CNTs- AND GNRs-BASED ELECTROMAGNETIC AND SPINTRONIC DEVICES: MODELS AND SIMULATIONS

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Fundamental electromagnetic and electromechanical properties of CNTs, graphene nanoribbons (GNR) and nanofibers (GNF), CNT- and graphene-based aerogels (CNTBA, GBA), CNT- and graphene-based 3D-nanofoams and carbon-based polymer nanocomposites 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. These nanomaterials are the basis for unique nanoelectronic devices 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. Electromagnetic properties of CNTs and GNRs nanostructures with functionalized atomic groups and their various interconnects with the essential concentration of 'dangling bonds' are very sensitive to local external perturbations. The induced changes of local electronic density of states lead to the correlated changes of current and spin states. Models of nanocarbon spintronic devices are developed as memory nanodevices, particularly, based on magneto-resistance phenomena. Models of nanocomposite carbon-based materials and nanodevices are proposed.

1. Introduction

The main objective of the current study is to demonstrate the implementation of advanced simulation models to ensure a proper description of the electronic properties, electrical conductivity, electromagnetic and electromechanical phenomena of functionalized CNT- and GNR-based nanostructures of different morphologies and their interconnects for nanosensor and nanomemory systems. The sensitivity of the local electronic density of states to external influences (mechanical, chemical, magnetic, etc) on the fundamental electromagnetic properties of CNTs, GNRs and their metal interconnects have been analyzed from the point of view of nanosensor applications [1,2]. We develop a set of prospective models of nanocarbon-based nanomaterials and nanodevices based on the various interconnects and interfaces (see Figure 1).

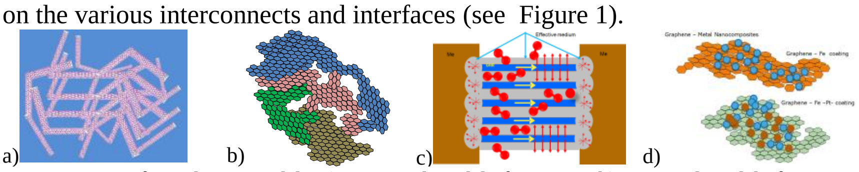

Figure 1 A set of simulation models: a) Structural model of CNTBA; b)Structural model of GBA; c) GNRs-based gas nanosensor device; d) Graphene-metal nanocomposites- Fe and Fe-Pt coatings.

Correlations between various external influences (mechanical, chemical, electromagnetic *etc* factors) and fundamental properties of nanocarbon materials are studied.

2. Memory nanodevices

Nanocarbon-magnetic metal interfaces open new possibilities for the creation of nanospintronic devices, e.g., nanomemory devices [1]. The model of CNTs growth with the predefined chiralities in a magnetically managed CVD process with the use of magnetically anisotropic Fe_xPt_{1-x} nanoparticles with various substitutional disorders has been developed (see Figure 2). The possibilities of CNT forest growth based on FePt nanoparticles for magnetic nanomemory are also evaluated [1], (see Figure 2).

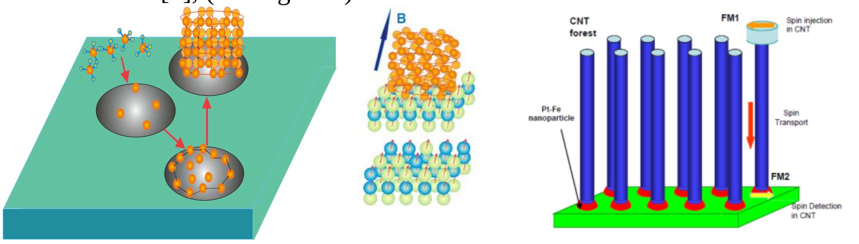

FIGURE 2 Model of CNTs growth in a magnetically controlled CVD process based on Fe-Pt nanodrops catalysts. CNTs forest is considered as a prototype of the magnetic memory, where ferromagnetic nanoparticles serve as cells of the magnetic memory.

Another possibility for the creation of magnetic memory devices is the magneto-resistance phenomenon [1] (giant magneto-resistance - GMR, tunnelling magneto-resistance TMR) consisting of sandwiches of two ferromagnetic metals separated by a thin spacer layer of **normal metal** (see, e.g., Figure 3) **or semiconductor.** They are of great industrial importance and are called spin-valves used as magnetic field sensors. The resistance of the device is dependent on the relative magnetization orientation of the ferromagnets. Our idea is to reach the same effect by introducing metal or semiconductor-like CNTs into the N space. The TMR signal operates in the same way as the GMR, where R_P and R_A are the resistances of the device for parallel and antiparallel orientations, respectively, of the ferromagnets magnetization (Figure 3).

