COMPUTATIONAL MICROMECHANICS OF NANOCOMPOSITES

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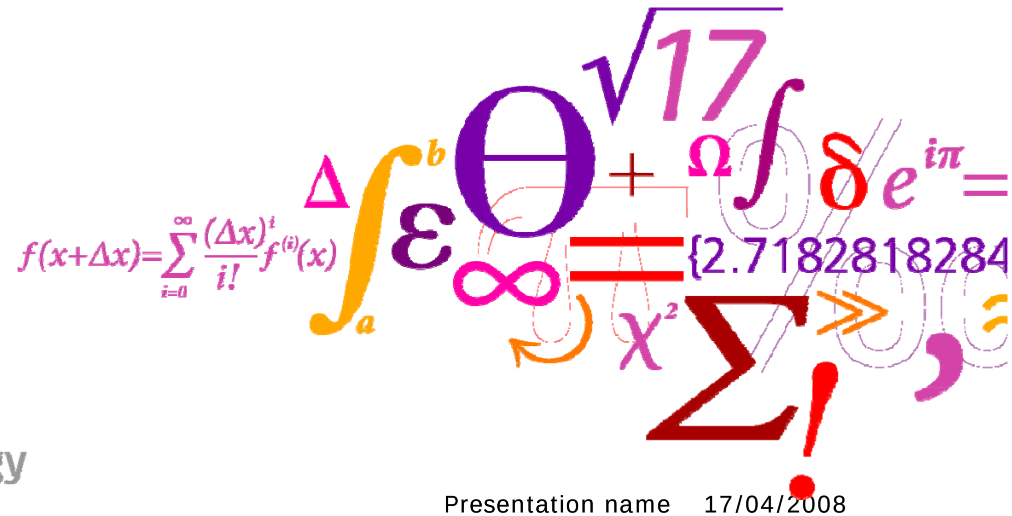
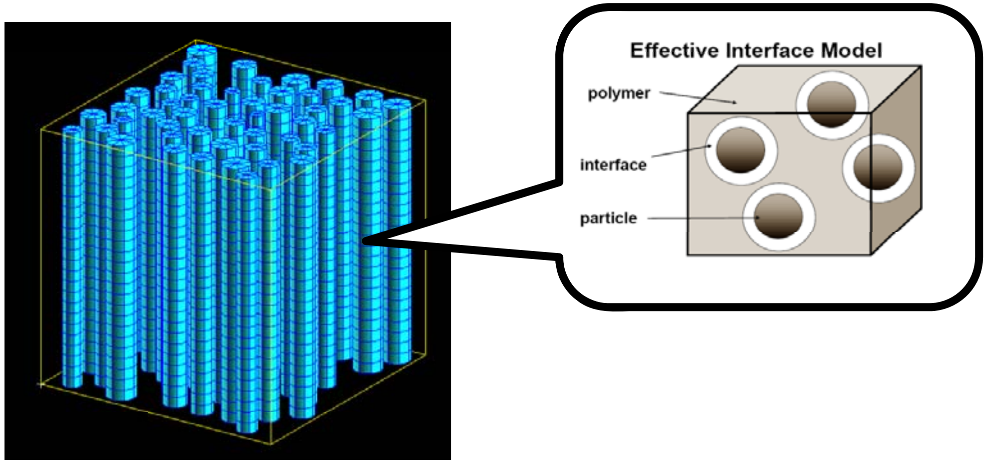


Risø DTU
National Laboratory for Sustainable Energy

Sino-Danish Collaborative project

3D VIRTUAL TESTING OF COMPOSITES FOR WIND ENERGY APPLICATIONS



Partner: Tianjin University of Commerce

Project duration: 1 year
Project Leaders: Leon Mishnaevsky Jr, Prof. Huaiwen Wang

NANOREINFORCED POLYMER COMPOSITES

Is the nanoclay reinforcement the way to enhance the properties of polymer composites for wind blades?

