PREDICTION OF PROPERTIES FOR THE PRODUCTION AND APPLICATION OF GRAPHENE REINFORCED METAL MATRIX COMPOSITES

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Abstract

This paper presents the development of finite element analysis (FEA) modelling for the prediction of the properties of the metal matrix composites (MMCs) reinforced with graphene. Process parameters taken into consideration were matrix metal (such as Al, Mg Ti, Ni, Cu and Fe) and volume fractions (1%, 5%, 10%, 15%, and 20%) of graphene. The FEA model was developed using ANSYS 14 based on the assumptions that it is free of voids and irregularities, and that the graphene sheets are perfectly aligned. Modelling results were discussed in relation to experimental data from the literature and also verified with theoretical methods; Rule of Mixtures (ROM) and Bettie's reciprocal theorem. The comparative study of results obtained from the analysis of composite has shown that the properties such as Young's moduli and Poisson's ratio and electrical conductivity of the material are significantly enhanced by the reinforcing graphene in the metal matrix. In particular, it was found that there is a significant increase of longitudinal Young's modulus with increasing volume fraction of graphene reinforcement. Graphene reinforced MMCs has the capability as an advanced composite material of being applied in many highly demanding advanced engineering applications in aero, auto and energy industries. In this paper, the case for application of aluminium-graphene metal matrix composite as the material of choice for power transmission lines is elaborated.

Keywords: Finite element method (FEM), metal matrix, reinforcement, volume fraction, graphene.

Annotations:

E_1 Longitudinal Young's modulus	k_m Matrix volume fraction of composite
E_2 Transverse Young's modulus	k_f Fibre volume fraction of composite
V_f Volume fraction of fibre	K_{el11} Lamina longitudinal electrical conductivity
V_R Volume fraction of reinforcement	K_{el22} Lamina transverse electrical conductivity
V_{12} Major Poisson's ratio	K_{el33} Lamina normal electrical conductivity
V_{21} Minor Poisson's ratio	RVE Representative Volumetric Element
E_f Young's modulus of fibre	CNT's Carbon Nano Tubes
E_m Young's modulus of matrix	MMC's Metal Matrix Composites
K_{em} Electrical conductivity of matrix	GO Graphene Oxide

1. INTRODUCTION

The discovery of graphene, which is well known for its excellent properties and named as a 'wonder material' has opened a new path to researchers for composite production [1]. Figure 1 shows the application of graphene in terms of weight percentage where it can be seen that 11% graphene is used for composite production, mainly for polymer matrix reinforcement. Only a small amount of investigation has been conducted to date for the production of graphene metal matrix composites. As reinforcements nano particles like fullerene, carbon nano tubes (CNT's) and graphene produce very different composite properties which is mainly due to their difference in their geometrical shape, for example CNT's are tube structured, graphene is plate structured and fullerene resembles the skin structure of a soccer ball. The possible effects of reinforcing a material can be understood by conducting suitable experiments which involves lots of time and cost. Simulation validated by previous experimental work provides an alternate way to understand select and optimise the composite.

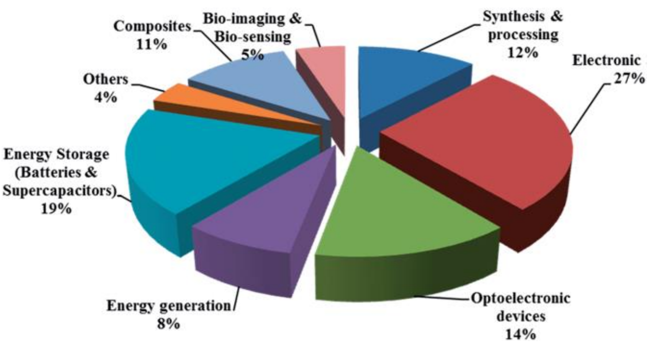

Figure 1: Percentage breakdown of applications of graphene based materials [2]

