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# Micro Mechanical Exploration of Composites for Superior Properties

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**Abstract:** The predictive engineering of materials is matured from predicting properties from known morphology or constituents to engineering novel morphology for superior properties. The focus of this paper is about implementation of computational material mechanics modeling method in COMSOL multiphysics software for engineering the constituents for superior properties. A brief review of property prediction methods, advantages and potential superior properties of composite materials are given. Numerical implementation of representative volume based computational micromechanics in COMSOL with periodic boundary condition is detailed. The prediction methodology and results of linear and nonlinear bulk material properties are provided. The effect of reinforcement shape, size, orientation and length is also investigated and reported with particular emphasis on superior properties. The advantages of windowing approach, COMSOL parametric models, and the ability to investigate materials at micro level for superior macroscopic performance is detailed.

**Keywords:** Composites, micromechanics, super properties, homogenization, polymer composites, Auxetic composites.

## 1. Introduction

It is a scientific quest to engineer materials with superior properties. Composite design concept enables us to design materials with superior properties by allowing us to engineer the constituents, morphology and processing methods. Computer Aided Material Mechanics (CAMM) is matured from predicting composite properties from known morphology or constituents to engineered material for superior properties [1-6]. The equation level multiphysics modeling capability of COMSOL enables to exploit the micro mechanical simulation methodology for engineering composite materials with superior property. The multiphysics capability can be exploited to predict, the structural, thermal, flow, acoustical, transport and electromagnetic properties prediction.

The focus is on the implementation of representative volume method for predicting the transverse structural properties of macro composites from the constituents. The modeling methodology and implementation in COMSOL will be detailed. The effect of shape, size, and volume fraction will be investigated and optimized for superior properties. The global performance and its linkage to the micro mechanical effects and the advantages of parametric numerical optimization method will be highlighted. The structural properties and performance will be used as a benchmark. Typical local von Mises stress distribution of glass polymer composites is shown for uniaxial macro loading. A parametric loading analysis will be performed to predict the load vs deflection performance of composites. Thus the nonlinear and superior performance of the composite can be predicted based on the constituent properties.

## 2. Computer aided micromechanics

The rule of mixture provides the first cut basis for the prediction of composite material properties. The iso-strain and iso-stress assumption provides upper bound and lower bound prediction capability, respectively. Analytical models based on effective medium theory also provide good capability to predict the composite properties. Eshelby's equivalent eigen stress method provides a strong theory of elasticity based foundation. The homogenization and periodicity methods provide strong first principle based foundation for micro mechanics. Homogenization method integrates the micro local strain displacement fields to macro strain and displacement fields. Extensive numerical methods are available to implement homogenization method in computer aided modeling environment.

The implementation of homogenization theory for composites is finite element method (FEM) based variational formulation (displacement and field equation). The selection of minimal RVE size to obtain realistic prediction along with periodic boundary condition enables simulation of composite microstructure for property prediction.

The Micromechanics is evolved much more than 'rule of mixtures', empirical, mean field and bounding methods of homogenization [1-6]. Homogenization theory integrated with FEM method will give unique advantage in virtual design of filler based materials. These are based on representative unit cell approach. These include representative volume element (Approximated by a unit cell, with periodicity and boundary effects), embedded cell, windowing, and multi scale models.

Bohm [3] provides a good overview of micromechanics models. Mean field theory is successful in thermo elastic response prediction. The current research focus is on non-linear properties. The variational bounding methods are useful for predicting upper and lower bounds. The representative volume element (RVE) or periodic micro field approaches (PMA) are approximated by a unit cell. In this case, the periodicity and boundary effects are critical. This method is suitable for bulk material property prediction. The embedded cell, based on unit cell, which is embedded in an outer homogenized region, is generally used for studying local properties such as stress concentration and failure. The windowing approach is another method, where sub regions are selected for upper and lower bounds prediction. In this paper, representative volume element with periodic boundary condition is adopted.