OVERVIEW

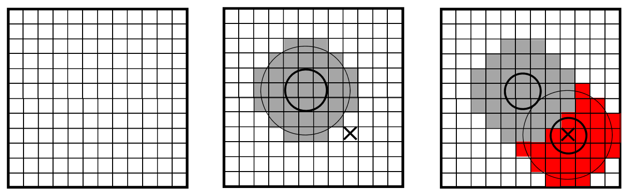
Material and shape	Method, Predicted properties	Conclusions/Remarks
polymer nanocomposites	Takayanagi's equation, -> tensile modulus	Three-phase model including the matrix, interfacial region, and fillers
Nano-platelets reinforced composites	Halpin-Tsai code LITAC; -> buckling, E	Comparison of tensile and compressive elastic moduli, and prediction of effects of incomplete exfoliation and imperfect alignment on modulus
Nylon 6/ layered aluminosilicates (MMT) Nylon 6/ glass fibers	Halpin-Tsai Mori-Tanaka Experiment- > E	The theories of Halpin–Tsai and Mori–Tanaka are used to evaluate the effects of filler geometry, stiffness, and orientation. Model predictions are compared to experimental morphological and mechanical property data
Nanoclay/P	Experiment Mori-Tanaka -> E	Three-phase model including the epoxy matrix, the exfoliated clay nanolayers and the nanolayer clusters was developed[4].
Nanotube/P	Mori-Tanaka FEM 3D-> E, waviness	The effect of waviness on effective moduli of CNT composites was determined by using FEM and the strain concentration tensor in a composite consisting of wavy carbon nanotubes was evaluated
Nanoclay/P	shear lag model-> load transfer	A concept of effective length of reinforcement was adopted to represent the load transfer efficiency
Montmorillonite silicate/ P	Mori–Tanaka-> Overall moduli	Formulas for the overall moduli of composite materials reinforced with transversely isotropic spheroids are derived; a hierarchical model is proposed to consider intercalated silicate stacks; a simple model containing constrained regions around the reinforcements is also proposed[
Nanoclay/P	Halpin-Tsai Mori-Tanaka Experiment FEM 2D-> E	Multiscale modeling was presented taking into account the hierarchical morphology of the nanoclay reinforcement; besides exfoliated nanoclay sheets, an 'effective particle' was proposed to represent the nanoclays distributed in the matrix with intercalation structure[
polymer–clay nanocomposites (PCNs)	FEM-> E	A locally orthotropic finite element model was developed, and then a number of flake groups with varied orientations were assembled to predict the actual moduli seen in PCNs
silica nanoparticle/poly imide spheres	MD Eshelby.-> E	A micromechanical model was suggested that includes an effective interface between the polyimide and nanoparticle with properties and dimensions that are determined using the results of molecular dynamics simulations; effect of the nanoparticle/Polyimide interface on elastic properties was determined.
polymer nanocomposites	FEM. -> E	A FEM model with emphasizing on the role of inclusion/matrix interphase was developed with different shapes including spherical, cylindrical, and platelet[

