of the global concentration tensors of Graphene and polymer phases. At this level, the multi-site version of the global concentration tensor is adopted by accounting for the topological (spatial orientation and distribution of the phases) and morphological (aspect ratio, volume fraction, mechanical properties) textures. Mean-fields approaches (Mori-Tanaka [11], Self-Consistent [12-14], Generalized Self-Consistent [15, 16], Incremental [17] or Differential [18] schemes) can therefore be applied for the overall response of the composite. A Double-scale approach combining Graphene Polymer composite developed above as matrix phase in which are embedded carbon fibres is used to carry out the effective response of a carbon fibre-reinforced Graphene Polymer composite.

Finally, the proposed constitutive law is proposed to be implemented within a finite element code as a user defined material subroutine (UMAT). The explicit nonlinear finite element code LS-DYNA represents 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. This 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.

6 IMPACT

This initiative will impact on the quality of life: ultra-light vehicles will offer low energy consumption, and low CO2 impact. The lightweighting of vehicles will accelerate their uptake in many market segments, and this in turn will have a direct positive impact especially on the quality of life in environments that today are suffering from excessive amounts of NOx and other unhealthy greenhouse gases (GHG), combined with excessive concentrations of diesel particles. The project will result in the development of the world’s first graphene-based polymer materials to be used in a large scale for vehicle bodies, in order to enhance their efficiency and safety standards. The results will benefit the automotive companies and relevant industries with optimised graphene-composite material properties in body parts, body-in-white, chassis and heavier interior systems. The development of novel materials will be of huge benefit to the global automotive industry. As the developed material could be used in several applications, the impact of the research will benefit a wide range of industry.

The main application targeted in this work is the automotive industry. This initiative also assures its impact in this sector by the inclusion of world-class academic and industrial partners within both automotive and materials sectors that, though focussing principally on passenger vehicle applications, will assure spin-off to their industrial vehicles affiliates. Higher performance composite parts offer a tremendous light-weighting benefit to transport vehicle sectors, of which automotive is by far the largest. Lightweighting is a top strategic and competitive priority for all transport vehicle industries, and cost effectiveness as well as industrialisation are key issues that remain as yet unsolved.

7 CONCLUSION

Lightweighting becomes an important issue for energy efficiency in automotive. It arises the need for developing a novel generation of materials that will combine both weight reduction and safety issues. Throughout this work, the applicability of Graphene-based polymer composite materials is discussed regards to the fulfilment of these requirements. For such a composite, open challenges concerning Graphene reinforcements need to be addressed. 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 is candidate for an implementation within a finite element code for instance LS-DYNA.

ACKNOWLEDGEMENTS

The research leading to these results has received funding from the European Union Seventh Framework Programme under grant agreement **no. 604391 Graphene Flagship.**

REFERENCES

[1] WilliamJ. Joost. Reducing vehicle weight and improving u.s. energy efficiency using integrated computational materials engineering. *JOM*, 64(9):1032–1038, 2012.

[2] Gundolf Kopp, Elmar Beeh, Roland Scholl, Alexander Kobilke, Philipp Strassburger, and Michael Krieschera. New lightweight structures for advanced automotive vehicles-safe and modular. *Procedia - Social and Behavioral Sciences*, 48(0):350 – 362, 2012.

[3] Shaik Amjad, S. Neelakrishnan, and R. Rudramoorthy. Review of design considerations and technological challenges for successful development and deployment of plug-in hybrid electric vehicles. *Renewable and Sustainable Energy Reviews*, 14(3):1104 – 1110, 2010.

[4] G.S. Cole and A.M. Sherman. Light weight materials for automotive applications. *Materials Characterization*, 35(1):3 – 9, 1995. Microstructural Characterization of Lightweight Structural Materials Transportation.

[5] Xiaohong An, Trevor Simmons, Rakesh Shah, Christopher Wolfe, Kim M. Lewis, Morris Washington, Saroj K. Nayak, Saikat Talapatra, and Swastik Kar. Stable aqueous dispersions of noncovalently functionalized graphene from graphite and their multifunctional high-performance applications. *Nano Letters*, 10(11):4295–4301, 2010. PMID: 20557029.

[6] Changgu Lee, Xiaoding Wei, Jeffrey W. Kysar, and James Hone. Measurement of the elastic properties and intrinsic strength of monolayer graphene. *Science*, 321(5887):385–388, 2008.

[7] J.R. Xiao, B.A. Gama, and J.W. Gillespie Jr. An analytical molecular structural mechanics model for the mechanical properties of carbon nanotubes. *International Journal of Solids and Structures*, 42:3075 – 3092, 2005.

[8] J. Cho, J.J. Luo, and I.M. Daniel. Mechanical characterization of graphite/epoxy nanocomposites by multi-scale analysis. *Composites Science and Technology*, 67(11â€“12):2399 – 2407, 2007.

[9] A. Tchalla, W.L. Azoti, Y. Koutsawa, A. Makradi, S. Belouettar, and H. Zahrouni. Incremental mean-fields micromechanics scheme for non-linear response of ductile damaged composite materials. *Composites Part B: Engineering*, 69(0):169 – 180, 2015.

[10] P. H. Dederichs and R. Zeller. Variational treatment of the elastic constants of disordered materials. *Zeitschrift für Physik A Hadrons and Nuclei*, Volume 259, Number 2, 103-116, DOI: 10.1007/BF01392841, 1973.

[11] T Mori and K Tanaka. Average stress in matrix and average elastic energy of materials with misfitting inclusions. *Acta Metallurgica*, 21(5):571 – 574, 1973.

[12] Av Hershey. The elasticity of an isotropic aggregate of anisotropic cubic crystals. *Journal of applied mechanics-transactions of the asme*, 21(3):236–240, 1954.

[13] E. Kröner. Effective moduli of random elastic media-unified calculation of bounds and self-consistent values. *Mechanics Research Communications*, 4(6):389 – 393, 1977.

[14] E. Kröner. Bounds for effective elastic moduli of disordered materials. *Journal of the Mechanics and Physics of Solids*, 25(2):137 – 155, 1977.

[15] E. Hervé and A. Zaoui. n-layered inclusion-based micromechanical modelling. *International Journal of Engineering Science*, 31(1):1 – 10, 1993.

[16] P. Lipinski, E.H. Barhdadi, and M. Cherkaoui. Micromechanical modeling of an arbitrary ellipsoidal multi-coated inclusion. *Philosophical Magazine*, 86(10):1305–1326, 2006.

[17] P. Vieville, A. S. Bonnet, and P. Lipinski. Modelling effective properties of composite materials using the inclusion concept. general considerations. *Arch. Mech.*, 58(3):207–239, 2006.

[18] S. Nemat-Nasser and M. Hori. *Micromechanics: Overall properties of heterogeneous materials*. 1993.