CNT-Fe-Pt interconnect electromagnetic simulations for magnetically stimulated CNT growth and novel memory nanodevices

Yu N Shunin[1, 2, 3*] S Bellucci[1], Yu F Zhukovskii[2], V I Gopejenko[3],
N Burlutskaya[3], T Lobanova-Shunina[4], A. Capobianchi[5], F Micciulla[1]

[1] *INFN-Laboratori Nazionali di Frascati, Via Enrico Fermi 40, I-00044, Frascati-Rome, Italy,*

[2] *Institute of Solid State Physics, University of Latvia, Kengaraga Str. 8, LV-1063 Riga, Latvia*

[3] *Information Systems Management Institute, 1 Lomonosov, Bld. 6, LV-1019 Riga, Latvia*

[4] *Riga Technical University, 1 Lomonosov, Bld. 4, LV-1019 Riga, Latvia*

[5] *Istituto di Struttura della Materia-CNR A.d.R. Roma, Via Salaria Km 29.300 Monterotondo Rome) Italy*

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Abstract

The parametrically controlled production of carbon nanotubes (CNTs) with predefined morphologies is a topical technological problem for modern nanoelectronics. The chemical vapor deposition (CVD) technique for single walled carbon nanotubes (SWCNTs) in the presence of various metal nanoparticle catalysts is generally used now. The application of a magnetically stimulated CVD process scheme and catalyst nanoparticles with a strong magnetism promises additional possibilities for the CVD process management and allows expecting a predictable growth of CNTs with set chiralities and diameters. The main attention is focused on the magnetically anisotropy Pt-Fe in L10 crystallographic phase nanoparticles effect research. The developed cluster approach based on the multiple scattering theory formalism, realistic analytical and coherent potentials, as well as effective medium approximation (EMA-CPA), can be effectively used for modeling of nanosized systems. It allows us to calculate the dispersion law E(k), electronic density of states, conductivity, etc. This theoretical approach is used for simulation of fundamental electromagnetic properties in Pt-Fe L10-CNT interconnects, which are responsible for developing CNTs morphologies. The developed model of 'effective bonds' and the model of magnetic stimulation for growing CNTs morphologies generated on the Pt-Fe nanoparticle surface are applied for the evaluation of the expected CNT chiralities distribution. The model and conditions controlled magnetically, which stimulate CNT growth in the CVD process, aimed at the predictable SWCNT diameter and chirality and based on Pt-Fe L10 catalyst are discussed. The possibilities of CNT forest growing on FePt nanoparticles for magnetic nanomemory are also evaluated.

Keywords: chemical vapor deposition (CVD), CNTs CVD magnetically controlled growth, arc discharge technique CNTs creation, Pt-Fe nanodrops –catalysts, fundamental electromagnetic properties in Pt-Fe L10-CNT interconnect, model of magnetically controlled CNTs growth

1 Introduction

Carbon nanotubes (CNTs) of various chiralities open new wide possibilities for modern nanoelectronics as promising candidates for nanointerconnects in a high-speed electronic nanosensoring and nanomemory devices [1-3].

We focus our current study on the implementation of advanced simulation models for a proper description of the fundamental electromagnetic properties (electrical resistance, capacitances and impedances) in contacts between carbon nanotubes of different morphologies and metallic substrates of different nature. We also present the model of magnetically stimulated CNT growth for a special case of Fe-Pt metallic nanoparticles, which have unique magnetic properties. We expect that in the presence of magnetic field, the CNTs growth will be more determined from the point of view of possible CNTs morphologies. Moreover, the creation of a CNT forest based on PtFe nanoparticles provides the possibilities to consider this kind of structure as the basic fragment of nanomemory devices, where information bits are located in nanoparticles and the CNT forest provides the necessary spin transport for reading and recording information.

Thus, in our simulations, we expect to reproduce not only a CNT forest with the predefined morphology but also to develop a prototype of a nanomemory device.

The adequate description of CNT chirality [2] is one of the key points for a proper simulation on electric properties of CNT-based nanoelectronic devices.

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[*] Corresponding author- Email: shunin@isma.lv

The electronic structure of CNT-Me interconnects can be evaluated through the electronic density of states (DOS) for a carbon-metal contact considered as a 'disordered alloy', where clusters containing both C and Me atoms behave as scattering centres. The computational procedure developed for these calculations [2, 4] is based on the construction of cluster potentials and the evaluation of both scattering (S) and transfer (T) matrices.

