

Nanoscale materials (nanocomposites, nanowires, carbon nanotubes, nanoparticles): Computational modeling and applications in molecular, cell biology and nanomedicine

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Discovering of carbon nanotubes (CNTs), by S. Iijima, [1] in 1991 was a revolution in nanoscience. (CNTs) possess extraordinary physico-mechanical properties, and could be used as reinforcement for nanocomposites (a matrix- polymer, ceramic etc. reinforced by CNTs). Recently has been discovered that these nanomaterials, could be used as constructive elements in many regenerative and tissue engineering problems. As has been proved nano and biocomposites, play an important role as successful tools in molecular and cellular biology and medicine. Moreover it has been established that nanoparticles (nanowires, nanoshells), could be considered as appropriate materials in cancer research. Nanotechnology based on nanoparticles, have been developed and in many cases they have been used for In Vitro and In Vivo Diagnostics, Therapy and Treatment of cancer. The aim of the work, presented could be formulated as follows: to give some basic studies, regarding to the mechanical behaviour of nanocomposites, and to present some new computational models regarding to molecular and cellular biology and medicine. Nanowires, as nanoscale materials also have very important applications, as field effect transistor (NWFET), for example [2]. Computational models, based on the classical mechanics theories and molecular dynamics for simulations of physico-mechanical, electronics, optical etc. properties of polymeric nanocomposites have been designed as well in the paper by authors. Numerical author's FORTRAN programs and algorithms have been developed by authors in the paper. Some basic definitions and applications of nanomedicine have been analysed too. Numerical results, obtained have been compared by the experiments in literature and they show a very good agreement. Applications of nanotubes, nanowires, nanorods, nanoparticles, nanodots, nanocomposites in engineering, technique, nanomedicine, molecular and cellular biology have been given, accounting for work

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