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Mechanical prediction of graphene-based polymer nanocomposites for energy-efficient and safe vehicles

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Abstract

This work investigates efficient ways of lightweighting vehicles structures based on Graphene Related materials (GRMs). An integration of Graphene as polymer reinforcements within composite materials for energy-efficient and safe vehicles (EESVs) is addressed with respect to some technological challenges for instance the lack of constitutive material models for high performance structural applications. Therefore, accurate material models need to be developed to support simulation of structural design for these vehicles. A multi-scale modelling of Graphene reinforced polymer composite is elaborated and using the Mori-Tanaka micro-mechanics scheme, the effective non-linear behaviour is predicted for various micro-parameters such as the aspect ratio and volume fractions. The results show an enhancement of the equivalent macro stress-strain response when the aspect ratio is low corresponding to platelets-like inclusions. Also, the volume fraction is seen to have a good improvement on the composite response. The results highlight the effect of Graphene platelets versus Carbon and Glass fibres in the design of lightweight structures with enhanced mechanical responses and by consequence a CO₂ emissions reduction.

Key words: Automotive applications, Energy efficient and safe vehicles, Graphene, Graphene composites, Mori-Tanaka scheme, Elasto-plasticity.

1. Introduction

Lightweighting is a priority for several sectors (e.g. automotive, rail, aerospace) and there is a global drive towards lighter structures for energy efficiency and reduction of carbon footprint. Development of advanced composite materials (ACM) that offer substantial weight reduction, while improving strength, is in a great demand by several industries. The automotive industry, as one of the largest and critical sectors within the global economy, is widely viewed as an area of the greatest volume use for ACM in the future for production of light vehicles. Nowadays, several advanced materials are widely used in the automotive industry; however, vehicle safety is usually compromised due to lightweighting [1]. Indeed, 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].

With the current pressure growing on automotive manufactures to have strong decarbonisation targets and to reduce annual CO₂ emissions and fuel consumption by developing environmentally-friendly, energy-efficient and safe vehicles (EESV), they are studying better alternatives to current design trends and ACM. Therefore, the design of the new generation of vehicles (namely EESV) should be developed aiming for individual mobility whilst also retaining safety, environmental friendliness and affordability [2]. However, the use of advanced composites in structural vehicle body applications has been far less extensive [3]. Significant hurdles remain with respect to their improved performance, manufacturability, cost, and modelling [1]. As a consequence, considerable materials science effort and new discovery need to be developed to overcome these hurdles.

Graphene is at the centre of an ever growing academic and industrial interest because it can produce a dramatic improvement in mechanical properties at low filler content [4]. Indeed, it is expected that one of the most immediate application for graphene will be in composite materials [5]. To take a full advantage of its properties, integration of individual graphene sheets in polymer matrices is important. Exceptional physical thermomechanical properties, a high surface/volume ratio and low filler content of graphene make it a promising candidate for developing the next-generation of polymer composites [6-8]. Graphene has been used to increase stiffness, toughness and thermal conductivity of polymer resins by a large margin [9-12]. However, many

challenges, including the lack of materials model on commercial explicit finite element software to model Graphene based composite materials for high performance structural applications can affect the final properties and applications of graphene composites.

In this work, it is aimed to analyse novel Graphene-based composite materials and their potential applications on EESVs. To this end, 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 multi-scale material modelling to pave the way of a better understanding of the contribution of Graphene in the enhancement of polymer matrix composites for high performance structural applications.

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 [13]. 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 [13]. An illustration of the use of MMCs in automotive is within the engine block cylinder liners. Indeed, Cole et al. [13] 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 [13].

3. Energy efficient and safe vehicles: general energy efficiency processing/solutions and their relations/trade off with safety

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].

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 initiative through the innovative **Graphene-based Polymer Composite** materials for **Automotive iGCAuto** applications propose to combine novel materials concepts with the latest safety design approaches through the development and optimisation 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.

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.

