MODELLING OF MECHANICAL BEHAVIOUR OF MXENE/POLYMER NANOCOMPOSITES

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1 Introduction

New two-dimensional transition metal carbides called MXenes [1] hold great promise for future applications in many science and technology areas. Unique compound of characteristics of MXenes such as conductivity, strength, hydrophilicity and electromagnetic interference (EMI) shielding give a possibility to create new high-tech multifunctional composite materials. As an example, conductive MXene/polymer nanocomposites with these unique properties could be used for structural health monitoring in an airplane wing or a wind turbine blade. The complexity in degradation process of composites filled with nanoinclusions brings a challenge for experimentalists. In order to understand the evolution of damage and determine mechanical properties, finite element (FE) modelling at microscale level can be useful.
The aim of this study was to find the mechanical properties of a single MXene nanosheet and interface layer between nanofiller and polymer matrix using strategy of inverse finite element modelling under static and dynamic loading.

2 Methods

The FE analysis was used to study the mechanical behaviour of a single MXene nanosheet and MXene/polymer nanocomposite. Simulations were carried out using ABAQUS CAE software. Different 2D and 3D models were analysed under tension conditions. Static general procedure was used for determination of elastic properties and dynamic explicit for strength characteristics of the nanocomposite. The inverse micromechanical modelling method [2] was used to clarify the mechanical properties of MXene and interface layer.

3 Results

The mechanical properties of a single MXene flake were determined and compared with molecular dynamic analysis [3]. Using obtained characteristics, a unit cell of MXene/polymer nanocomposite was created. According to the experimental data [4] the unit cells were build taking into account the interface layer. Using the inverse modelling technique, the properties of interface layer were evaluated.

Conclusions

Obtained mechanical properties of MXene nanosheet had a good agreement with theoretical data, calculated by molecular dynamics analysis.
It was found that stacking effect of MXene flakes have a high weakening factor for composite strength characteristics due to less adhesive surface with polymer matrix.

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