## 3. Numerical Implementation

The micromechanics formulation with a representative volume element was implemented in COSMOL [7]. The basic assumption in homogenization of micromechanics is as follows. The variation of the stress and strain fields at micro scale influences the macro scale only via their volume averages. The gradients of stress and strain field at macro scale are not significant at micro scale. Macro field can be cast into a form of uniform applied or far field stresses and strains. The selection of region that is representative of micro geometry of the material is critical. A RVE based on available micro geometry based statistical information can help to decide a suitable volume. The microstructure of reinforcement distribution in a composite system can be simplified to square, hexagonal and realistic random packaging for simulation purpose. Square and hexagonal packing are idealistic packaging model. Realistic random distribution is challenging to model analytically. However, computer aided micromechanics combined with image processing, allows to directly model the micrograph based realistic reinforcement distribution.

On a representative volume element, the macroscopic strain $\langle \varepsilon \rangle$ and stress $\langle \sigma \rangle$ can be related to microscopic strain $\varepsilon(x)$ and stress $\sigma(x)$ as follows,

$$\varepsilon(x) = A(x)\,\langle \varepsilon \rangle$$
$$\sigma(x) = B(x)\,\langle \sigma \rangle$$

Where, A(x) and B(x) are called mechanical strain and stress concentration tensors. The homogenization relationship of macro and micro stress strain relationship can be written as follows,

$$\langle \varepsilon \rangle = \frac{1}{\Omega_S} \int_{\Omega_s} \varepsilon(x)\, d\Omega = \frac{1}{2\Omega_S} \int_{\Gamma_s} \left( u(x) \otimes n_\Gamma + n_\Gamma \otimes u(x) \right) d\Gamma$$
$$\langle \sigma \rangle = \frac{1}{\Omega_S} \int_{\Omega_s} \sigma(x)\, d\Omega = \frac{1}{\Omega_S} \int_{\Gamma_s} t(x) \otimes x \, d\Gamma$$

Where, $\Omega_S$ represents volume region, $\Gamma_S$ represents surface region, u(x) is the deformation vector, t(x) surface traction vector, $n_\Gamma$ are surface normal vectors, $\otimes$ is dyadic product of vectors. This formulation is based on the assumption that the macroscopic heterogeneous material is statistically homogeneous. The representative volume should be selected to represent a statistically homogeneous microstructure.

Many methods are proposed for the implementation of homogenization by a representative volume element along with periodic boundary condition in a finite element formulation [2, 6]. We have implemented generalized unit cell proposed by Li [6]. The implementation in COMSOL model involves, digitizing a typical representative volume of composite and including the periodic boundary condition in the analysis procedure. A 2D plain strain element based model is implemented with periodic boundary condition. The global and local stress and strain components are simulated. The parametric simulation data is also used to predict the bulk property. The parametric load and displacement data is used for simulating the stress strain behavior. A 3D model is also under development.

## 4. Results and Discussion

The methodology developed in the previous section is used to evaluate the effect of constituent properties on composite property. The linear elastic modulus is studied in detail. The transverse properties of composites are one of the weakest link and hence the investigation is focused on evaluating and improving the transverse properties. A polymer matrix system with glass fiber reinforcement is considered.

A typical stress distribution results on a representative volume is shown in figure 1. The elastic modulus is predicted for polymer glass composites with 18% volume fraction. The stress strain behavior and stress distribution pattern for all the three systems were predicted. The modulus predicted by the simulation is 72 and 2.4 GPA for glass and polymer, respectively. This is calculated by giving same elastic property for fiber and matrix in the RVE simulation. The isotropic system shown uniform stress distribution within the unit cell. However, the glass polymer composite system shows stress concentration effects. The figure 1 clearly shows the bulk macro property prediction capability and the local stress and strain pattern for micro level exploration.

The effect of fiber volume fraction on properties is investigated. A glass polymer system with a volume fraction of 10% and 30% is also predicted. The modulus predicted for 30% and 10% volume fraction is 4.78 GPa and 2.96 GPa, respectively. The higher volume fraction increases the modulus and the stress concentration effects. The predicted results are comparable to experimental results and within the lower and upper bound prediction of properties. An elastoplastic analysis would provide the nonlinear performance of the composites. The micro mechanical exploration allows to zoom into local stress and strains for the global loads to design novel materials with superior properties.

