MODELLING OF THE MECHANICAL BEHAVIOUR OF CORROSION PROTECTIVE COATING BASED ON NOVEL POLYMER NANOCOMPOSITE

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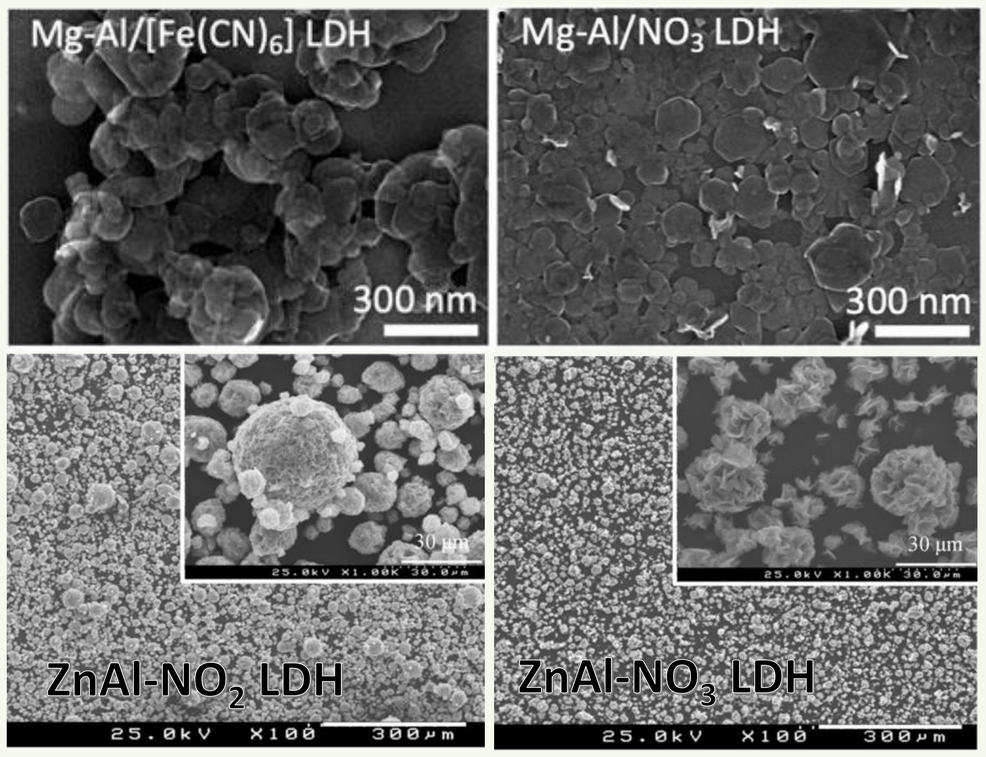
AIM

To perform predictive analysis of mechanical properties of corrosion protective coating based on novel double layered hydroxides (LDH) polymer nanocomposite using numerical finite element modelling.

NANOMATERIALS



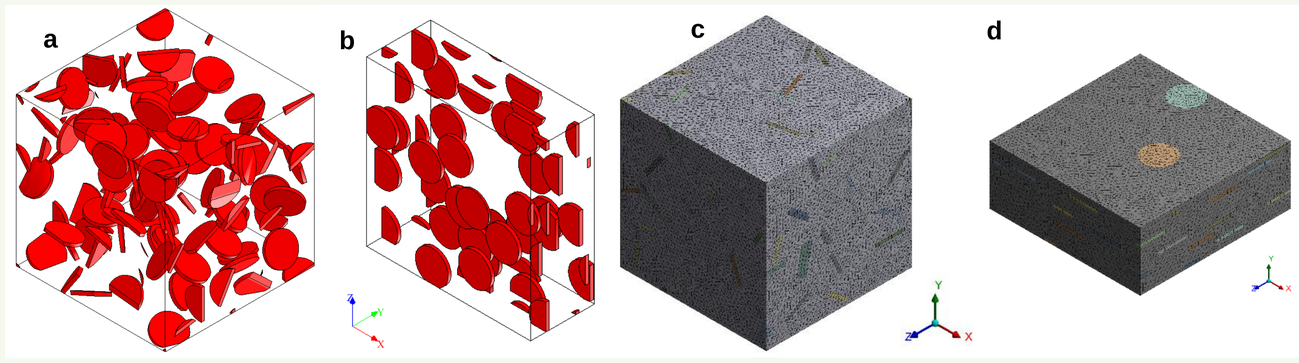
Sushkova A, *et al* (2023), Front. Chem. Eng. 5:1145049, doi: 10.3389/fceng.2023.1145049
Gomes C, *et al* (2020), Materials, 13: 1769; doi:10.3390/ma13071769

MODELLING

Material property	Materials	
	MgAl-LDH	Epoxy
Young's modulus (MPa)	3.3	1060
Poisson's ratio	0.25	0.4

