# HOMOGENIZATION METHOD FOR 2-D NANOSTRUCTURE REINFORCED EPOXY

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# HOMOGENIZATION METHOD FOR 2-D NANO-STRUCTURE REINFORCED EPOXY

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## Introduction

Graphene flakes are being used as base resin additives in epoxy to improve the properties of the material for aerospace applications [1]. The concentrations of the flakes should be optimized to create material properties that meet the design and cost requirements of the components. A predictive modeling approach is needed to aid in the design of these composite materials for increased stiffness. Using a 2D representation, the mechanical properties of a representative area element of epoxy embedded with graphene flakes can be predicted.

## Experimental Development of Graphene-Epoxy Composites

Graphene flakes supplied by 2D fab were dispersed in liquid epoxy resin with the aid of an ultrasonic horn for 30 minutes. After the addition of the hardener, the mixture was molded into the shape of a 3.2 mm thick plate and cured at 25 °C for 24 hours and post-cured at 100 °C for 4 hours. The content of graphene flakes in the cured composite was 1 wt%. Flexural tests of the composite and the neat resin were carried out at a crosshead speed of 1.35 mm/min. Samples were ground, polished and sputter-coated with gold for scanning electron microscopy (SEM) observation (Figure 1).

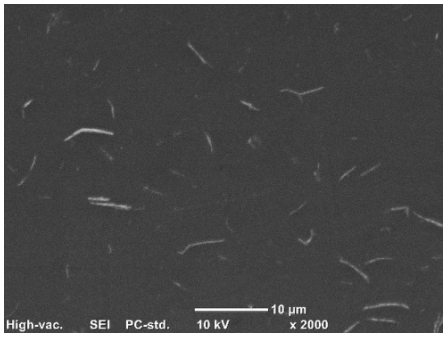



Fig. 1: SEM image of the 1 wt% graphene-epoxy composite

## Computational Homogenization of Graphene-Epoxy Composites

To predict the theoretical increase in stiffness of the reinforced matrix, an FE-model based method has been developed. In this method, the effective elastic representation of the graphene enhanced epoxy composite is homogenized using computational homogenization, cf. ref. [3]. In the homogenization, the graphene flakes are modelled as 2D "stiffening" elements embedded in the neat resin, cf. ref [2]. As alluded to in Figure 2, the effective stiffness properties of the graphene-epoxy composites can then be used to create computational models of fiber-reinforced composites with a graphene-enhanced matrix. This allows the graphene additive to be efficiently incorporated into traditional laminated composite analysis techniques.

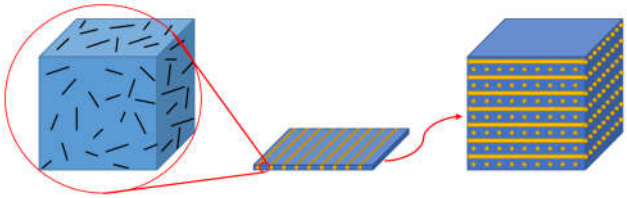


Fig. 2: Multiscale composite material analysis, from micro to macro level

This approach uses experimental microscopic images of graphene-epoxy composites to create a virtual representation of the experimental material microstructure. The micrographs are analysed systematically with a series of image analysis techniques. Systematic image analysis increases repeatability, reduces errors in flake extraction, and allows large numbers of images to be process relatively quickly. The series of image analysis steps are as follows. First, if needed, images are converted to 8-bit grayscale. Then, the physical scale of pixels per micrometer is set and the image is cropped to the prescribed size. Next, Fiji's Renyi Entropy automatic threshold is used [4]. Then, the flakes are selected automatically using particle analysis. Finally, the Feret's diameter of each flake is output as the result

[4]. These lines are then used directly as flake representations in the computational homogenization.