OVERVIEW

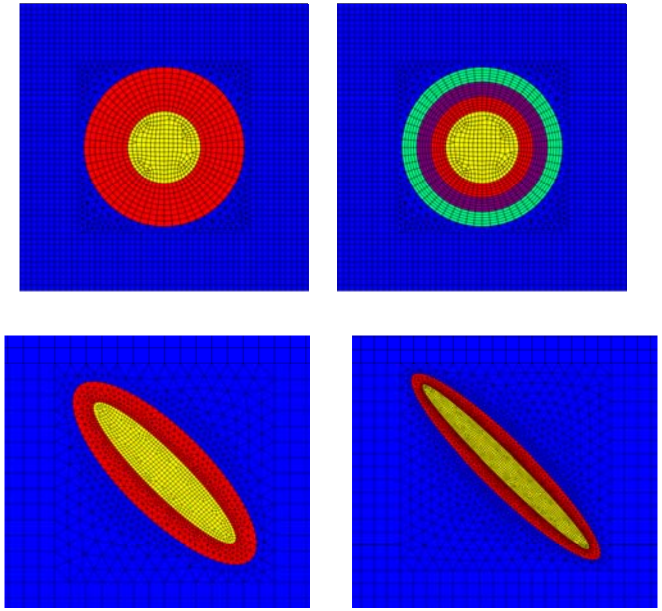
Material and shape	Method, Predicted properties	Conclusions/Remarks
polymer nanocomposites	FEM. -> E	A FEM model with emphasizing on the role of inclusion/matrix interphase was developed with different shapes including spherical, cylindrical, and platelet
Nanoclay/ P	Mori-Tanaka FEM 2D & 3D-> stiffness	Both two-dimensional and three-dimensional finite element models are presented for aligned and randomly oriented clay particles which are randomly distributed; the differences between simulation results and Mori-Tanaka model were discussed and owing to the clusters of nearly aligned particles that formed at high volume fractions
Nanocomposites	stochastic Monte-Carlo approach, -> E	At the same volume fraction, platelets are generally more efficient than fibers in improving composite modulus; low interfacial adhesion and poor dispersion of inclusions lead to decrease in reinforcement efficiency
CNT/epoxy	Experiment Micromechanics-> E	A new micromechanical model denominated Dilute Suspension of Clusters was developed to consider the heterogeneous dispersion of nanoreinforcement of the composite and the clusters formation
Nanotube Nanoplatelet	Mori-Tanaka-> E	The mechanical reinforcing efficiencies of two types of nanoparticles, nanotube and nanoplatelet, are compared. Additionally, the interphase zone in the vicinity of the nanoparticles is addressed
P nanocomposites sphere	Mean-field (MF) FEM-> E	Modeling of nanocomposites using the mean field approach
P nano-composites Circular	FEM 2D-> viscoelastic properties	The influence of the interphase and its structure was studied
Nanoclay/ P	Experiment Eshelby FEM 2D-> E	A micromechanical analytical approach based on a multiscale framework is presented in which special attention is devoted to the constrained region around reinforcements
SWCNT/PET	Experiment Cox and Krenchel Halpin-Tsai Mori-Tanaka-> E	Elastic constants of SWCNT-reinforced PET composites were determined by tensile tests. The experimental results were compared to some micromechanical models which take into account orientation and aspect ratio of the nanotubes but not curvature of the nanotubes, and as a result it was addressed that the waviness of nanotubes is an important factor that influences the reinforcing efficiency

2D COMPUTATIONAL MODEL OF NANOCLAY REINFORCED POLYMERS

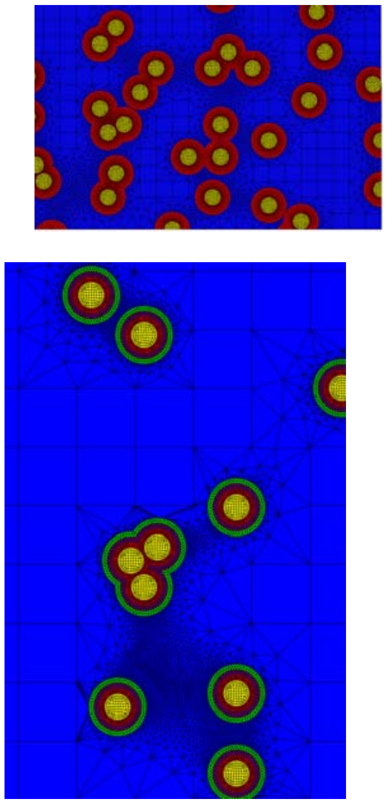
Random arrangement of unit cells with overlapping interfaces