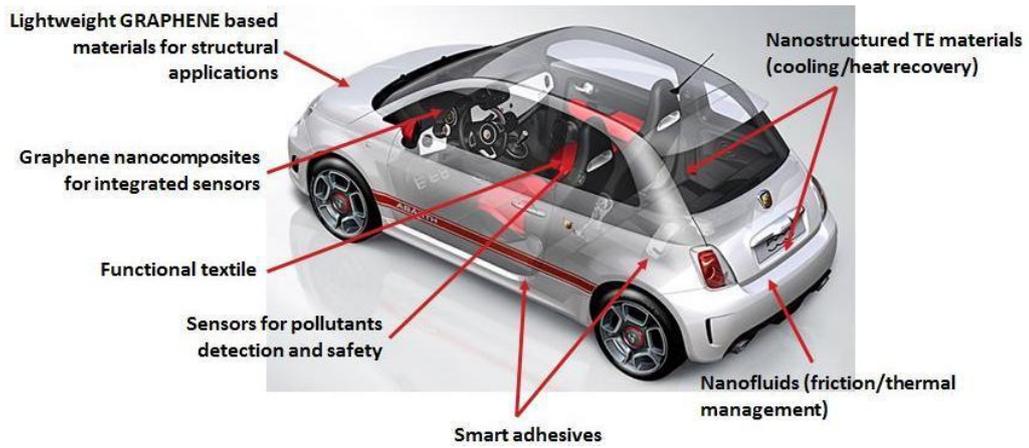
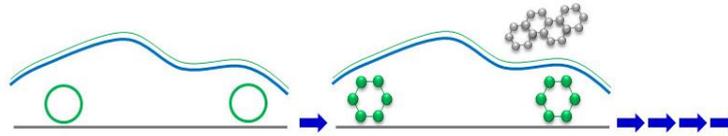


Figure 1: Potential applications of Graphene-based composite in automotive



Towards a new generations of EESVs

Figure 2: Moving towards Graphene-based composite Car

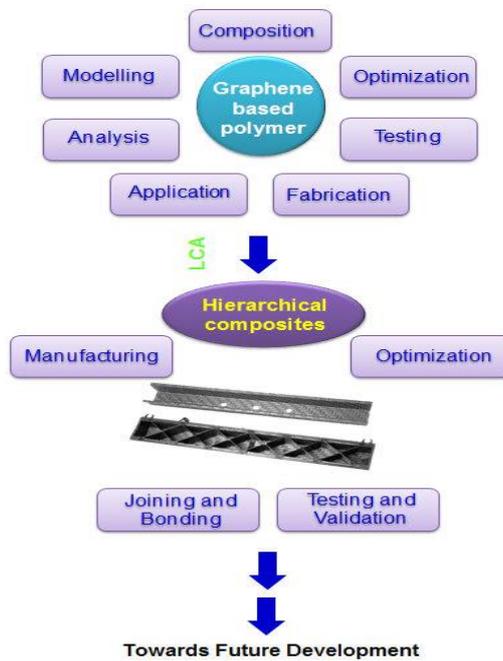


Figure 3: Approach for Automotive Graphene Composites

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 [14]. 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 CO₂ in overall LCA within lightweighting process; however, no solid info on how to evaluate pro's and con's inside design process.

In addition, efforts need to establish and develop reliable material models and constitutive laws combining several modelling techniques ranged from molecular models to continuum models using smooth transition analysis considering combination of both meso-scale and multi-scale modelling. In the sequel, an application example of constitutive modelling is done by using a multiscale approach

5. Modelling application on graphene composite materials

The multiscale modelling strategy is depicted by Figure 4. It is consisted on:

- the modelling of *2-phases Graphene/polymer* composite. The mechanical properties of the Graphene which are widely derived at the atomistic scale [15, 16] are considered through graphene platelets GPL as continuum phases interacting with the polymer matrix.