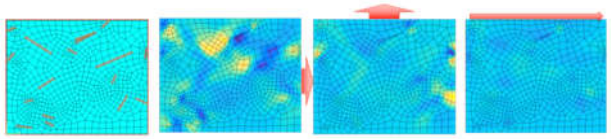
The flexural modulus obtained in this study for the neat epoxy and the 1 wt% graphene composite were 2510 and 2643 MPa, respectively. It is known that epoxy has approximately a 5% increase in tensile modulus when compared with the flexural modulus for pure resin. Therefore, the tensile modulus (E11 & E22) was calculated accordingly. The epoxy Poisson's ratio (v12) used was obtained from literature [5]. The shear modulus (G12) was then calculated as 967 MPa using these stiffness properties. The epoxy stiffness properties used for the homogenization are as follows, Table 1.

| | | |
|---|---|---|
| E11 | 2.635 | GPa |
| E22 | 2.635 | GPa |
| G12 | 0.967 | GPa |
| v12 | 0.363 | |

Table. 1: Semi-empirical Resin Properties

## Results

The computational homogenization was conducted on three SEM micrographs from the graphene-epoxy composites. A representative homogenization sample can be seen in Figure 3.



a) b) c) d)

Fig. 4: Computational homogenization: a) undeformed mesh, b) extension 11, c) extension 22, d) shear 12.

The homogenization results can be seen in Table 2. If the graphene epoxy composite is isotropic at a large scale, then the elastic modulus in the vertical direction (E11) and the elastic modulus in the horizontal direction (E22) terms should converge at some large sample size. In the table, we can see this convergence happening when the averages of the results are calculated. The elastic constants calculated for the composite are very similar to the semi-empirical ones obtained from the experimental results. These homogenized properties can then be used as matrix material properties in a full laminated composite simulation.

| | E11 | E22 | G12 | |
|---|---|---|---|---|
| GExp1 | 3.02 | 2.65 | 1.04 | GPa |
| GExp2 | 2.80 | 2.70 | 1.01 | GPa |
| GExp3 | 2.69 | 2.78 | 1.00 | GPa |
| | | | | |
| Avg | 2.84 | 2.71 | 1.02 | GPa |

Table. 2: Results from computational homogenization.

The three samples analysed each had an approximate area of 2500 $\mu m^2$. The graphene flakes were dispersed and the flake metrics are tabulated in Figure 5. These have been averaged for the three experimental micrographs. Flakes under 3µm had a negligible effect on resultant stiffness and were therefore omitted.

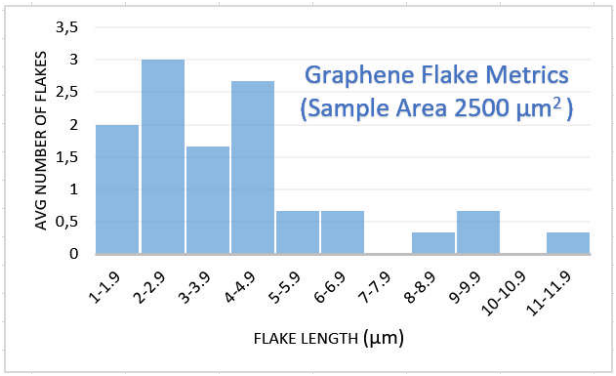



Fig. 5: Graphene Flake Metrics

Limitations of this method include image variation throughout the material and correlation between the 2D and true 3D properties. The image variation throughout the material can be smeared through the averaging of several samples. However, if the nanocomposite has a high level of inhomogeneity, then more samples or larger volumes may be required to calibrate the homogenization. The method proposed here uses a 2D representation which artificially creates infinite plate structures (of the 1D flakes) that run out of plane. This may overpredict the resultant stiffness.

## Conclusion

This work uses a computational homogenization of a representative volume element (RVE) in order to calculate representative stiffness properties of graphene enhanced epoxy. The method utilizes micrographs of experimental samples and resin stiffness properties as inputs. The output is a homogenized nanocomposite that can be used as a resin in traditional CLPT analysis.


## Acknowledgements

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