Suitable modelling involves the application of appropriate boundary conditions, loading and proper modelling of the constituents. Two different modelling techniques are used for the composite materials, one is continuum modelling which assumes a continuous material structure and the second approach is molecular which considers the molecular behaviour to obtain global response. The present work is based on the continuum approach. The main focus in this paper is given to aluminium as the matrix material because of its unique combination of good corrosion resistance, low electrical resistance, and excellent mechanical properties. The low density of aluminium also enables its usage within many MMCs applications. Additionally, it is inexpensive in comparison to other low density metals such as Ti and Mg. Ti is more expensive and Mg is only slightly more expensive, though Mg processing cost is higher than Al due to the reactivity of Mg. Aluminium has a density of 2700 kg m^{-3}, approximately one third that of steel (7830 kg m^{-3}), copper (8930 kg m^{-3}), or brass (8530 kg m^{-3}). Density of Magnesium, Titanium and Nickel are 1780, 4500, 8908 kg m^{-3} respectively. Magnesium is the lightest structural metal, approximately 35 % lighter than aluminium, and is also used commercially in specific automotive application as a matrix material for composites. Aluminium can display excellent corrosion resistance in most environments, including atmosphere, water (including salt water), petrochemicals, and many chemical systems. Titanium has been examined for use in aero-engines, mainly for compressor blades and discs, due to its higher elevated temperature resistance property. The melting point of titanium is relatively higher than aluminium, so the strength of titanium is retained to higher temperatures than for aluminium. Corrosion and oxidation resistance of titanium is also good. Ni-based composites have been widely adopted in automobile and aerospace industries because of their high specific strength, favourable corrosion resistance and toughness. Conductivity of aluminium is more than twice of copper, per pound [3]. Copper-clad aluminium wires are used in high frequency coaxial applications such as power cables, CATV distribution cables and RF antennas. These wires are less expensive and lighter than pure copper and possess higher strength and electrical conductivity than aluminium [4]. Aluminum offers nearly 30-40% of cost savings compared to copper. Cost analysis of different types of cables per kg of weight are given in Table 1 [5].

Table 1. Cost analysis of cables [5]

Cable	Price (per kg weight)
Bright copper wire	£ 2.80
PVC wire	£ 0.80
Low grade cables	£ 0.60
High grade PVC wire	£ 2.00
Aluminum cable with copper	£ 0.65

Researchers have shown by experimental work that the performance of conventional fibre composites can be enhanced by addition of small (0.025, 0.05 and 0.1 % wt) amounts of CNT's to epoxy resins [6]. Using micromechanics approach, the longitudinal and transverse properties of composites materials by reinforcing graphene and CNT's were calculated to know which material is the best reinforcement, The effects of uniform and random distribution of these CNTs nano reinforcements have also been examined [7]. The coefficient of thermal expansion, shear modulus and Young's modulus of CNT's and graphene sheet were evaluated by the finite element method and the variation of mechanical properties with size of CNT's was predicted [8]. The elastic properties of fibre reinforced composite lamina for longitudinal loading using finite element modelling has shown that for better analysis of fibre reinforced composite materials the finite element method can provide a large property data set for analysis [9]. There is no similar evidence of conductivity analysis by using pure graphene. In recent experiments on aluminum matrix composite with graphene nanosheets as reinforcement there was an increase of tensile strength from 154 MPa to 249 MPa [10]. This demonstrated GNS's as a promising reinforcement material for composites. Researchers have fabricated aluminum nanocomposites by milling, hot isostatic pressing, and hot extrusion. Their results indicate an increase of tensile strength of aluminum by up to ∼12% [11]. Graphene/nickel composites were prepared by electrodeposition in a nickel sulfamate solution with graphene oxide (GO) sheets in suspension. This preliminarily study of the composites' properties and measurements showed that the thermal conductivity of Ni-based graphene composite films was improved by 15% over that of pure Ni electrodeposits. The hardness value of the composites was almost 4-fold higher than that of pure electrodeposited Ni [12].

Though graphene itself has huge potential to be used as reinforcement, there is very little available literature to back that claim [figure 2] [1], especially for metal matrix composites that is even less. Therefore, the objective of the present work is to predict the effectiveness of graphene reinforcement on properties such as Young's modulus and Poisson's ratio of composite materials using finite element method and also to explore their potential applications.