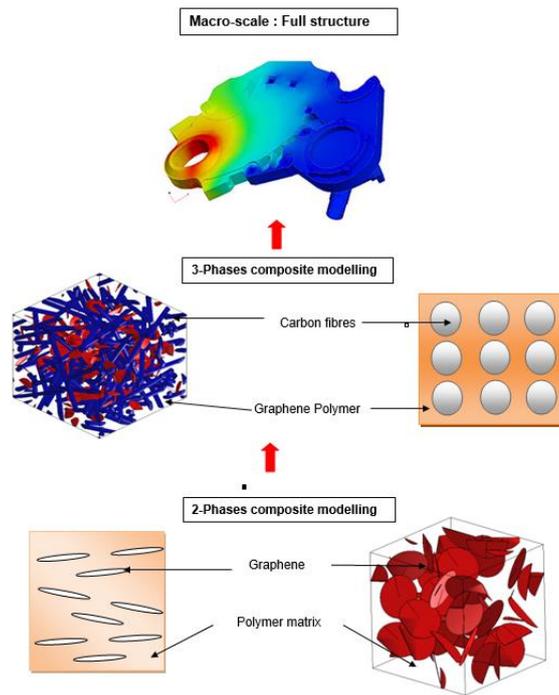


Figure 4: Multiscale modelling of Graphene/polymer composites

- The modelling of *3-phases Carbon fibres/Graphene polymer* composite. It consists on a double-scale approach combining the *2-phases Graphene Polymer* composite developed above as matrix phase in which are embedded the Carbon fibres. The derivation of the effective properties remains analytical-based micromechanics formalism.
- And the *full structure* simulation by a multiscale strategy. At each Gauss integration point within a macro model, will be implemented the above constitutive laws for *3-phases Carbon fibres/Graphene polymer* composite using a User-defined Materials UMAT subroutine.

To pave the way for a better understanding of the GPL influence in the enhancement of mechanical properties of the hierarchical composite, the *2-phases composite* is studied in the sequel of this work through a mean-field homogenisation formalism.

5.1. Mean field homogenisation formalism

A macroscopic homogeneous and microscopic heterogeneous materials is selected under a representative volume element RVE as depicted by Figure 5. The associated boundary-value problems are formulated, in the terms of uniform macro field traction vector or linear displacement fields. The RVE is assumed to be in equilibrium and its overall deformation compatible. Also the body forces and inertia term are absent.

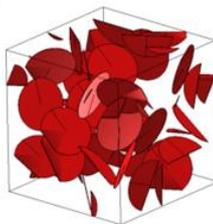


Figure 5: 3D schematics of a RVE of platelets reinforced polymer

These general considerations are restricted to the case of a linear constitutive law under small transformation

approximation. They can be summarised like:

$$\sigma_{ij,j} = 0 \quad (1)$$

$$\varepsilon_{ij} = \frac{1}{2}(u_{i,j} + u_{j,i}) \quad (2)$$

where σ_{ij} , ε_{ij} and u_i represent respectively the components of the stress and strain tensors and the elastic displacement. At each point r in the RVE, the local elastic constitutive law is written such as:

$$\sigma_{ij}(r) = c_{ijkl}(r)\varepsilon_{kl}(r) \quad (3)$$

The scale transition is now introduced to make the relationship between the micro scale (local) and macro scale (global) elastic properties. It consists firstly in the *localisation* of the global strain tensor by the introduction of a fourth order global strain concentration tensor \mathbf{A} such as:

$$\varepsilon_{ij}(r) = A_{ijkl}(r)E_{kl} \quad (4)$$

The second part of the scale transition is the *homogenisation* which employs averaging techniques to approximate the macroscopic behaviour:

$$\Sigma_{ij} = \frac{1}{V} \int_V \sigma_{ij}(r) dV \quad (5)$$

$$E_{ij} = \frac{1}{V} \int_V \varepsilon_{ij}(r) dV \quad (6)$$

Replacing Eq. (4) in Eq. (3) and combining the result with Eq. (5), leads to the effective properties given by:

$$C_{ijkl}^{eff} = \frac{1}{V} \int_V c_{ijmn}(r) A_{mnkl}(r) dV \quad (7)$$

Or in others terms

$$\mathbf{C}^{eff} = \sum_{I=0}^N f_I \mathbf{c}^I : \mathbf{A}^I \quad (8)$$

with \mathbf{c}^I , \mathbf{A}^I , f_I the uniform stiffness tensor, the strain concentration tensor and the volume fraction of phase I respectively. Using, the Eshelby's inclusion concept [17], the final expression of the global strain concentration tensor is given by an iterative procedure [18] such as:

$$\left\{ \begin{array}{l} \mathbf{A}^I = \mathbf{a}^I : \langle \mathbf{a}^I \rangle^{-1} \\ (\mathbf{a}^I)_0 = \mathbf{I} \\ (\mathbf{a}^I)_{i+1} = (\mathbf{I} + \mathbf{T}^{II} : \Delta \mathbf{c}^I)^{-1} : \left(\mathbf{I} - \sum_{\substack{J=0 \\ J \neq I}}^N \mathbf{T}^{IJ} : \Delta \mathbf{c}^J : (\mathbf{a}^J)_i \right) \\ I = 0, 1, 2, 3, \dots, N \end{array} \right. \quad (9)$$

