NEMESYS: Non Equilibrium dynamics Models and Excited state properties of low dimensional SYStems

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Progress in 2017

We have formulated the approach of conductivity calculations for carbon-based polymer nanocomposites using the effective media cluster approach, disordered systems theory and conductivity mechanisms analysis, and obtained the calibration dependences. Providing a proper description of electric responses in nanosensoring systems, we demonstrated the implementation of advanced simulation models suitable for real time control nanosystems [1].
Also, we modeled two electronics systems based on few-layer graphene flakes, i.e. a voltage-controlled tunable attenuator [2] and a voltage-controlled tunable planar antenna [3], with the strategy to exploit the variation of graphene resistance with the applied bias voltage.
By a multiphysics modeling method at the nanoscale, we evaluated Carbon Nanotube-based Interconnects, thus elaborating a numerical tool suitable to characterize hybrid Carbon Nanotube-Copper Interconnects [4].
We discussed tthe two convergent areas of real-time control nanosystems-for ecological monitoring and medical applications. Functionalized Carbon Nanotubes and Graphene Nanoribbons serve as a basis for the creation of physical pressure and temperature nanosensors [5]. The development of bio-nanosensors (e.g. glucose biosensors) based on polymer nanotracks with various enzymes was considered from the modelling and simulation poin of view. Both nanosensor models were successfully analyzed in comparison with available experimental data, thus validating the proposed model [5].
One of the most appealing properties of carbon nanotube interconnects is the possibility of exhibiting, under certain circumstances, a negative temperature coefficient of the electrical resistance, i.e., a resistance that decreases as temperature increases. In the past, this behavior has been theoretically predicted and experimentally observed, but only for a certain class of nanotubes, with short lengths (up to some micrometers) and in a limited range of temperature. We demonstrated the possibility of obtaining such a desirable behavior in a larger scale (up to fractions of millimeters). An accurate electrothermal model was set up to define the conditions under which a negative derivative of the resistance may be observed. Then, a novel bottom-up technique was proposed to realize the interconnect, by self-assembly of short CNTs. The experimental results of an electrothermal characterization demonstrated the possibility of obtaining a negative temperature coefficient of the resistance and confirmed the validity of the theoretical model [6].
Noise and electrical transport properties of composites based on epoxy resin filled with various carbon

inclusions (single-walled carbon nanotubes, high surface area carbon black, and exfoliated graphite) were also investigated in depth. The temperature dependence of resistivity showed that Mott's hopping and tunneling between conductive carbon particles dominate the charge carrier transport at low temperature, whereas a positive temperature coefficient effect occurs at higher temperature. Low-frequency noise spectra of the investigated materials comprise 1/fα type components. The noise level is the highest for composites close to the percolation threshold. The percolation threshold value of the system also strongly impacts both the temperature dependence of the noise level and the resistivity. Close to the percolation threshold, the noise level increases due to the carrier tunneling throughout the polymer matrix and decreases due to the rapid expansion of the polymer matrix. In contrast, the latter has almost no influence on the noise level far above the percolation threshold, and the small kink in the temperature dependence of the noise level indicates a crossover between tunneling and thermally activated electron transport mechanisms [7].
We modeled the effect of different mixing regimes on the dynamic moduli and viscosity of nanocomposites, thus assessing the degree of the filler dispersion inside the matrix. The rheological percolation threshold and relaxation time spectra are determined, in order to evaluate the internal structure of the nanodispersions. The relaxation spectrum is highly efficient to probe the effects of interfaces and interconnections on the relaxation dynamics of molecules in nanodispersions. Rheological results combined with transmission electron microscopy (TEM) observations confirm that the low frequency dynamic viscosity and moduli strongly increase, with increasing the degree of dispersion due to the exfoliation of graphene sheets. The rheological percolation threshold was found at very low concentration depending from the processing conditions [8].

The book [9] presents a systemic view of nanophenomena in terms of disordered condensed media with characteristics arising at various hierarchical levels from nanoagents/nanoparticles through multiple technological interfaces to the creation of micro-or mesostructures with essential nanodimensional effects. These properties can be seen in various schemes for the functionalization of nanocarbon systems, namely, CNTs, GNRs, GNFs, carbon-based nanoaerogels, nanofoams, and so on, where nonregularities characterize surface nanointeractions and various nanointerconnects, resulting in both predictable and unpredictable effects. Beginning with nanosensing and finishing with other forms of functionalized nanomaterials, these effects will define the prospective qualities of future consumer nanoproducts and nanodevices.

Other studies in nanotechnology topics are presented in [10-14].

