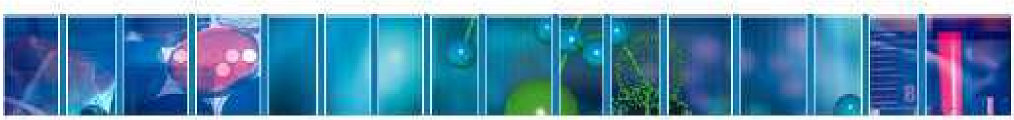

2012 Spring Meeting

May 14 – 18
Strasbourg, France

PROGRAMME

CONFERENCE SYMPOSIA

MATERIALS FOR ENERGY

A Advanced Silicon Materials Research for Electronic and Photovoltaic Applications III
B Thin Film Chalcogenide Photovoltaic Materials
C Solid State Ionics: Mass and Charge Transport across and along Interfaces of Functional Materials
D Unconventional Thermoelectrics: from new materials to energy conversion devices
E Actinide compounds and properties
F Solid proton conductors (In honor of Prof. G. Alberti)

BIO / ORGANIC / POLYMERIC MATERIALS

G Functional Biomaterials
H Organic and Hybrid Materials for Flexible Electronics: Properties and Applications
I Biological applications for organic electronic devices
J DNA Directed Programmable Self-assembly of Nanoparticles into Meta Materials for energy and other applications
K Surface modifications of carbon-related materials II

MATERIALS FOR ELECTRONIC / PHOTONIC / PLASMONIC

L Novel Functional Materials and Nanostructures for innovative non-volatile memory devices
M More than Moore: Novel materials approaches for functionalized Silicon based Microelectronics
N Control of light at the nanoscale: materials, techniques and applications
O Applied Nanoplasmonics: Nanoplasmonic Functional Materials and Devices

ADVANCED MATERIALS AND NANO MATERIALS

P Advanced Hybrid Materials II: design and applications
Q Novel materials and fabrication methods for new emerging devices
R Science and technology of nanotubes, graphene and 2D layered materials
S Novel materials for hetereogeneous catalysis
T Physics and Applications of Novel gain materials based on Nitrogen and Bismuth Containing III-V Compounds
U Carbon- or Nitrogen-Containing Nanostructured Thin Films

METHODS AND ANALYSIS

V Laser materials processing for micro and nano applications
W Current Trends in Optical and X-Ray Metrology of Advanced Materials for Nanoscale Devices III
X Quantitative Microscopy of Energy Materials
Y Advanced materials and characterization techniques for solar cells

16:20

GPGPU-assisted polymer nanocomposite modelling and characterisation

Authors : Sergey V. Pyrlin[1,2]; Marta M.D. Ramos [1]; Anna Y. Matveeva [2]; Ferrie W.J. van Hattum[2]
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Resume : 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. This work is a part of Marie Curie Initial Training Network "CONTACT" (FP7-PEOPLE-ITN-2008-238363) http://www.contactproject.eu/.

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GPGPU-assisted polymer nanocomposite modeling and characterization

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.

1. Predefined distribution density
2. "CNT web" following the distribution
3. Intersection correction
4. Periodic conditions
5. "Real-like" system for simulation & analysis

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

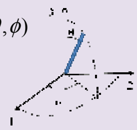
NVIDIA GTX 480	0.5 vol % uniform distribution	$18*10^6$ inclusions	5.0 min	NVIDIA Tesla C2050	1.0 vol % uniform distribution	$36*10^6$ inclusions	33.5 min
NVIDIA GTX 480	0.5 vol % nonuniform distribution	$18*10^6$ inclusions	9.2 min	NVIDIA Tesla C2050	1.0 vol % nonuniform distribution	$36*10^6$ inclusions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

Examples of applications:

Estimation of composite mechanical properties depending on CNF orientation:

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

$$\rho(\theta,\phi)$$



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

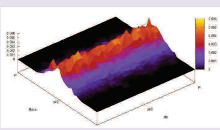
(Mori-Tanaka theorem of averages stresses in matrix)

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

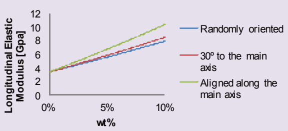
(Eshelby Equivalent inclusion method)

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

Simulated orientation distribution:

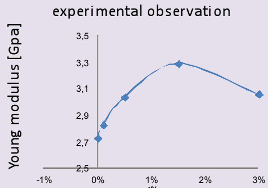


Elastic modulus depending on the orientation state

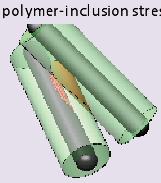


Inclusions' contact surface area evaluation and properties correction:

Tensile tests (CNF/Epoxy) – experimental observation

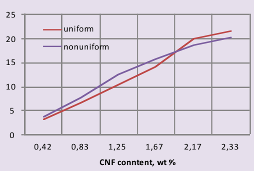


The fiber surface area between 2 fibers doesn't participate in polymer-inclusion stress transfer



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.

% of ineffective area



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:

1. The work is a part of the CONTACT project for the tailored supply-chain development of CNT-filled composites with improved mechanical and electrical properties funded by Marie Curie Initial Training Network "CONTACT" (FP7-PEOPLE-ITN-2008-238363) http://www.contactproject.eu/;
2. The Center of Physics of University of Minho research is partially sponsored by FEDER funds through the program COMPETE- Programa Operacional Factores de Competitividade and by national funds through FCT-Fundação para a Ciência e a Tecnologia, under the projects CONC-REEQ/443/EEI/2005 and PEst-C-FIS/UI607/2011-2012.