2. PROBLEM DESCRIPTION

To achieve the objective of the present problem, micro mechanical analogy associated with finite element method was applied for graphene reinforced metal matrix composites. The Young's modulus and Poisson's ratio in both

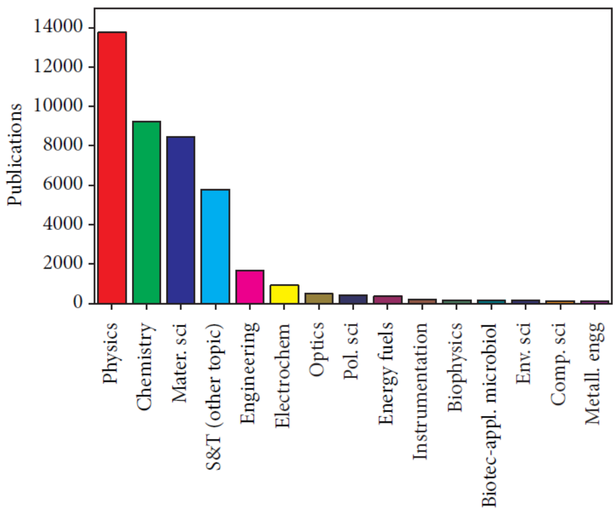

Figure 2: Graphene has been extensively used in these top 15 research areas since 2000–2012 [1]

longitudinal and transverse directions for composites with different metal as matrix and graphene as reinforcement at different volume fractions (1%, 5%, 10%, 15%, and 20%) were calculated. To simplify the problem, it was solved in two different phases. In first phase the continuum model of graphene reinforced aluminium matrix composite was modelled to determine the effective properties of nano composites and the results obtained were validated through rule of mixtures and Bettie's reciprocal theorem. The second phase of this study examined the prediction of the properties of different metal matrix composites reinforced with graphene.

2.1 Model set-up

Graphene was idealized as a plate with uniform thickness and plate shaped representative volume element was considered for the present analysis. Due to the symmetry of the problem in geometry, loading and boundary conditions, one-fourth portion of Representative Volumetric Element (RVE) were used for the analysis in FE software ANSYS 14.

2.1.1 Materials

The properties of graphene used as reinforcement for the present analysis were Young's modulus of 1TPa and Poisson's ratio of 0.186 and conductivity of 1×10^8 S/m at 20°C. Properties used for metal matrix are shown in Table 2. Melting point for Al, Mg, Ti, Ni, Cu and Fe are 660, 650, 1660, 1450, 1100, 1530°C respectively.

Table 2. Properties of materials

Matrix (Metal)	Young's modulus (GPa)	Poisson's ratio	Conductivity (S/m) at 20^0C
Al	70	0.35	3.55×10^7
Mg	45	0.29	2.07×10^6
Ti	116	0.32	2.38×10^6
Ni	200	0.31	1.47×10^7
Cu	110	0.34	5.95×10^7
Fe	211	0.29	1.00×10^7

2.2 Geometry and element type

As one fourth portion of unit cell is considered for the modelling, a size of the Representative Volumetric Element (RVE) was calculated for the percentage volume fraction of reinforcement. The element used for the present analysis was SOLID 185 of ANSYS; it was based on 3D elasticity theory and was divided into number of nodes with an edge length of 0.25nm with three degrees of freedom at each node. Figure 3 shows a typical finite element mesh of the model for the composite at 10% volume fraction of graphene as reinforcement with aluminium and is converged.

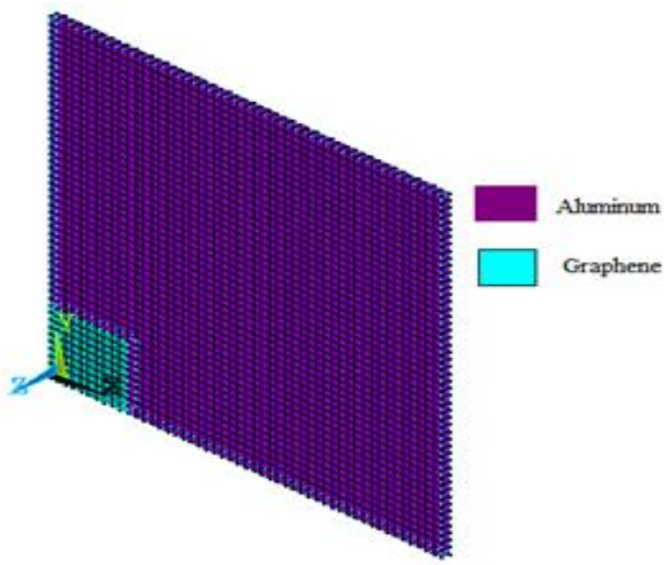

Figure 3. FEA mesh for 10% graphene reinforced Al composite

2.3 Boundary conditions

The following assumptions were made for the model set-up.