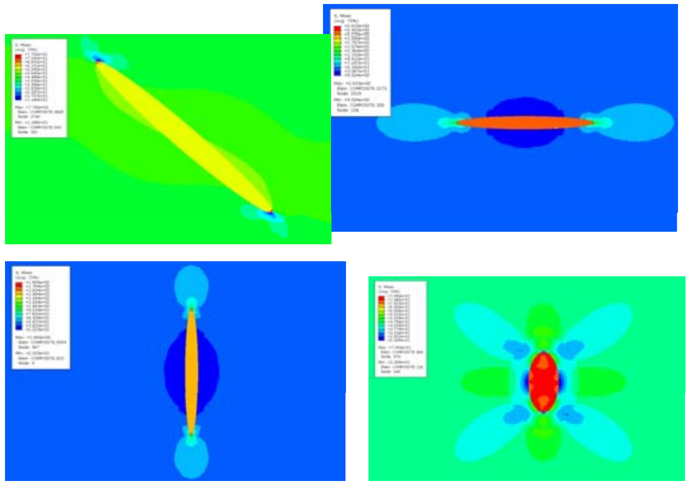
Unit cell model with effective interface (based on Odegard et al., 2005)



Randomly arranged round nanoclay particles

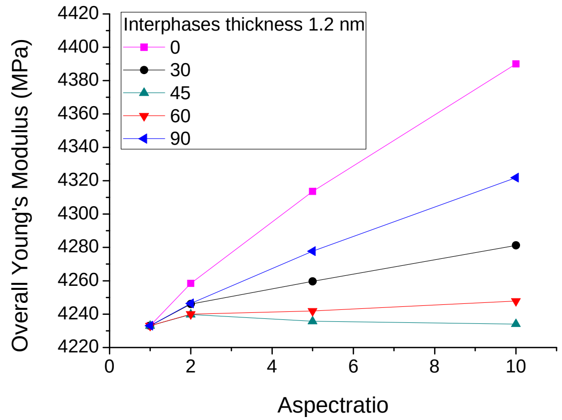


Mises stress

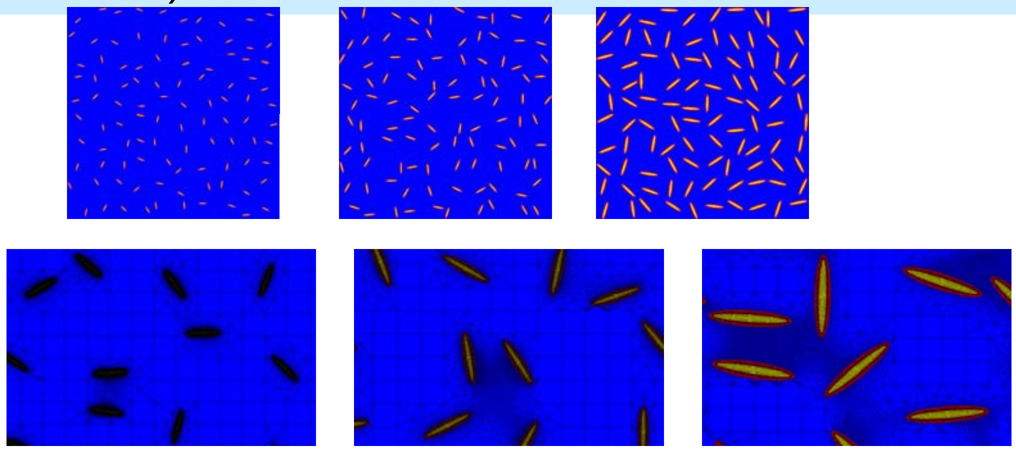


2D COMPUTATIONAL MODEL OF NANOCLAY REINFORCED POLYMERS

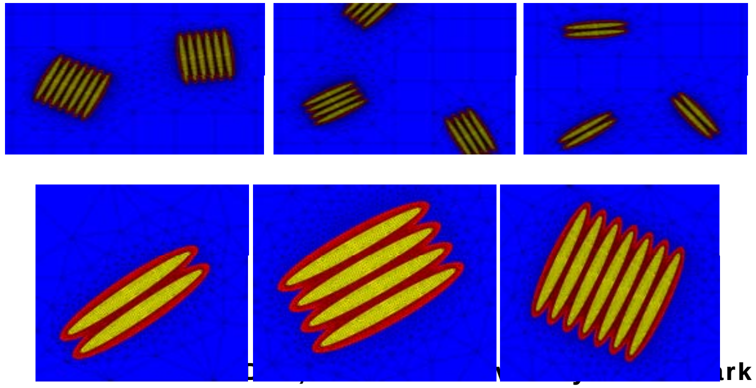
Effect of aspect ratio of particles

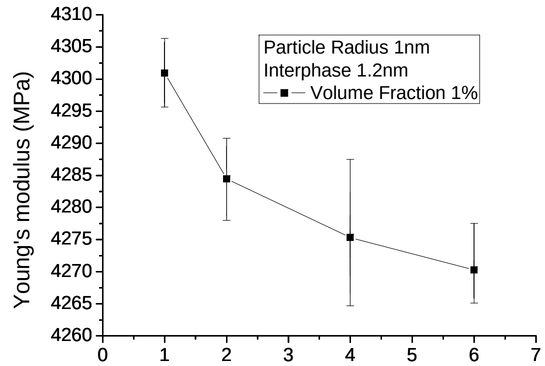


Randomly oriented nanoparticles (exfolliated structure)