Labuschagne J, et al (2019), Macromolecular Symposia, 384: 1800148
Pinto R, et al (2022), J. Comp. Mat. 56: 951, doi.org/10.1177/00219983211065206

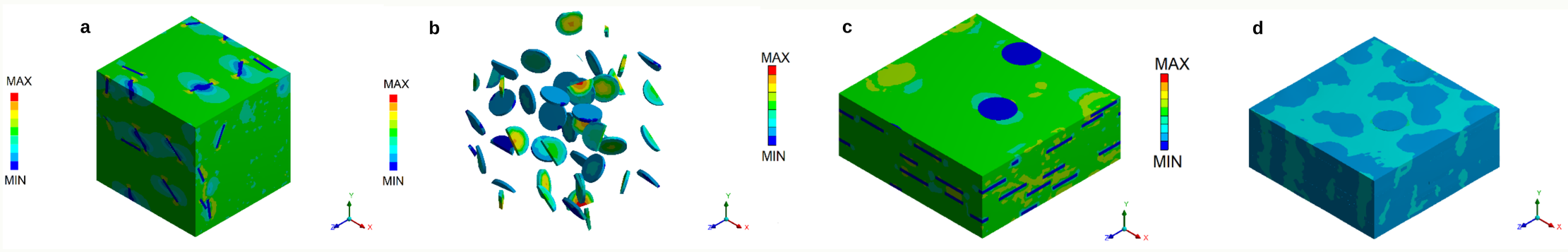
A series of three dimensional computational microstructural models, representative volume elements (RVEs), were developed using Digimat-FE (Extreme Engineering, MSC Software, Belgium).The size of the RVE with randomly distributed LDH particles is 15.4 µm. The dimensions of the RVE with aligned LDH particles are 15.4x6x15.4 µm. The diameter of the particle is 3.08 µm. A computational model of elastic behaviour was developed and solved by using the commercial finite element software ANSYS.



Examples of modelled RVE's: (a) randomly oriented MgAl-LDH particles 5%vf, AR=10; (b) aligned MgAl-LDH particles 5%vf, AR=10

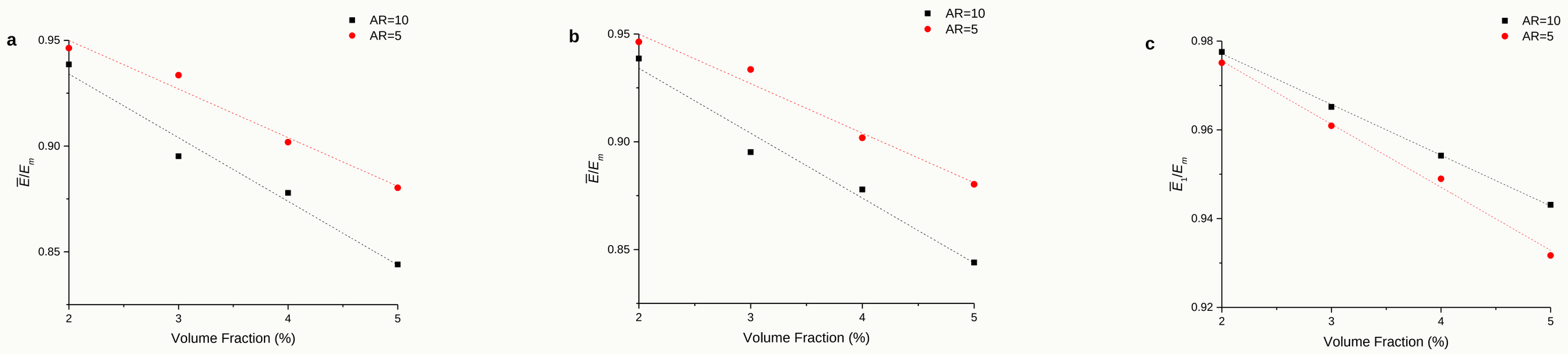
Meshed RVE models: (c) with randomly oriented MgAl-LDH particles 5%vf, AR=10; (d) with aligned MgAl-LDH particles 5%vf, AR=10

RESULTS



Max. principal stress contours for the RVE with randomly distributed MgAl-LDH particles (2%vf, AR=10): (a) whole RVE; (b) LDH particles

Max. principal stress contours for the RVE with aligned MgAl-LDH particles (5%vf, AR=10) as load applied along: (c) x-direction; (d) y-direction



Normalised Young's modulus (a, b) vs %vf under different aspect ratios of randomly distributed MgAl-LDH particles (a) and normalised transverse Young's modulus (c) of aligned particles

CONCLUSIONS

A suitable methodology based on the multiscale FE homogenisation approach for the prediction of elastic properties and micro-structural damage behaviour of polymer nanocomposites filled with LDH was developed. The representative volume elements were modelled using various aspect ratios of nanoparticles, as well as various alignments and volume fractions. After the models' validation, the predictive analysis of developed nanocomposites' mechanical behaviour was performed.

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