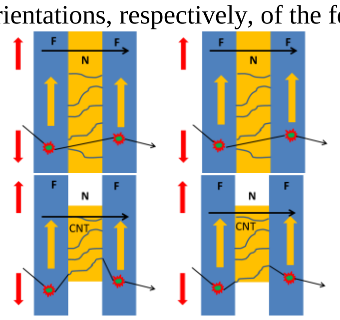

FIGURE 3a Giant magneto-resistance (GMR) device. *Current perpendicular to the plane* (CPP) spin-valve. A thin normal metal spacer (N-e.g.,CNT metal-like:) separates two ferromagnets (F).

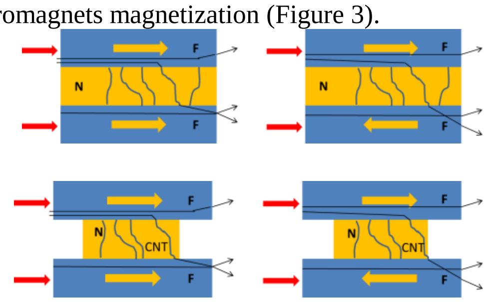

FIGURE 3b *Current in the plane* (CIP) spin-valve. Separate channels are for minority and majority spins. The electrons scatter from one F layer to the other on the way through the sandwich.

The next object of our interest and simulation is Fe-Pt-graphene nanocoatings for various Fe_xPt_{1-x} compounds where electrical and magnetic properties of Fe-Pt-graphene nanofilms (see Figure 1d) are essentially dependent on the morphology and composition of this nanosystem. Percolation thresholds are inverstigated. These nanosystems are also considered as prospective elements of spintronic nanodevices.

3. Nanoporous and nanocomposite material models

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 (Fig.1a,1b,1c). Interconnects are essentially local quantum objects and are evaluated in the framework of the developed cluster approach based on the multiple scattering theory formalism as well as effective medium approximation [1]. Particular properties of carbon-based nanoporous systems in dependence on the porosity extent, morphology and fractal dimension are practically studied to find useful correlations between their mechanical and electrical properties.

The model of nanocomposite materials based on carbon nanoclusters suspension (CNTs and GNRs) in dielectric polymer environments (e.g., epoxy resins) is considered as a disordered system of fragments of nanocarbon inclusions with different morphology (chirality and geometry) in relation to a high electrical conductivity in a continuous dielectric environment. Presumably, the electrical conductivity of nanocomposite material will depend on the concentration of nanocarbon inclusions (in fact, carbon macromolecules).

Isolated nanocarbon inclusions will provide conductivity due to the hopping conductivity mechanism through dangling bonds up to the percolation threshold, when at high concentrations (some mass %) a sustainable ballistic regime appears, which is characteristic of pure carbon systems. The hopping mechanism is regulated by the hopping of electron between 'nanocarbon macromolecules': $\sigma_{IC} = \sigma_0 \cdot \exp(-\frac{4}{3}\left(\frac{4\alpha r_{IC}}{a}\right)^{3/4}\left(\frac{W_0}{kT}\right)^{1/4})$, where r_{IC} - is the length of the tunnel 'jump' of the electron equal to the distance between 'nanocarbon' clusters, σ_0 - normalization constant which means the conductivity of monolithic dielectric medium. Added to this is the effect of intrinsic nanocarbon cluster conductivity, which is dependent on its morphology. The electric conductivity will also depend on the spatial orientation of nanocarbon inclusions. It will be greater for the longitudinal electric field orientations and lower for the transverse ones. Of course, any spatial orientations are technologically possible. The overall conductivity of nanocomposite material is: $\Sigma \approx \Sigma_D + \sum_{k=1}^{L} R_k^{-1}$,

$$R_k = \sum_{j=1}^{M}\sum_{i=1}^{N}(\sigma^{-1}_{nano,i.j,k} + (N_{eff-in,i\,j,k}\sigma_{IC-in,i,j,k})^{-1} + (N_{eff-out,i,j,k}\sigma_{IC-out,i,j,k})^{-1}),$$

where M - is the number of conductivity channels, N – is the number of nanocarbon clusters in the conductivity channel, N_{eff} is the number of effective bonds of tunneling bonds, $\Sigma_D = (R_D)^{-1}$ is the conductance of dielectric medium, σ_{nano} is the conductivity nanocluster, σ_{IC} - the hopping conductivity of the *in-* and *out-type* effective bond, which for large nanocarbon inclusion concentrations create their interconnect. A natural application of this kind of nanocomposite materials are nanosensors of pressure and temperature.

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