Intercalated (clustered) microstructures: effect of nanoparticle clustering



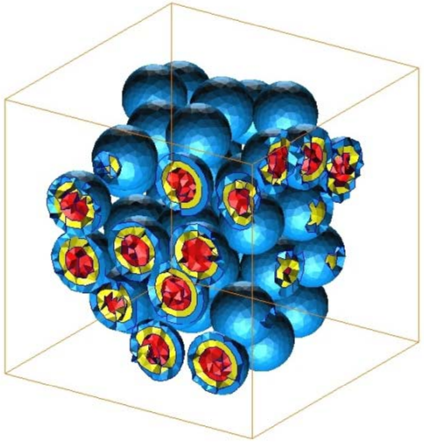


3D MODELLING OF NANOREINFORCED POLYMER COMPOSITES

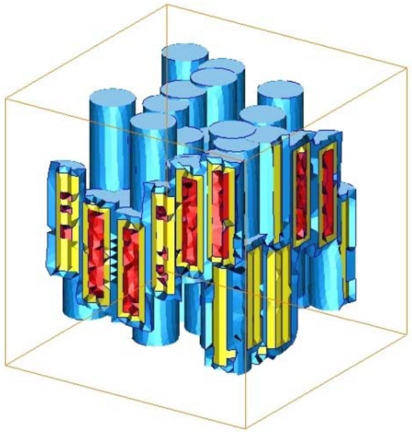
- H. Wang, P. Peng, H.W. Zhou, L. Mishnaevsky Jr, in preparation

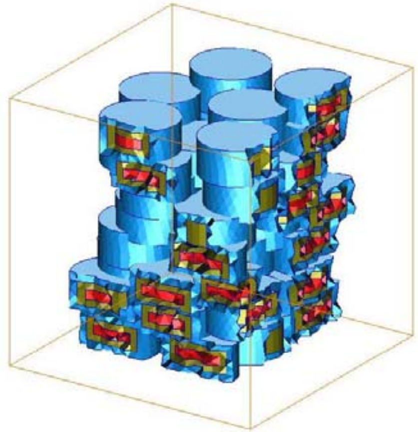
3D COMPUTATIONAL MODELS

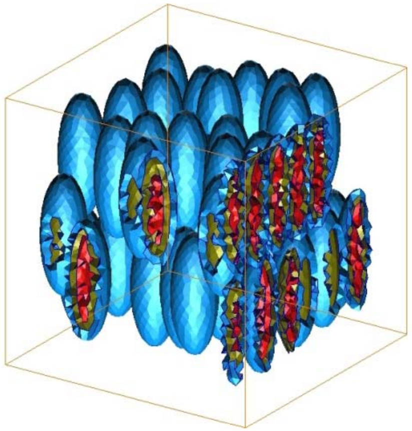
Round nanoparticles



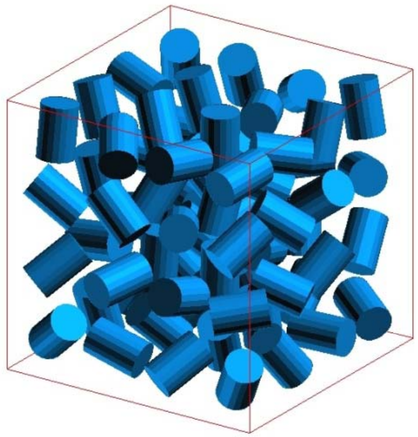
Aligned cylindrical, disc-shaped and ellipsoidal nanoparticles



