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# SIMULATION OF FUNDAMENTAL PROPERTIES IN CNT- AND GRAPHENE-BASED NANOPOROUS MATERIALS: *ELECTROMECHANICS AND ELECTROMAGNETICS*

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**ABSTRACT**

Electromechanical and electromagnetic properties of CNTs and graphene-based nanoporous materials are essential for various nanotechnology applications, e.g. for engineering new classes of ultra-light, highly conductive nanomaterials with exceptional mechanical strength, flexibility, and elasticity. We pay major attention to CNTs, graphene nanoribbons and nanofibers (GNR and GNF), CNT- and graphene-based aerogels (CNTBA, GBA), CNT- and grapheme-based 3D-nanofoams and carbon-based polymer nanocomposites, as to the basis for the unique nanoelectronic devices, revolutionary membrane materials (due to their strength and atomic thickness) and nanosensors. Particular properties of carbon-based nanoporous systems in dependence on porosity extent, morphology and fractal dimension allow finding practically useful correlations between their mechanical and electrical properties

*Keywords:* CNT- and graphene-based aerogels (CNTBA, GBA), CNT- and grapheme-based 3D-nanofoams, carbon-based polymer nanocomposites

## 1 INTRODUCTION

Technological interest in contacts of CNTs or GNRs with other conducting elements in nanocircuits [1], FET-type nanodevices, CNTBA and GBA, carbon-based nanofoams constitutes the reason for estimating their electromagnetic properties including interconnect impedances, which depend on chirality effects and electromechanical properties as some integrated effect of macroscopic structural deformations. One of the likely applications of CNTs and graphene nanofoams (see Figures 1 and 2) is in chemical sensing. These sensors are able to detect gases at room temperature, while many commercial sensors today require high temperatures to work properly. The porous CNTs and graphene are not only more effective than current commercial sensors it also can easily be reused, e.g., in order to "empty" the graphene of trapped gas molecules, all the graphene needs is an electric shock. CNTs and graphene nanafoams graphene may also be used in energy storage, such as supercapacitors and batteries, accumulators of massive amounts of

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energy, (e.g., hydrogen). The CNTs and graphene nanafoams have a high surface area thanks to its porous nature, providing their high electrochemical capacitance.

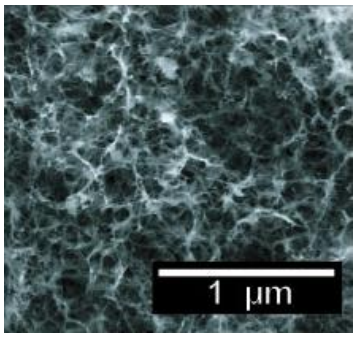


FIGURE 1 CNTS BASED NANOAEROGEL IMAGE (M B BRYNING, D E MILKIE, M F ISLAM, L A HOUGH, J M KIKKAWA, A G YODH 2007 CARBON NANOTUBE AEROGELS *ADVANCED MATERIALS* **19**(5) 662)

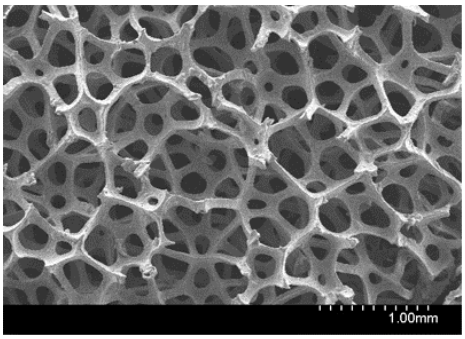


FIGURE 2 GRAPHENE BASED NANOFOAM IMAGE HTTPS://GRAPHENE-SUPERMARKET.COM/3D-GRAPHENE-FOAMS

## 2 MODELS OF CARBON BASED NANOPOROUS MATERIALS

Nanoporous systems are considered as complicated ensembles of basic nanocarbon interconnected elements (e.g., CNTs or GNRs with possible defects and dangling boundary bonds) within the effective media type environment (see Figures 3and 4). Interconnects are essentially local quantum objects and are

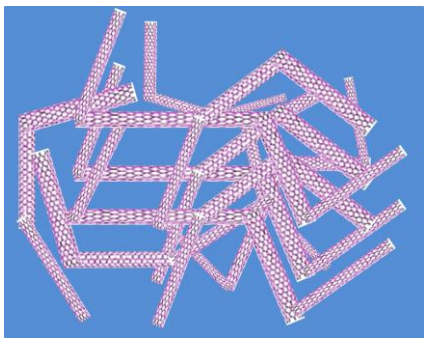

FIGURE 3 STRUCTURAL MODEL OF CNTBA: COVALENT BONDING IN INTERCONNECTS BETWEEN STATISTICALLY PARAMETRIZED CNTS AND VAN DER VAALSE TYPE SIDE BONDING OF CNTS

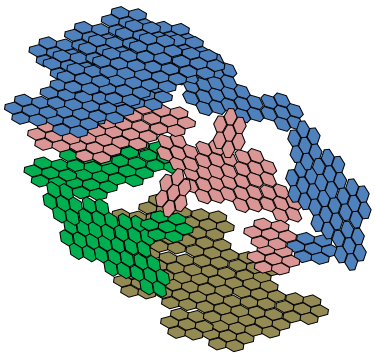

FIGURE 4 STRUCTURAL MODEL OF GBA: COVALENT BONDING IN INTERCONNECTS BETWEEN STATISTICALLY PARAMETRIZED GNRS AND VAN DER VAALSE TYPE BONDING OF GNRS LAYERS

evaluated in the framework of the developed cluster approach based on the multiple scattering theory formalism as well as effective medium approximation [1], which allows calculating the above mentioned nanosized systems' local electronic densities of states, conductivity, force interaction constants, etc. Technological interest in contacts of CNTs or GNRs with other conducting elements in nanocircuits [2], FET-type nanodevices, CNTBA and GBA, carbon-based nanofoams constitutes the reason for estimating their electromagnetic properties including interconnect impedances, which depend on chirality effects and electromechanical properties as some integrated effect of macroscopic structural deformations.

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