where \mathbf{a}^I states for the local strain concentration tensor and $\Delta \mathbf{c}^J = \mathbf{c}^J - \mathbf{c}^0$. \mathbf{T}^{IJ} represents the interaction tensor between inclusions. In the case where the interactions between inclusions are neglected i.e $\mathbf{T}^{IJ} = 0$ (most of case in the open literature), the local concentration tensor \mathbf{a}^I reads more simple expression:

$$\mathbf{a}^I = \left[\mathbf{I} + \mathbf{T}^{II} : \Delta \mathbf{c}^I \right]^{-1} = \left[\mathbf{I} + \mathbf{S} : (\mathbf{c}^0)^{-1} : \Delta \mathbf{c}^I \right]^{-1} \quad (10)$$

where \mathbf{S} represents the Eshelby's tensor [17]. Its expression depends on the aspect ratio $\alpha = c/a$ of the ellipsoidal inclusion of semi-axis (a, b, c) and the material properties of the surrounding matrix \mathbf{c}^0 . Under the Mori-Tanaka MT [19] assumptions, the global strain concentration tensor of the matrix is expressed as [18, 20]:

$$\mathbf{A}^0 = \mathbf{a}^0 : \langle \mathbf{a}^I \rangle^{-1} = \left(f_0 \mathbf{I} + \sum_{I=1}^N f_I \mathbf{a}^I \right)^{-1} \quad (11)$$

leading to the effective MT properties through Eq. (8) such as:

$$\mathbf{C}^{MT} = \sum_{I=0}^N f_I \mathbf{c}^I \mathbf{A}^I = \left(f_0 \mathbf{c}^0 + \sum_{I=1}^N f_I \mathbf{c}^I \mathbf{a}^I \right) : \mathbf{A}^0 \quad (12)$$

5.2. Derivation of non-linear tangent operators

Within the RVE, let assume that one or more phases behave elasto-plastically. Referring to the work by Doghri and Ouair [21] at least two tangent operators can be defined: the ‘‘continuum’’ (or elasto-plastic) \mathbf{C}^{ep} tangent operator, which is derived from the rate constitutive equation, and the ‘‘consistent’’ (or algorithmic) \mathbf{C}^{alg} tangent operator, which is solved by a discretisation in the time interval $[t_n, t_{n+1}]$. These tangent operators are related to the rate of the constitutive equation as follows:

$$\begin{cases} \dot{\boldsymbol{\sigma}} = \mathbf{C}^{ep} : \dot{\boldsymbol{\varepsilon}} \\ \delta \boldsymbol{\sigma}_{n+1} = \mathbf{C}^{alg} : \delta \boldsymbol{\varepsilon}_{n+1} \end{cases} \quad (13)$$

They are derived from the classical J_2 flow rule:

$$\begin{cases} \boldsymbol{\sigma} = \mathbf{C}^{el} : (\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^p) \\ f = \sigma_{eq} - R(p) - \sigma_Y \\ \dot{\boldsymbol{\varepsilon}}^p = \dot{p} \mathbf{N}, \quad \mathbf{N} = \frac{\partial f}{\partial \boldsymbol{\sigma}} = \frac{3}{2} \frac{dev(\boldsymbol{\sigma})}{\sigma_{eq}} \\ \sigma_{eq} = \left(\frac{3}{2} \mathbf{s} : \mathbf{s} \right)^{1/2} \end{cases} \quad (14)$$

The ‘‘continuum’’ (or elasto-plastic) \mathbf{C}^{ep} tangent operator yields:

$$\begin{cases} \mathbf{C}^{ep} = \mathbf{C}^{el} - \frac{(2\mu)^2}{h} \mathbf{N} \otimes \mathbf{N} \\ h = 3\mu + \frac{dR}{dp} > 0 \end{cases} \quad (15)$$

while the ‘‘consistent’’ (or algorithmic) \mathbf{C}^{alg} tangent operator is given by:

$$\begin{cases} \mathbf{C}^{alg} = \mathbf{C}^{ep} - (2\mu)^2 \Delta p \frac{\sigma_{eq}}{\sigma_{eq}^{tr}} \frac{\partial \mathbf{N}}{\partial \boldsymbol{\sigma}} \\ \frac{\partial \mathbf{N}}{\partial \boldsymbol{\sigma}} = \frac{1}{\sigma_{eq}} \frac{3}{2} \mathbf{I}^{dev} - \mathbf{N} \otimes \mathbf{N} \end{cases} \quad (16)$$