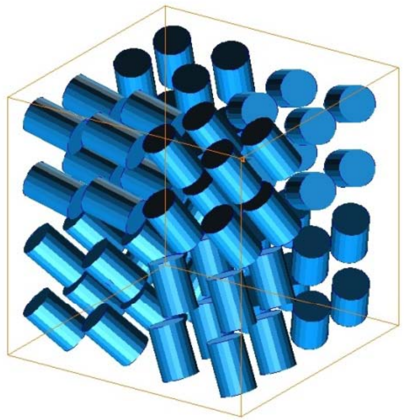




Randomly oriented particles

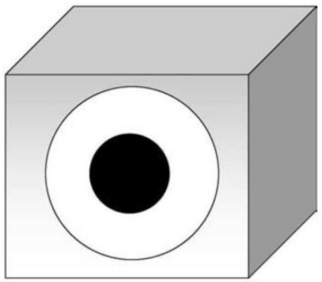


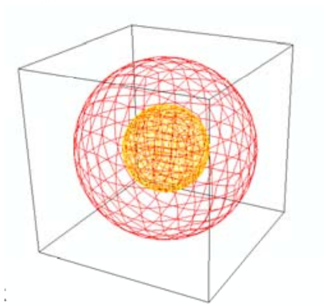
Randomly/correlated oriented particles



ENHANCED EFFECTIVE INTERFACE MODEL

Effective interface model (EIM) was proposed by Odegard and his colleagues to take into account the interface/interphase effects in nanocomposites. In this model, the homogeneous region of finite size represents molecular structure of the perturbed polyimide and interfacial molecules with a gradual transition to the bulk molecular structure. The “effective interface layer” is considered here as a region of finite thickness around nanoparticle, which contains interphases, and/or other structural deviations, or has atomistic structures and properties different from those of both matrix and particles.



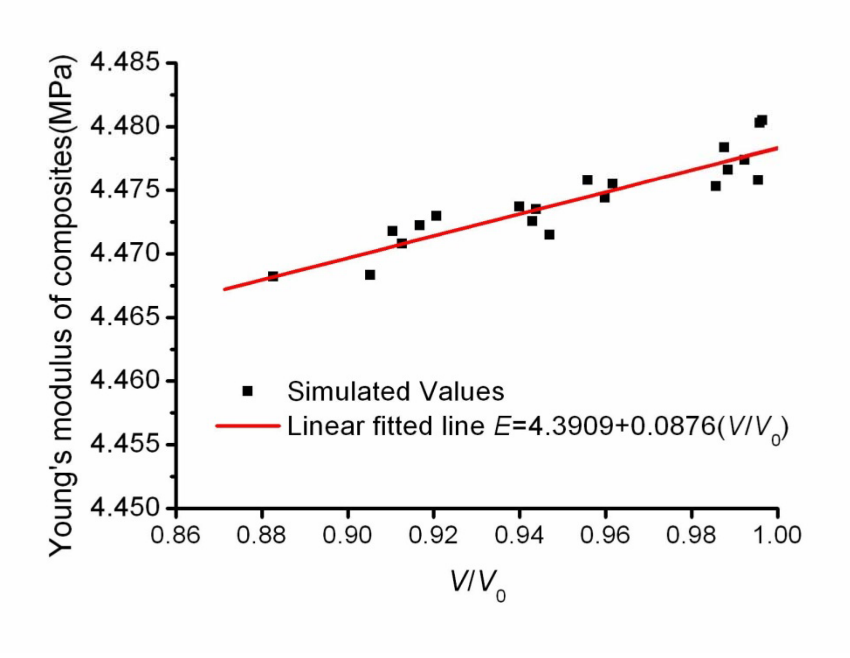


Generalized effective interface model:

