

Editorial

# Nanoscience and Nanotechnology, Proceedings of the INFN-LNF 2018 Conference

Stefano Bellucci 

INFN-Laboratori Nazionali di Frascati, Via E. Fermi 40, 00044 Frascati, Italy; bellucci@lnf.infn.it

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**Abstract:** The NEXT Nanotechnology group at INFN-Laboratori Nazionali di Frascati (LNF) has organized, since the year 2000, a yearly series of international meetings in the area of nanotechnology. The 2018 conference has been devoted to recent developments in nanoscience and their manifold technological applications. These consisted of a number of tutorial/keynote lectures, as well as research talks presenting frontier nanoscience research developments and innovative nanotechnologies in the areas of biology, medicine, aerospace, optoelectronics, energy, materials and characterizations, low-dimensional nanostructures and devices. Selected, original papers based on the 2018 conference talks and related discussions have been published, after a careful refereeing process, in the MDPI journal *Condensed Matter*, and are currently included in the present dedicated issue.

**Keywords:** chemical stability; graphene; temperature dependence in HOPG; electrodeposition process; boron sheet's electronic structure

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## 1. Introduction

The Physics and Chemistry of Nanostructures, a fast-growing research field which has attracted increasing attention over many years, especially for many promising nanotechnological applications, led me in 1999 to plan, install, and coordinate the so-called NEXT nanotechnology Laboratories, hosted within the INFN-Laboratori Nazionali di Frascati, near Rome (Italy).

One of the main objectives of such Laboratories is to allow us, on the one hand, experimental tests of theories, models, and simulations and, on the other hand, to design and realize devices, which may yield a prototype for industrial exploitation, in such a way as to constitute a basis for Technology Transfer.

At NEXT, we always believed to be of crucial importance, for the quality of the research, to work in a national or international context which, through collaborations and public research financed projects, can promote professional growth, yielding results with a high impact on the scientific community, producing, whenever possible, useful applications [1,2]. Training and, in general, teaching have always occupied a central place in the NEXT activities, as we believe it is imperative to make the developed methods, and the obtained results, available to younger generations.

Working actively in such a multidisciplinary field led us, also in this respect, into the parallel activity of schools and workshops organization, as well as editorial projects. Hence, we organized, since the year 2000, a series of international meetings in the area of nanoscience and its nanotechnological applications. The conferences have been held under the patronage of INFN (Italian Institute for Nuclear Physics), CNR (Italian Research Council), and various universities, in close collaboration with industrial partners, including 3M, MTS, RS Components, VARIAN, MICOS, Newport, Veeco, and many more.

The 20 yearly meetings on nanoscience and nanotechnology (n&n) 2000–2019, hosted important lecturers, e.g., O. Groening, P. Kelires, I. Berbezier, R. Garcia, J. Gonzalez, J. Solyom, R. Cingolani, J.

Kirschner, K. Takayanagi, M. Terrones, L. Vescan, B. Yakobson, U. Valbusa, R. Egger, M. Pimprikar, N. Pugno, V. Balzani, P. Baglioni, B. Fubini, J.M. Kenny, M.S. Sarto, F. Beltram, P. Milani, K. Wandelt, B. Voigtlaender, L. Balents, G. Grasso, targeting as an audience young postdocs and PhD students, assessing the state-of-the-art of frontier nanoscience research developments and innovative nanotechnologies in the areas of biology, medicine, aerospace, optoelectronics, energy, materials and characterizations, low-dimensional nanostructures and devices.

From this activity, many proceedings collections, as well as 3 Springer-edited volumes, originated [3–13]. Of the latter volumes, the book on biomedical applications of nanoparticles—*Nanoparticles and Nanodevices in Biological Applications: The INFN Lectures*—is one of the very first attempts to write a series of books on selected topics in Nanoscale Science and Technology based on lectures given at the well-known INFN schools of the same name. The aim of this collection is to provide a reference corpus of suitable, introductory material to relevant subfields, as they mature over time, by gathering the significantly expanded and edited versions of tutorial lectures, given over the years by internationally known experts. A recent example can be found in [14].