a. The composite considered for the analysis is free of voids
b. Matrix is homogeneously reinforced with the reinforcement
c. The load applied on the composite is within the elastic limit

Due to the symmetry of the problem, the following symmetric boundary conditions were applied, at X=0 U_x=0; at Y=0, U_y=0; at Z=0 U_z=0 and on the positive faces (X, Y & Z) of RVE, multipoint constraints were imposed. The uniform tensile load was applied on the positive Z-plane.

3 ANALYTICAL SOLUTION

The elastic properties of composites were calculated using ROM and the FE model of the composite was verified with these results as well as with Bettie's reciprocal theorem.

3.1 Rule of mixture (ROM)

General equations to solve Young's modulus in fibre direction, $E_1 = \frac{\sigma_1}{\varepsilon_1}$ and Young's modulus in transverse direction, $E_2 = \frac{\sigma_2}{\varepsilon_2}$

where,

$V_f + V_m$=1

V_f Volume fraction of fibre

V_m Volume fraction of matrix

E_f Young's modulus in fibre direction

E_m Young's modulus in matrix direction.

Equations to calculate the electrical conductivity of composite (neglecting voids) are [9],

Longitudinal electrical conductivity,

$$Ke_{l11} = K_f\, Ke_{f11} + K_m\, Ke_m$$

Transverse electrical conductivity,

$$Ke_{l22} = (1 - \sqrt{K_v}\,) + \frac{\sqrt{K_f}Ke_m}{1-\sqrt{K_f}(1-\frac{Ke_m}{Ke_{f22}})}$$

where,

K_{em} Electrical conductivity of matrix

k_m Matrix volume fraction of composite

k_f Fibre volume fraction of composite

K_{el11} Lamina longitudinal electrical conductivity

K_{el22} Lamina transverse electrical conductivity

K_{el33} Lamina normal electrical conductivity

3.2 Bettie's Reciprocal Theorem

Bettie's reciprocal theorem states that whenever an object is subjected to tensile loading, the ratio of longitudinal Young's modulus to major Poisson's ratio will be equal to the ratio of transverse Young's modulus to minor Poisson's ratio [13] i.e. $\frac{E_1}{v_{12}}=\frac{E_2}{v_{21}}$ where,

v_{12} Major Poisson's ratio
v_{21} Minor Poisson's ratio

4 RESULTS

The value of longitudinal Young's modulus of the composite calculated from ROM matches exactly with the value obtained from ANSYS. The transverse Young's modulus of the composite were also predicted and validated with Bettie's reciprocal theorem, see Figure 4. The graphene reinforced composite is shown to be a stiffer material than SiC reinforced aluminium composites, see Figure 5. The reinforcements are used to enhance the properties of the materials; the question arises to what extent enhancement is possible. The first step to solve that problem is to calculate the properties and observe how the properties changes with volume fraction. When metal matrix is reinforced with graphene the longitudinal Young's modulus increased gradually with increase in percent of reinforcement, see Figure 6. The increase in major Poisson's ratio was not significant for any of the matrix materials, see Figure 7. The significant increases predicted in electrical conductivity of the composite with aluminum and copper as matrix materials at different percentage of reinforcement are shown in Figure 8.