In equations (15) and (16), μ denotes the material shear modulus while \mathbf{C}^{el} represents the elastic stiffness tensor and $R(p)$ is the hardening stress function with p the accumulated plastic strain. \mathbf{N} represents the

normal to the yield surface in the stress space. σ_{eq}^{tr} denotes a trial elastic predictor of σ_{eq} . \mathbf{I}^{dev} stands for the deviatoric part of the fourth order symmetric identity tensor. The knowledge of internal variables such as Δp and σ_{eq}^{tr} is important for computing the algorithmic tangent operator in Eq. (16). A detailed procedure about the update of internal variables can be found in Azoti et al. [22]. \mathbf{C}^{alg} will be later used to determine the overall composite behaviour using the MT scheme by Eq. (12).

5.3. Numerical results and discussions

The numerical algorithm for solving the overall response of the *2-phases composite* material is shown by Figure 6. The start point of the algorithm is the partition of strain increment $\Delta \mathbf{E}$ between the matrix phase and inclusions. To this end, Voigt assumption is used to state the strain increment in the inclusions (GPL) while an average technique expresses the strain increment in the matrix (Polymer). Next, the algorithmic tangent operator of each phase is computed using Eq. (16). Due to its robustness, the generalised mid-point rule used by Doghri and Ouair [21] is applied on the algorithmic tangent operator to derive the strain concentration tensor \mathbf{A}^I . Finally, the effective properties are obtained using Eq. (12) after a convergence checking.

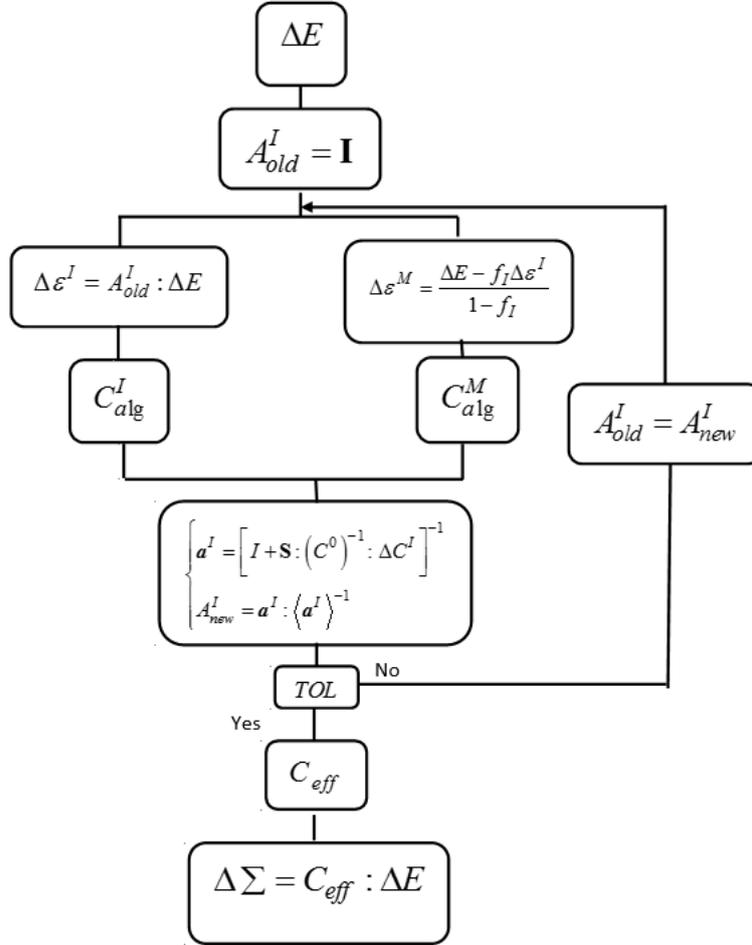


Figure 6: Numerical algorithm for overall response of 2-phases composite

For application, 2-phases composite is considered. The RVE is subjected to uniaxial loading. The load is given in terms of macro strain increment $\Delta \mathbf{E} = \Delta \mathbf{E} \cdot \boldsymbol{\psi}$ with $\boldsymbol{\psi} = e_1 \otimes e_1 - \frac{1}{2} [e_2 \otimes e_2 + e_3 \otimes e_3]$. The matrix is an

elasto-plastic Polymer PA6-B3K with an isotropic hardening in power-law $R(p) = kp^m$ whereas the Graphene inclusions are considered elastic. The properties of the matrix and the inclusions are reported in Table 1

