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VIRTUAL NANOTITANIUM: **THEORETICAL ANALYSIS, DESIGN AND VIRTUAL TESTING OF BIOCOMPATIBILITY AND MECHANICAL PROPERTIES OF TITANIUM-BASED NANOMATERIALS**

International Conference on

COMPUTATIONAL MODELLING OF NANOSTRUCTURED MATERIALS

ICCMNM - 2013

September 3 - 6, 2013
Frankfurt Institute for Advanced Studies,
Frankfurt am Main, Germany

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Mechanics of rolling of nanoribbon on tube and sphere

MULTISCALE MODELLING OF ELECTRON TRANSPORT IN CARBON NANOTUBE REINFORCED COMPOSITES

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Development of functional composite materials by addition of inorganic inclusions to polymer matrix attracts growing attention in last decades and carbon nanotubes (CNT) attract particular interest as reinforcement material due to their unique properties tunable by doping and functionalization. However such material characteristics depend not only on the concentration and properties of nanoinclusions but also on their distribution inside embedding polymer, mutual orientation, interaction with surrounding matrix etc., which complicates prediction and optimization of composite properties and leads to large discrepancies in experimental data [1]. Different properties of carbon nanotubes were successfully studied in silico in numerous papers by atomistic calculations. However computational chemistry is limited to systems containing hundreds to several thousands of atoms so only fragments of polymer chains and nanotubes are accessible. Meanwhile optical microscopy analysis shows that industrial-scale CNT-polymer composites contain distribution irregularities and agglomerates of CNTs up to ~10 micron size [2].

Charge transport in such composites mostly explained by electron tunneling between conductive inclusions, probability of which depends on nanotube's electronic structure as well as on tunneling distance and local electric field in the contact region, affected by the presence of other conducting inclusions. To facilitate the investigation of CNT-polymer composites' electric properties a two-level modeling procedure is suggested: first, local density of states (LDOS) around CNT's Fermi level is evaluated from *ab initial* calculations including the effect of doping and functionalization, then a Monte Carlo simulation of charge transport between CNTs is carried out where the tunneling probability is estimated using previously calculated LDOS and simplified representation of electronic wave functions in the inter-CNT space as spherical or cylindrical waves. The suggested procedure, although very simplistic, allows charge transport studies on a length scales of ~100 um compared to the scale of CNTs' distribution irregularities in composites and direct comparison with experimental data. In this work we study the impact of nanotube agglomerates' size and volume fraction on the composite electrical conductivity by computer modeling. Model samples are created by home-developed tool to generate non-uniform filler particle distribution according to a predefined probability map avoiding unphysical intersection of inclusions. Variations of as generated samples due to change in filler content and agglomerates' amount and size distribution is then studied by three methods: finite difference solution of Kirchhoff's current equation using continuum percolation-like local conductivity dependence on CNT volume fraction, construction of equivalent resistor network and statistical simulation of electron tunneling using Monte Carlo approach.

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GPGPU-assisted polymer nanocomposite modeling and characterization

CONTACT

E-MRS Spring Meeting Strasbourg 05/2012

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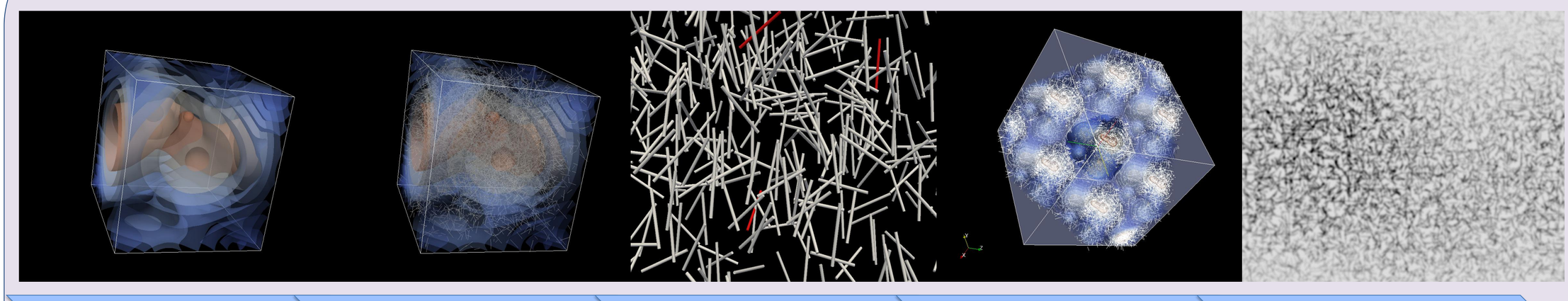
Abstract: Development of the hybrid materials with predefined properties by addition of inorganic nanoinclusions to a polymer material constitutes a hard challenge due to significant properties' variations depending on inclusion's distribution and interaction. To understand structure-property relations in such materials optical image analysis and numeric modeling are widely used, however matching such data with properties' measurements for industrial nanocomposites requires a link to be established between experimental and modeling length scales. In this work a computer code was developed to create a model composite structure with a predefined distribution probability of inclusions using NVIDIA CUDA GPGPU approach. The code is capable of randomly populating and analyzing samples of the typical size of microphotographs used for experimental characterization and typical nanoinclusions' concentrations avoiding unphysical intersections and thus allow correlating the results of both optical characterization and statistical computer modeling. The initial probability distribution can be taken from experimental samples and further varied to investigate the effect of distribution on a desired property. Application to study the effect of carbon nanotubes and carbon nanofibers in a polymer matrix on the composite electrical and mechanical properties is discussed.