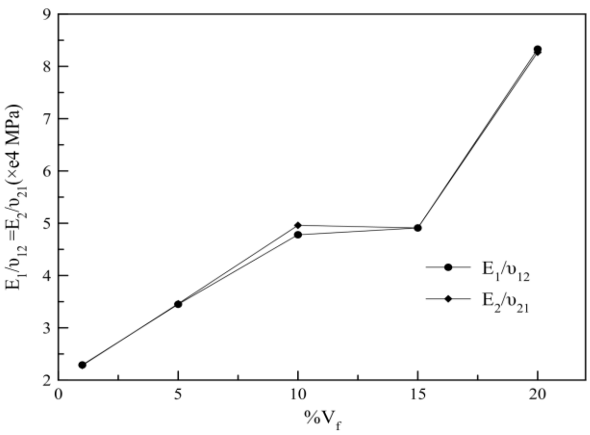

Figure 4. Verification with Bettie's Reciprocal theorem

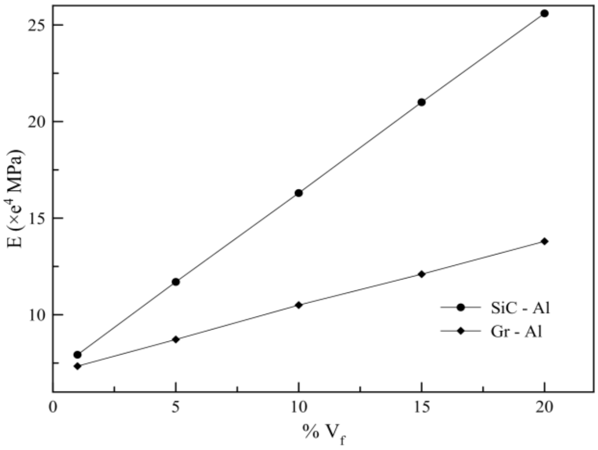

Figure 5. Comparison of Young's modulus for graphene reinforced aluminium composites with traditional reinforcement SiC in aluminium matrix for different vol % of reinforcement

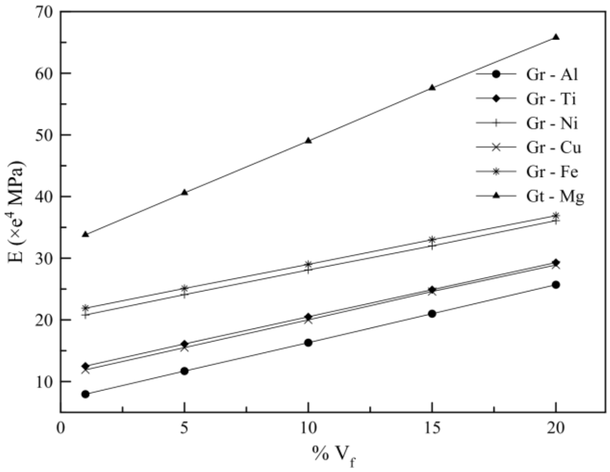

Figure 6. Comparison of Young's modulus of different matrix materials with different vol % of graphene reinforcement (1%, 5%, 10%, 15%, and 20%)

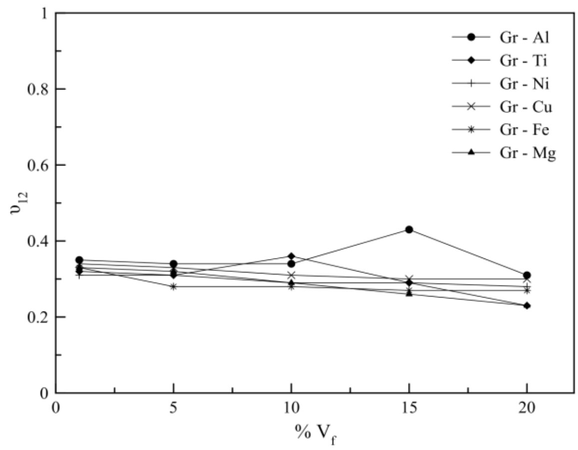

Figure 7. Comparison of major Poisson's ratio of different matrix materials with

different vol % of reinforcement (1%, 5%, 10%, 15%, and 20%)

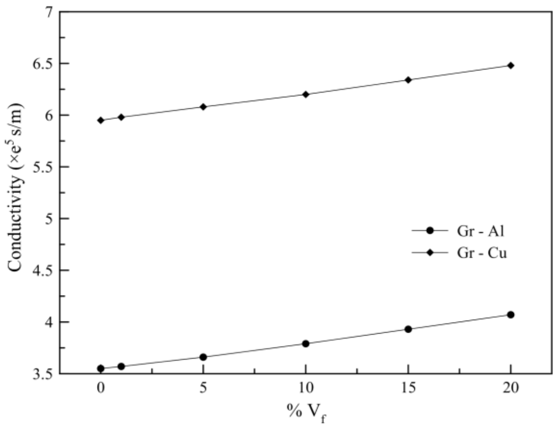

Figure 8. Comparison of conductivity of aluminium & copper with different vol % of reinforcement (1%, 5%, 10%, 15%, and 20%)