Table 1: Phases properties of a Graphene-reinforced polymer composite

Matrix (Polymer PA6-B3K)					Inclusions (Graphene G2NAN)	
E_0	ν_0	σ_Y	k	m	E_I	ν_I
2000 MPa	0.39	60.5 MPa	63 MPa	0.4	1000 GPa	0.22

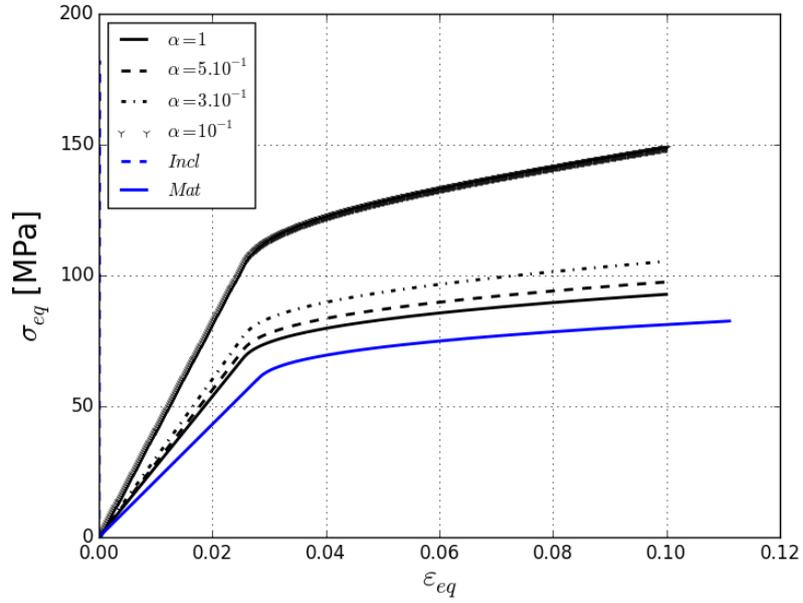


Figure 7: Aspect ratio variation for $f_I = 0.1$

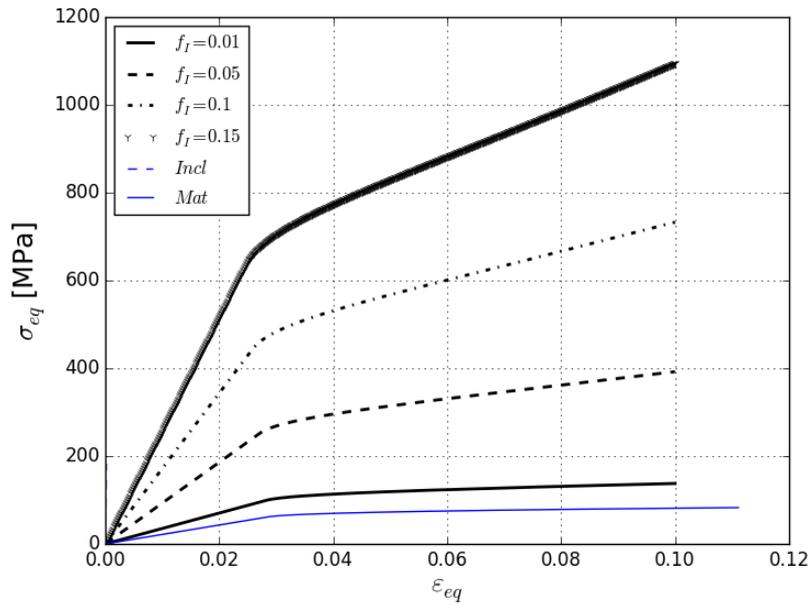


Figure 8: Volume fraction variation for $\alpha = 0.01$

Figure 7 depicts the evolution of the effective equivalent stress-strain behaviour versus the Graphene aspect ratio α . For different α the overall response is well bonded between the responses of the matrix as well as the Graphene. Also, it can be observed an increase in the overall response with respect to the decrease of α . Therefore, lower values of $\alpha = 0.1$ corresponding to *platelets-like* inclusions show a good reinforcement character than *circular-like* inclusions i.e $\alpha = 1$. In addition, the variation of the volume fraction is analysed. The equivalent macro stress-strain response versus different volume fractions $f_I = 0.01; 0.05; 0.1; 0.15$ is shown by Figure 8. The model predictions reproduce a trend similar to that of the matrix. The composite stress-strain response shifts towards higher stresses with the increase of the inclusions volume fraction. An enhancement of the mechanical properties is therefore noticed with the volume fraction. Herein the predicted stress-strain curves are also well bounded between the matrix and inclusions responses. Also, due to its low density and high Young modulus ($\rho_I = 1.06 \text{ g/cm}^3$; $E_I = 1000 \text{ GPa}$) compared to its counterpart fillers like carbon fibres ($\rho_{cf} = 1.76 \text{ g/cm}^3$; $E_{cf} = 240 \text{ GPa}$) or glass fibres ($\rho_{gf} = 2.6 \text{ g/cm}^3$; $E_{gf} = 85 \text{ GPa}$) for nearly same Poisson's ratio, Graphene platelets