## 2. Fluctuation Theory in Chemical Kinetics

In the paper [15], stability properties of chemical reactions of arbitrary orders have been considered. In each chemical experiment, the formation of a chemical equilibrium can be studied by optimizing the reaction rate. Under infinitesimal simultaneous variations of the concentrations of reacting species, the binary component equilibrium is achieved when either one of the orders or concentrations of reactants vanishes. The chemical concentration capacities of the components are calculated to describe the local stability of the equilibrium. The correlation between the components is obtained as the mixed second-order derivative of the rate with respect to concentrations. The global stability analysis is performed by introducing a symmetric matrix with its diagonal components as the chemical capacities and off-diagonal components as the local correlation. It turns out that the local chemical stability requires the orders of the reactants to be either negative or larger than unity. The corresponding global stability requires the positivity of a cubic factor over the orders of the reactants. This illustrates how a chemical reaction takes place by attaining its activation state and asymptotically approaches the equilibrium when two components are mixed with arbitrary orders. Qualitative discussions are provided to support our analysis towards the formation of an optimized equilibrium. Finally, along with future directions, verification of the model is discussed towards the formation of carbon-based reactions, formation of organic/inorganic chemical equilibria, and catalytic oxidation of CO–H<sub>2</sub> mixtures in presence of Pt.

## 3. Effect of High-Temperature Annealing on Graphene with Nickel Contacts

Graphene has shown great potential for ultra-high frequency electronics. However, using graphene in electronic devices creates a requirement for electrodes with low contact resistance. Thermal annealing is sometimes used to improve the performance of contact electrodes. However, high-temperature annealing may introduce additional doping or defects to graphene. Moreover, an extensive increase in temperature may damage electrodes by destroying the metal–graphene contact. In the work [16], the effects of high-temperature annealing on graphene and nickel–graphene contacts were studied. Annealing was done in the temperature range of 200–800 °C, and the effect of the annealing temperature was observed by two and four-point probe resistance measurements and by Raman spectroscopy. It is observed that the annealing of a graphene sample above 300 °C increased the level of doping, but did not always improve electrical contacts. Above 600 °C, the nickel–graphene contact started to degrade, while graphene survived even higher process temperatures.

## 4. Temperature Effects on the HOPG Intercalation Process

Graphite intercalation via chemical strategies is a common procedure to delaminate stratified crystals and obtain a suspension of graphene flakes. The intercalation mechanism at the molecular

level is still under investigation in view of enhancing graphene production and reducing damage to the original pristine crystal. The latter can undergo surface detriment due to both blister evolution and carbon dissolution. The role of the electrolyte temperature in this process has never been investigated. In work [17], by using an in situ atomic force microscopy (AFM) apparatus, the surface morphology changes after the application of fast cyclic-voltammeteries at 343 K have been explored, in view of de-coupling the crystal swelling phenomenon from the other electrochemical processes. It was found that blisters do not evolve because of the increasing temperature, while the quality of the graphite surface becomes significantly worse, due to the formation of some adsorbates on possible defect sites of the electrode surface. These results suggest that the chemical baths used in graphite delamination must be carefully monitored in temperature for avoiding undesired electrode detriment.

### 5. Model of Nano-Metal Electroplating Process in Trapezoid Profile Groove

The principle of the electrodeposition method is to immerse the coated products in a water electrolyte solution, the main components of which are salts or other soluble compounds—metal coatings. The process of electrodeposition of metals is important in micro- and nano-electronics, as it is used in the production of multilayer printed circuit boards (MPC). MPCs consist of many layers, most of which are complex electrical circuits. The simplicity, availability, and technological capabilities of the electrodeposition process make it possible to use it for local electrochemical deposition, especially with an unchanged decrease in topological dimensions. Electrodeposition is a complex process occurring at the interface of type 1 and 2 conductors, and depends on various factors such as temperature, mixing rate, and electrolyte composition, as well as ion solvation processes, adsorption at the phase boundary, the state of the double electric layer, the phenomena of electrode polarization, diffusion, and convection flows near the deposition surface. However, the process of local metallization is affected by a complex surface relief.