5 DISCUSSION

From the results determined and potential applicability to real world applications, aluminium presents as a good matrix material choice to examine further with graphene reinforcement. Higher temperature melting alloys would present greater difficulty in making the composite due to destructive effects on the graphene sheet [14], one reason being due to the formation of carbides at high temperatures. The mechanical properties of fibre reinforced composites using Buckminster fullerence as reinforcement were studied with the help of micro mechanical and continuum approaches, no significant effect of nano particles on longitudinal properties were observed whereas enhancement of transverse properties was observed [15]. Form the results present in this paper, showed that graphene reinforcement enhances the properties of composites above those achievable from the widely used SiC reinforcement. Due to the huge density difference between graphene nano sheets and metal matrix, the dispersion of graphene in MMC with the existing metallurgical methods is challenging [16]. In transverse direction the lateral strain dominates the longitudinal strain, which in turn decreases the Poisson's ratio. Graphite aluminium composite is used for antenna boom for Hubble space telescope; the energy transmission between antenna dish and spacecraft was enabled by the excellent electrical conductivity of MMC [17]. Graphene reinforced Al matrix composite possess the potential to replace the antenna booms as graphene highly conductive compared to graphite. To perform thermal, structural and EMI-shielding functions Gr/Al composites are widely used [18]. Due to excellent combination of high conductivity and low density, discontinuously reinforced aluminium composites were used in packing & thermal managing applications [19]. Graphite copper MMC's were developed for high temperature structural radiators [20]. Aluminium matrix composites were used in flywheel enables smaller flywheels compared to polymer composites [21]. For certain applications copper alloy conductors are preferred instead of pure copper, especially when higher strengths or improved abrasion and corrosion resistance properties are required. Electrolytic tough pitch copper is used for power distribution and telecommunications [22]. In Briton, post office communications used cadmium copper aerial lines with 1% cadmium for extra strength, for local lines 0.01124 kg/m and for toll lines 0.0196 kg/m [23]. The experiments done on Al-Ni stabilized Nb-Ti/Cu superconducting cable have shown that the mechanical and resistivity characteristics depends on certain parameters of work-hardening process and the produced composite was a promising material for low temperature applications [24]. High purity aluminium nearly 99.99% is being used as a stabilizer material in composite conductors for high-energy physics magnets [25]. The study of effect of intermetallic compound on electrical and mechanical properties of bimetallic friction of Al-Cu joints were studied which leaded to the designing of new screwed Al-Cu connections for aluminium cables. The experimental results at same loading and environmental conditions for these different junctions have shown that the design was advantageous than existing [26]. The effect of adding metal impurities of Al, Cu and Fe in the insulation layer of distribution cables was studied and the results have shown the relation between forward and reverse charging currents, the effect of impurities on charging current was illustrated [27]. The reliability of cables will be effected by cyclic loading and presence of electrical joints inside remoulded rubber. Experiments were conducted until electrical breakdown of three different kinds of joints, bolted Cu to Cu, crimped Al to Al and bolted Al to Al and illustrated the evidence of self healing, wear and corrosion damage [28]. The study of aluminium alloy conductors for communication cables with respect to electrical, mechanical and processing properties have shown that the best composition for 24-gage conductor was Al-0.84, Fe-0.12 and Mg alloy. The tests conducted on the wire showed that the failures were less compared to copper conductors [29]. Graphene as a reinforcement provides less weight and more strength and high conductivity to the composite material, which possess the potential to replace the conventional materials used in flywheels and cables. There is still a long way to go in area of MMC's to develop a feasible process to produce and distribute reinforcement in matrix homogenously. The current experimental focus from researchers internationally is to develop graphene reinforce aluminium MMCs through powder metallurgical or severe plastic deformation routes.

6 CONCLUSION

A FEA model has been developed in ANSYS for the prediction of structural and electrical properties of graphene reinforced metal matrix composites. For most metal matrix, a significant increase in both of these properties were observed. Transverse mechanical properties were increased greatly compared to a lower increase in longitudinal properties across the investigated volume fractions. The results have shown that the electrical conductivity of MMC's increases with the percentage increase of graphene reinforcement. In future work, the analysis method developed in this paper could be extended to the examination and comparison of crack or delamination in graphene reinforced metal matrix composites.

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