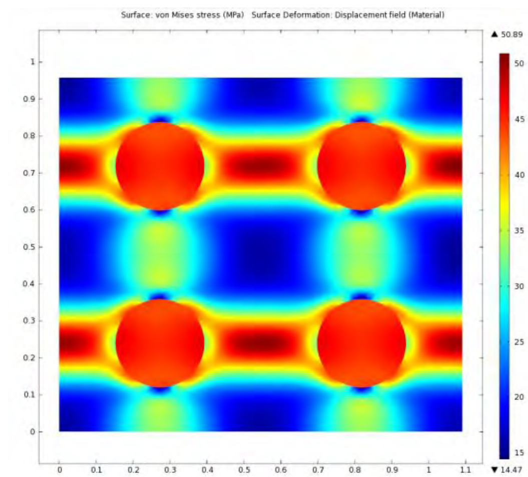


**Figure 1. Typical local stress distribution of glass polymer composites (vf =0.18) representative volume with periodic boundary conditions.**

| Matrix Poisson ratio | Fibre Poisson's Ratio | Composite Elastic modulus Predicted (GPa) | % of increase in Modulus |
|---|---|---|---|
| 0.3 | 0.2 | 2.536 | 0.0 |
| 0.3 | -0.5 | 2.576 | 1.6 |
| 0.3 | -0.9 | 2.602 | 2.6 |
| 0.4 | 0.2 | 2.762 | 8.9 |
| -0.4 | 0.2 | 2.879 | 13.5 |
| -0.5 | 0.2 | 3.206 | 26.4 |
| -0.6 | 0.2 | 3.701 | 45.9 |
| -0.7 | 0.2 | 4.496 | 77.3 |
| -0.8 | 0.2 | 5.937 | 134.1 |
| -0.9 | 0.2 | 9.352 | 268.7 |

**Table 1. Effect of NPR matrix and fiber on composite property**

Conventional materials usually exhibit positive Poisson's ratio. However, theoretically it is possible to have Negative Poisson's Ratio (NPR) from 0.5 to –1. Recently, there has been increased research activity about Auxetic or negative Poisson's ratio (NPR) material for its counter intuitive property and novel applications

[5]. Micromechanics based numerical simulation methodology is used to evaluate NPR materials for improving the modulus of polymer matrix based composites materials.

The natural material, which shows NPR effect are Iron pyrites, single crystal material such as Arsenic, Cadmium, Cubic elemental metals, Polymorph of crystalline silica. Certain unidirectional and angle ply laminated composite configuration also shows NPR. Ceramics such as vanadium dioxide, YBa2 Cu3O2 exhibits NPR. The molecular negative Poisson ratio materials include cyclic hexamers and carbon nitride. Zeolites which widely used as filler material in composites also exhibit NPR.

Table 1, shows the effect of NPR matrix and fibers on composite property for a typical glass polymer system. The polymer matrix and fiber reinforcement modulus considered for this investigation is 2 GPa and 72 GPa, respectively. A fiber volume fraction of 10% is used for this investigation. For high modulus glass fiber reinforcement with NPR as high as –0.9 did not show significant improvement in modulus. However, the effect of negative poisons ratio matrix on composite property is significant. Composite property enhancement potential of around 270% (~ 3 times) is possible with negative Poisson ratio matrix material. The increase in modulus is hypothesized to be due to increase in the internal stiffness of the composites by the counter resisting internal forces between fiber and matrix. This novel exploration shows that fibers or matrix with negative Poisson's ratio can increase the property significantly. The NPR polymer in polymer composites shows good potential for enhanced modulus and failure strain. The computer aided micromechanics model enables to virtually explore the material space for super properties of composites.

## 5. Conclusions

The computer aided micromechanics and its benefits for engineering super property materials are given. The paradigm shift to use material mechanics for engineering novel property than predicting property is detailed. An overview of computer aided micro mechanics is given starting with rule of mixtures, bound theorems and representative volume elements methods. A detailed overview of homogenized representative volume element method with periodic boundary condition is given. The methodology developed was used to evaluate the effect of constituent properties on composite property. The liner elastics modulus is studied in detail. The effect of negative Poisson's ration material on composite property is explored in detail, which shows excellent potential for performance improvement of polymer composites.

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## 7. Acknowledgements

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