In some cases, mathematical modeling methods can replace a full-scale experiment, saving material and time costs. In this article, we consider the possibility of mathematical modeling of electrochemical deposition of copper and silver under local metallization in a hollow trapezoidal profile groove using the basic package of COMSOL Multiphysics. The software COMSOL Multiphysics was utilized in [18] to perform a simulation of the processes of electrodeposition of the metals copper and silver in the groove of the trapezoidal profile. The results obtained for the thicknesses of the deposited layers of copper and silver can optimize the deposition regimes. For example, it is advisable to carry out metal deposition in a periodic mode, changing the polarity of the electrode to the opposite. This should ensure the alignment of the concentration of metal ions in the depth of the groove, and thus reduce the thickness variation of the layers on the vertical walls.

### 6. Electronic Structure of Boron Flat Holeless Sheet

The electronic band structure, namely energy band surfaces and densities-of-states (DoS), of a hypothetical flat and ideally perfect, i.e., without any type of holes, boron sheet with a triangular network is calculated in [19] within a quasi-classical approach. It is shown to have metallic properties as is expected for most of the possible structural modifications of boron sheets. The Fermi curve of the boron flat sheet is found to be consisted of 6 parts of 3 closed curves, which can be approximated by ellipses representing the quadric energy-dispersion of the conduction electrons. The effective mass of electrons at the Fermi level in a boron flat sheet is found to be too small compared with the free electron mass and to be highly anisotropic. The low effective mass of conduction electrons indicates their high mobility and, hence, high conductivity of the boron sheet. The effects of buckling/puckering and the presence of hexagonal or other type of holes expected in real boron sheets can be considered as perturbations of the obtained electronic structure and theoretically considered as effects of higher order.

## 7. Simulation of the Process of Obtaining Nanoparticles by Thermal Decomposition

Today, nanopowders are in great demand for the creation of new materials and technologies, fundamentally new devices. The process of obtaining nanopowders is therefore an important direction in nanotechnology.

The synthesis of nanocrystalline powders of metals and compounds using pyrolysis is associated with the use of complex and organometallic compounds. Numerous studies show that thermal decomposition is a complex process, depending on a variety of parameters. Therefore, the current task is to develop synthesis methods, that is, the simulation of deposition modes in which the most accurate particles can be obtained. By changing the conditions for thermal decomposition and input parameters, one can control the quality and morphology of the resulting metal nanoparticles.

The goal of the work [20] was to analyze a model for obtaining nanopowders by thermal decomposition. The relevance of the pyrolysis process is that the rate of the formation and growth of metal nanoparticles is regulated by changes in the ratio of the number of reactants and the process temperature. In the work [20], the possibility of modeling the process of thermal decomposition in the COMSOL Multiphysics program for the preparation of nanoparticles of metals and their alloys was determined. To identify the most suitable pyrolysis medium, two environments were presented: A water solution and ethanol.

## 8. Conclusions

With the advent of the era of nanotechnology, many new possibilities emerged to find manifold applications from enabling technologies stemming out of innovative materials [21,22]. An example is graphene, a two-dimensional carbon allotrope, which is characterized by light weight, strength, and very high electrical and thermal conductivity [23,24]. Graphene can be utilized in nanoelectronics to replace conventional materials (e.g. copper), which suffer many limitations, for example in applications involving small sizes and high frequencies [25,26].

The results presented in the present book highlight some of the most recent advances in nanoscience and nanotechnology studies, from both the physical and chemical point of view, with an eye also to possible engineering applications.

These studies demonstrate directly how effective, and at the same time stimulating, implementing the “cross fertilization” procedure is. Indeed, multidisciplinary research allows one to catch more easily the analogies’ inherent different areas of science, as well as to take advantage and optimize different methods and techniques, often borrowed from other research areas.

In the present special issue, we included six published papers. The latter contributions, on the one hand, are developed at the theory level and, on the other hand, show experimental results on realization and experimental characterization of nanostructured systems, suitable of yielding progress towards the realization of systems and devices, that can ultimately lead to industrial applications. The results show that recent scientific research advances in these areas may provide important steps in the direction of fostering innovation and technological development.

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