

# NUMERICAL INVESTIGATION ON MECHANICAL PROPERTIES OF POLYMER COMPOSITES REINFORCED WITH MXENE NANOSHEETS

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## Introduction

Recently a new class of two-dimensional (2D) nanomaterials, called MXenes, was discovered [1]. MXenes are transition metal carbides or nitrides produced by etching of the A element from the MAX phases. MXenes behave as “conductive clays” because of the combination of the metallic conductivity of transition metal carbides and the hydrophilic nature of their hydroxyl or oxygen terminated surfaces [2]. MXenes have already found various applications from electromagnetic interference shielding, energy storage, to antibacterial coatings, and water purification [3]. However, the possibilities of this material as a filler for nano-engineered structural polymer composites have not been studied yet, but these opportunities of MXenes are very promising and relevant.

This study is addressed to identify a suitable methodology based on finite element (FE) homogenization approach for prediction of mechanical properties of polymer composite reinforced with MXene 2D nanosheets.

## Materials and Mechanical Properties

As it was intended to develop the material for nano-engineered structural polymer composite, the Epoxy/MXene composite was analysed. Till now MXenes as nanofillers were investigated only for matrices of polydiallyldimethylammonium chloride and polyvinyl alcohol [4]. For this investigation the Biresin® CR122 epoxy resin and hardener Biresin® CH122-5 were used. The main mechanical properties

of this epoxy resin system are: Young’s Modulus of 2.8 GPa; Tensile Strength of 80 MPa; Tensile Elongation (at break) 5.6 %.

The mechanical properties of MXene nanosheets were predicted by simulation on classical molecular dynamics (MD) [5] and only elastic properties were obtained experimentally by nanoindentation with the tip of an atomic force microscope [3]. According to MD simulation the modulus of the most important MXene material ( $\text{Ti}_3\text{C}_2$ ) is 0.502 TPa, but experimentally was obtained modulus of  $0.33 \pm 0.03$  TPa. For our investigation these MXene properties were used: Young’s Modulus of 0.33 TPa; Tensile Strength of 20 MPa; Tensile Elongation (at break) 4.5 %.

The interaction effects between nanofillers and surrounding polymer matrix were taken into account, as this interface has a significant influence on the strength of nanocomposites [6]. Here, we used several approaches for the investigation of interface effect on nanocomposite properties. The inverse micromechanical modelling method [7] based on experimentally obtained macro mechanical properties of composite was used to clarify the mechanical properties of Epoxy/MXene interface layer.

## Numerical Models and Homogenization Approach

The FE analysis of mechanical behaviour of Epoxy/MXene composite was based on the micro-macro homogenization strategy. The analysis was performed by FE code DIGIMAT™ and ABAQUS. The effects of MXene nanosheet aspect ratio, shape, clustering, orientation, and volume fraction on the

elastic and strength properties of nanocomposite under static loading conditions were investigated. Due to this, a number of 3D representative volume element (RVE) models were generated (Fig. 1).

According to the deterministic theory of averaging, the components of the macroscopic stress tensors were defined as the suitable average over the volume occupied by the RVE of the microscopic stress components. The macroscopic stress tensor was computed as the appropriate volumetric averages of their corresponding local quantities.

### Conclusions

FE model for mechanical properties optimization of Epoxy/MXene composite was proposed. The results of simulation demonstrated good agreement with experimental data.

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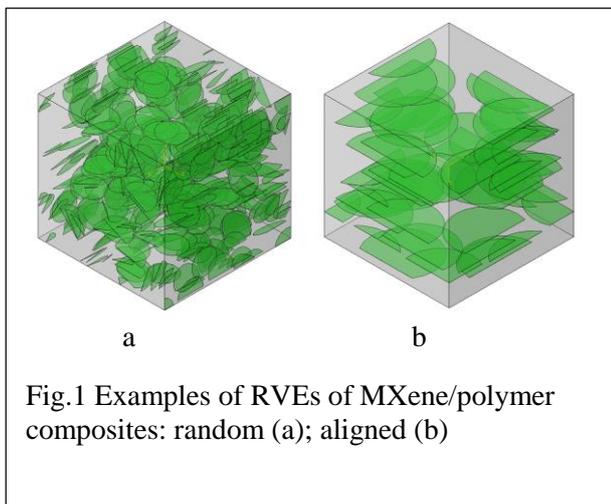


Fig.1 Examples of RVEs of MXene/polymer composites: random (a); aligned (b)

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