J Nanomed Nanotechnol 2013, 4:6
http://dx.doi.org/10.4172/2157-7439.S1.015

OMICS Group Conferences
Accelerating Scientific Discovery

3rd International Conference on
Nanotek & Expo

December 02-04, 2013 Hampton Inn Tropicana, Las Vegas, NV, USA

Multiscale modeling of the atomic layer deposition of HfO_2 thin film grown on silicon: How to deal with a kinetic monte carlo approach

Ahmed Dkhissi
AgroParistech, France

In this presentation we discuss briefly the principles of the multiscale modeling and its applications in nanomaterials and nanoscience through selected applications. Indeed, to investigate the atomic layer deposition (ALD) of HfO_2 on Si(100) surface, an original integrated approach developed within a multiscale strategy, which combines first-principles quantum simulations and kinetic Monte Carlo (KMC), is presented. Density functional theory within the hybrid functional is used to determine the detailed physicochemical mechanisms and associated energetics of the two half cycles taking place during the initial stage of film growth. A kinetic Monte Carlo model is then proposed that deals with the stochastic nature of the calculated DFT mechanisms and barriers. Beyond the chemical information emanating from DFT calculations, the lattice-based KMC approach requires preliminary physical considerations issued from the crystal structures that the system is intended to adopt. This is especially critical in the case of heterogeneous systems like oxides deposited on silicon. We also describe (i) how atomistic configuration changes are performed as a result of local events consisting in elementary reaction mechanisms occurring on specific lattice sites, (ii) the temporal dynamics, governed by transition probabilities, calculated for every event from DFT activation barriers, and (iii) the relation of KMC with the ALD experimental procedure. Some preliminary validation results of the whole multiscale strategy are given for illustration and pertinence with regard of the technological main issues.

Biography

Ahmed Dkhissi received a Ph.D. in Physics from the University of Paris XI in 1996. After postdoctoral studies at the University of Leuven and the University of Mons, he became a senior researcher. The main activity of his research is focused on multiscale modeling and simulation of nanomaterials and biological systems. Modeling methods include atomistic, quantum simulations, kinetic MonteCarlo, statistical mechanics and macroscopic simulations. Structure-property relationships of Molecules, biomolecules, nanoparticles, ?-conjugated materials and nanoscale interfaces are the main focus of modeling research. He is (co)author of over 55 papers in international peer-reviewed journals and more 1000 citations. He is member of Editorial board of ISRN Physical and Chemistry, and International Journal of Renewable and Sustainable Energy (IJRSE).

adkissi@laas.fr

Super paramagnetic iron oxide Fe_3O_4 nanoparticle-induced hyperthermia treatment under magnetic resonance imaging

Ahmed Elshahawy
Misr University for Science and Technology, Egypt

Super paramagnetic iron oxide Fe_3O_4 nanoparticles prepared via photochemical reaction in pure form were used for inducing hyperthermia to treat subcutaneous Ehrlich carcinoma implanted in female mice. Our results indicate that the mean temperature profiles at the rectum, periphery of the tumor surface and at the center of the tumor during hyperthermia treatment increased gradually. The maximum temperature achieved in the tumor center was 47±1°C after 20 min with radiofrequency exposures at 25 kW. The acquired magnetic resonance images identified apoptotic cells in the center of the tumor which were exposed to magnetic resonance hyperthermia (MRH). Apoptotic cells presented as dark signal intensity in the T1-weighted images that were further confirmed by pathological examinations. Also, the results revealed that the tumor size in the all mice exposed to MRH is still as the same as before the treatment, but the rate of tumor growth was very slow by comparing with the growth rate of control group.

Biography

Ahmed Elshahawy has acquired his BS and MS in Biophysics then Ph.D. in Nanotechnology and Applied Medical Physics from Fculty of Science, Cairo University in 2012. Ahmed thesis was evaluated externally from the Department of Medical Applied Physics and Material Science, Johns Hopkins University, USA and Department of Medical Applied Physics, Lab of Nanotechnology & Magnetism (NANOMAG) Research Technological Institute, University of Santiago de Compostela, Spain. Ahmed has over 15 years superintending the MRI & CT Scan in several sites in Cairo. Ahmed is a Biomedical physics consultant & applications developer at the Children Cancer Hospital 57357. Shahawy is a lecturer at Misr University for Science and Technology (MUST) and applications consultant at Siemens healthcare.

aabdelwahab73@yahoo.com