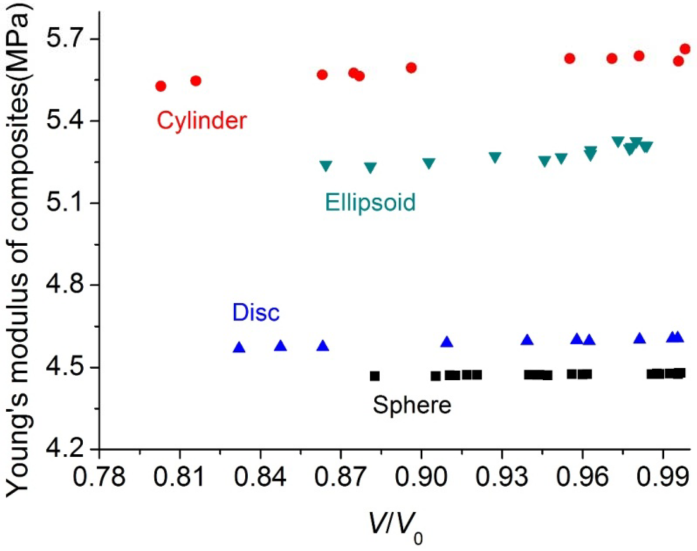
- the interface/interphase layer between the matrix and a particle consists of two layers, which have different properties, one of the stronger (outer layer) and one of them weaker (inner layer).
- While the outer interface layers are allowed to overlap, the inner layers do not overlap with those of neighboring particles. The idea was that the clustering of nanoparticles (which leads to the overlapping out effective interface layers) should ensure a lower and not a higher stiffness. With the bilayer effect interface model, where only the outer, stiffer layers can overlap, the clustering leads to the lower stiffness of the nanocomposites. The thickness of the effective layer was taken 12Å , each sublayer having the thickness of 6 Å.

RESULTS

The relation between Young's modulus of the composite and the degree of interphase intersection

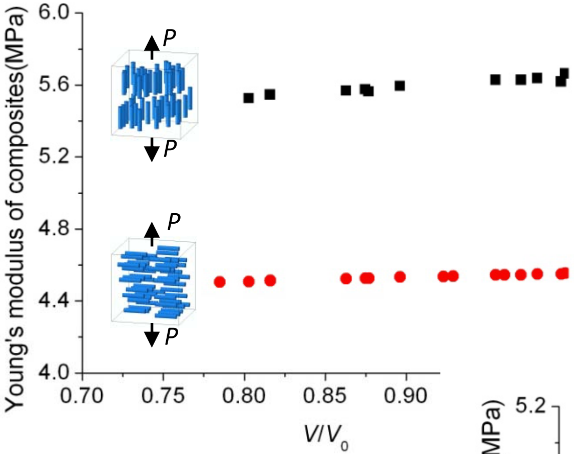


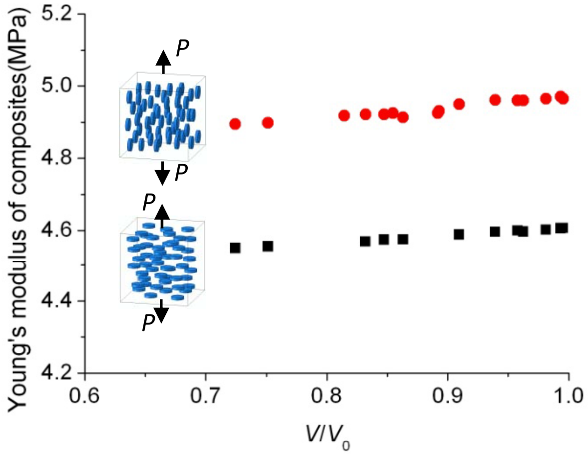
Elastic properties and typical overlapping coefficients for the composites with nanoparticles of different shapes