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[10] A Sindona, M Pisarra, CV Gomez, P Riccardi, G Falcone, S Bellucci, Calibration of the fine-structure constant of graphene by time-dependent density-functional theory
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Physical Review B 96 (20), 205414, 2017

[12] Radiation modification and radiation hardness of microwave properties for some polymer nanocomposites under Co-60 gamma irradiation
A Lobko, V Kazhuro, N Valynets, S Bellucci, A Celzard, J Zicans, P Kuzhir
Nuclear Instruments and Methods in Physics Research Section B: Beam

[13] F Micciulla, P Ulpiani, A Cataldo, S Bistarelli, S Bellucci, Ageing effects on composite nano carbon based materials, Semiconductor Conference (CAS), 2017 International, 37-42, 2017

[14] S Bellucci, Graphene-based tunable microstrip attenuators and patch antenna
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List of Conference Talks in the Year 2017

	Speaker	Conferenza	Data	Sigla	Titolo	Luogo	Nazione
1	Maffucci A	Applied Computational Electromagnet...	26-03-	NEMESYS	Carbon nanotube interconnects with	Firenze	Italia

			2017		negative temperature coefficient of the resistance		
2	Micciulla F	Semiconductor Conference (CAS), 201...	11-10-2017	NEMESYS	Ageing effects on composite nano carbon based materials	Sinaia	Romania
3	Bellucci S	Semiconductor Conference (CAS), 201...	11-10-2017	NEMESYS	Graphene-based tunable microstrip attenuators and patch antenna	Sinaia	Romania

Publications by LNF Authors in the Year 2017

	Titolo	Autori	Sigla	Rivista	Autori NEMESYS	Autori Totali
3	A Planar Antenna With Voltage-Controlled Frequency Tuning Based on Few-Layer Graphene	**Yasir, Muhammad** et al.	NEMESYS	IEEE ANTENN WIREL PR , **-16**	3	7
4	Ageing effects on composite nano carbon based materials	**Micciulla, F.** et al.	NEMESYS	INT SEMICONDUCT CON , **-**	1	5
5	Bridging between integral equation technique of classical electrodynamics and Landauer-Buttiker formalism for quantum transport	**Shuba, M. V.** et al.	NEMESYS	, **-**	1	8
6	Calibration of the fine-structure constant of	**Sindona, A.** et al.	NEMESYS	PHYS REV B , **20-96**	1	6

	graphene by time-dependent density-functional theory					
7	Carbon Nanotube Interconnects with Negative Temperature Coefficient of the Resistance	**Maffucci, A.** et al.	NEMESYS	, **-**	1	5
8	Cluster microstructure and local elasticity of carbon-epoxy nanocomposites studied by impulse acoustic microscopy	**Levin, Vadim** et al.	NEMESYS	POLYM ENG SCI , **7-57**	4	7
9	Enhanced Tunable Microstrip Attenuator Based on Few Layer Graphene Flakes	**Yasir, Muhammad** et al.	NEMESYS	IEEE MICROW WIREL CO , **4-27**	1	6
10	Fermionic currents in AdS spacetime with compact dimensions	**Bellucci, S.** et al.	NEMESYS	PHYS REV D , **6-96**	1	3
11	First-principles calculations on Fe-Pt nanoclusters of various morphologies	**Platonenko, Alexander** et al.	NEMESYS	SCI REP-UK , **-7**	1	6
12	Graphene nanoplatelets: Thermal diffusivity and thermal	**Potenza, M.** et al.	NEMESYS	AIP ADV , **7-7**	2	6

	conductivity by the flash method					
13	Graphene-based Tunable Microstrip Attenuators and Patch Antenna	**Bellucci, Stefano**	NEMESYS	INT SEMICONDUCT CON , **-**	1	1
14	Highly tunable and Large Bandwidth Attenuator Based on Few-Layer Graphene	**Yasir, Muhammad** et al.	NEMESYS	, **-**	1	6
15	Integral equation technique for scatterers with mesoscopic insertions: Application to a carbon nanotube	**Shuba, M. V.** et al.	NEMESYS	PHYS REV B , **20-96**	1	9
16	Modeling, Fabrication, and Characterization of Large Carbon Nanotube Interconnects With Negative Temperature Coefficient of the Resistance	**Maffucci, Antonio** et al.	NEMESYS	IEEE T COMP PACK MAN , **4-7**	1	5
17	Plasmon properties of doped or gated graphene nanoribbon arrays with armchair shaped edges	**Sindona, A.** et al.	NEMESYS	, **-**	1	7

18	Real time polymer nanocomposites-based physical nanosensors: theory and modeling	**Bellucci, Stefano** et al.	NEMESYS	NANOTECHNOLOGY , **35-28**	1	6
19	Resistivity and low-frequency noise characteristics of epoxy-carbon composites	**Pralgauskaite, Sandra** et al.	NEMESYS	J APPL PHYS , **11-121**	1	11
20	RHEOLOGICAL BEHAVIOR OF GRAPHENE/EPOXY NANODISPERSIONS	**Ivanov, E.** et al.	NEMESYS	APPL RHEOL , **2-27**	1	7
21	Tunable and Input-Matched Attenuator Based on Few-Layer Graphene	**Yasir, Muhammad** et al.	NEMESYS	EUR MICROW CONF , **-**	1	6