demonstrate, in Figure 9, a better enhancement of the overall mechanical properties at very low volume fraction $f_I = 0.01$. This observation leads to the consideration of GPL in the design of high strength lightweight components for EESVs and by consequence the reduction of CO₂ emissions.

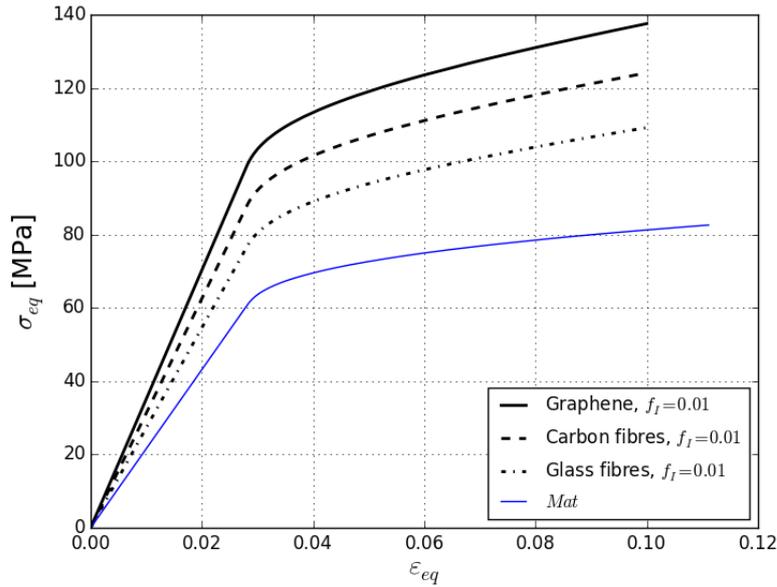


Figure 9: Overall response versus the nature of reinforcement for $\alpha = 0.01$

6. Conclusion

The applicability of Graphene-based polymer composite materials has been discussed regards to the fulfilment of lightweight requirements for energy efficiency in automotive. For such a composite, open challenges concerning Graphene reinforcements need to be addressed. From modelling view point, the development of appropriate constitutive models to integrate the macro-scale behaviour is elaborated. These strategies bind combination of several techniques from molecular mechanics to continuum mechanics. An application example is made by studying the non-linear effective behaviour of the Graphene sheet-polymer composite. The properties of the Graphene are assumed continuous while an elasto-plastic polymer is considered for the matrix. The Mori-Tanaka micro-mechanics scheme derives the effective response of the composite versus the aspect ratio of the Graphene sheet and its volume fraction. The results show an enhancement of the equivalent macro

stress-strain response when the aspect ratio is low corresponding to platelets-like inclusions. Also, the volume fraction is seen to have a good improvement on the composite response. With respect to CO₂ emissions reduction, the results highlight the effect of GPL reinforcements versus Carbon and Glass fibres in the design of lightweight structures with high mechanical responses.

Acknowledgments

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