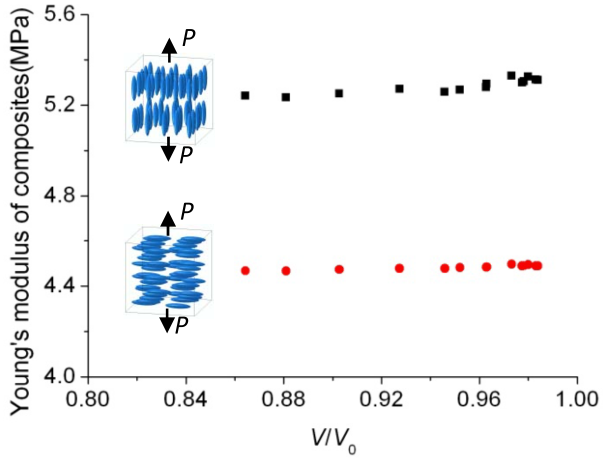


RESULTS

Effect of the vertical versus horizontal loading of aligned elongated particles: cylindrical (a), disc-shaped (b) and ellipsoidal nanoparticles (c).

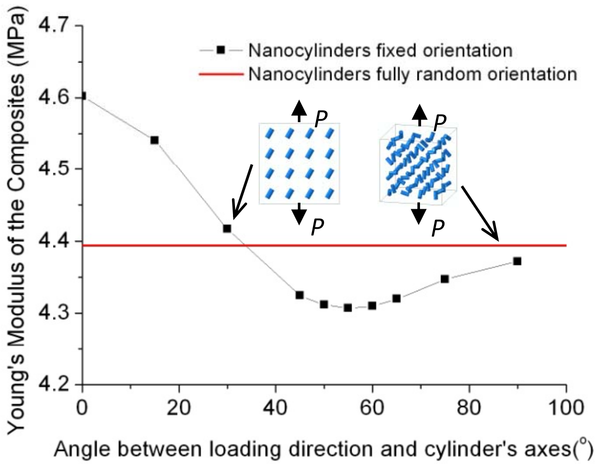




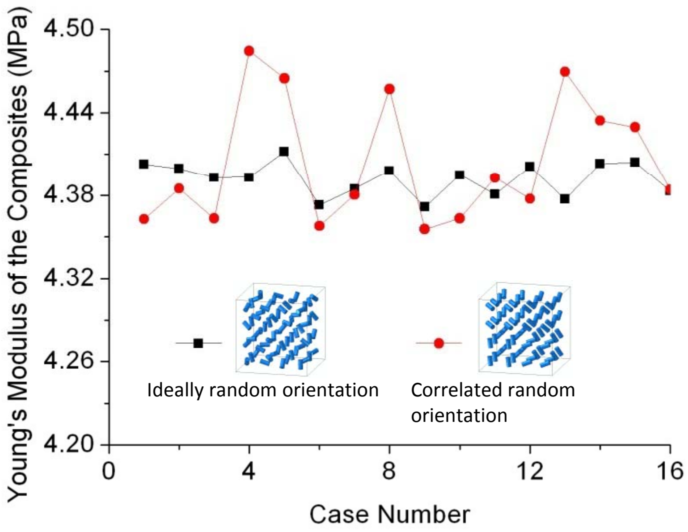


RESULTS

Comparison between the cases of random orientation of nanoparticles and the cases of fixed orientation of nanoparticles



Comparison between the cases of ideally and correlated random orientation of nanoparticles



CONCLUSIONS

- The small amount of nanoreinforcement can lead to drastic enhancement of composite properties, if the corresponding interface and clustering parameters are ensured.
- The clustering of nanoparticles leads to the reduction of the composite stiffness
- The elastic modulus of composites remarkably enhanced with the increasing of aspect ratio of nanoparticles. Thus, high aspect ratio nanoparticles such as nanoplatelets and nanotubes are most efficient enhancement filler among all the shapes
- In intercalated structures, overall elastic modulus of nanocomposite decreases with increasing the number of ellipsoid particles in each cluster