Sequence of generation of microphoto-scale computational models for analysis and simulation.



Predefined distribution density → "CNT web" following the distribution → Intersection correction → Periodic conditions → "Real-like" system for simulation & analysis

Rates of filling 168 um cube with 4um x 10 nm cylindrical inclusions:

NVIDIA GTX 480	0.5 vol % uniform distribution	18*10^6 inclusions	5.0 min	NVIDIA Tesla C2050	1.0 vol % uniform distribution	36*10^6 inclusions	33.5 min
NVIDIA GTX 480	0.5 vol % nonuniform distribution	18*10^6 inclusions	9.2 min	NVIDIA Tesla C2050	1.0 vol % nonuniform distribution	36*10^6 inclusions	155 min

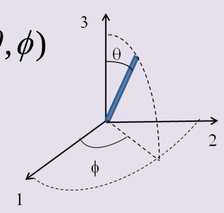
Examples of applications:

Estimation of composite mechanical properties depending on CNF orientation:

$$C = (V_m C_m + V_f \langle C_f A^{MT} \rangle)(V_m I + V_f \langle A^{MT} \rangle)^{-1}$$

$$\langle A^{MT}(\theta,\phi) \rangle = \frac{\int_0^{2\pi}\int_0^{\pi} \overline{A}^{MT}(\theta,\phi)\rho(\theta,\phi)\sin(\theta)d\theta d\phi}{\int_0^{2\pi}\int_0^{\pi}\rho(\theta,\phi)\sin\theta \mathrm{d}\theta\mathrm{d}\phi}$$

$\rho(\theta,\phi)$



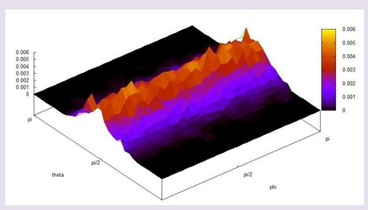
(Mori-Tanaka theorem of averages stresses in matrix)

$$A^{MT} = A^{Eshelby}((1-V_f)I + V_f A^{Eshelby})^{-1}$$

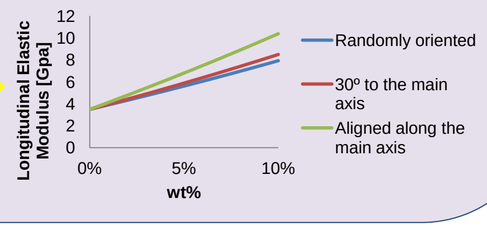
(Eshelby Equivalent inclusion method)

$$A^{Eshelby} = (I + ES_m(C_s - C_m))^{-1}$$

Simulated orientation distribution:

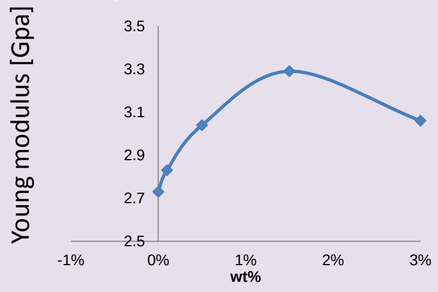


Elastic modulus depending on the orientation state

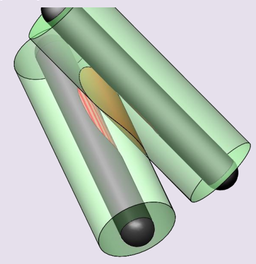


Inclusions' contact surface area evaluation and properties correction:

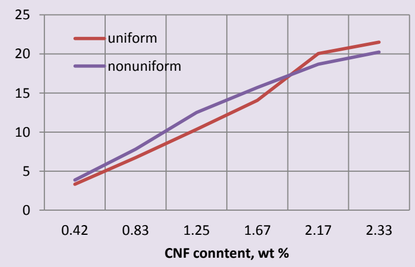
Tensile tests (CNF/Epoxy) – experimental observation



The fiber surface area between 2 fibers doesn't participate in polymer-inclusion stress transfer



% of ineffective area



With the increase of nanofiber content the ineffective surface area increases up to 20 % by 2 wt%.
Change in total ineffective area depending on nanofiber distribution can be observed directly.

To be added soon: various inclusion shapes (only spherically capped cylinders are implemented at the moment);
equivalent resistance network building;
equivalent continuum distribution of mechanical properties;

Acknowledgements:

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