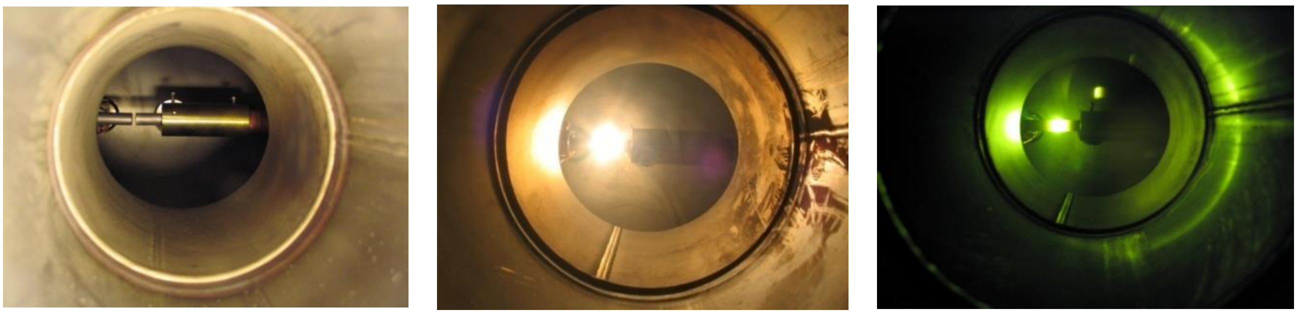
The cluster formalism was successfully applied, e.g., for metallic Cu [4], as well as for both elemental (Ge, Si, As, Se, Te) and binary (As_xSe_{1-x} and Sb_xSe_{1-x}) semiconductors [4, 5]. When using the coherent potential approach (CPA) as EMA approximation, the resistance of interconnect can be evaluated through the Kubo-Greenwood formalism [6] and Ziman model [7].

The further development of the cluster approach allowed us to formulate the 'effective bonds' model and to carry out a cycle of simulations on electromagnetic properties in various CNTs- and graphene (GNRs - graphene nanoribbons) -based metal interconnects (Me = Fe, Cu, Ag, Pt, Au, Pd, Ni) [3, 8]. We consider that this model serves as a tool for understanding the process of CNT growth adequate to CVD process.

2 Research motivation

The main goal of the current research is to understand if there is a relationship between the use of magnetic catalysts and the CVD growth of CNTs, taking into account that most commonly used materials for the growth of CNTs are just Fe, Co and Ni nanoparticles. The nanoparticles of these catalysts are magnetically isotropic. The key question arises: What would happen if one used instead of Fe, Co, and Ni nanoparticles, magnetically anisotropic nanoparticles such as those in the alloy Fe-Pt? The anisotropy of Fe-Pt alloy is due to a spin-orbit coupling of Fe and Pt orbitals. This coupling takes place only if the alloy is formed of alternating planes of Fe and Pt. This particular structure is called L10. In this way, because of the different sizes of the atoms of Fe and Pt, the structure is crushed and attomi of Fe and Pt are close forming a centred tetragonal phase (fct). This rapprochement allows the coupling and then the magnetic anisotropy with the magnetization axis perpendicular to such planes. It is essential in this case to find conditions to control the growing CNT chirality. We also should take into account a possible substitutional disorder of FexPt1-x alloy, when the stoichiometry number 'x' becomes an additional parameter of CNT growth. No doubt, the diameter of the grown CNT is also an essential parameter, which is evidently pre-defined by the created nanoparticle diameter. But again, we should discuss some limitations in the creation of Fe-Pt nanoparticle sizes in connection with the Fe-Pt melting point. However, Fe-Pt nanoparticles demonstrate an extremely strong coercing field (about, for the phase fct in some special compositions and this promises definite hopes for the controlled CNT growth in the CVD process. We also consider the CVD process of CNT growth as a more predictable one from the point of view of the expected growing CNT parameters (diameter, chirality, morphology of SW or MW CNTs)).

Our experience with the nanotubes synthesis by means of the arc discharge brought about large doubts in the possibilities of CNTs growth control. Two cathodes of pure graphite (99.7%) were taken φ = 6mm (cathode) and φ = 10mm (anode) in diameter. Carbon Black was added to iron – platinum powder, after which the mixture was introduced to complete the filling of the hole. At this point the whole mass was placed in the room. The synthesis was carried out according to the parameters presented here: Current 90 A, Voltage ~ 18 ÷ 20V DC, Vacuum ~ 2x10-4 mbar, Gas: He, Work Pressure 600 mbar, arc duration ~ 15 min.



a) b) c)

FIGURE 1

a) Cathode and anode aligned before the synthesis
b) Synthesis, arc,
c) arc with a glass front. Once you open the synthesis chamber it is possible to identify the growth of "filamentous" retiring from the anode

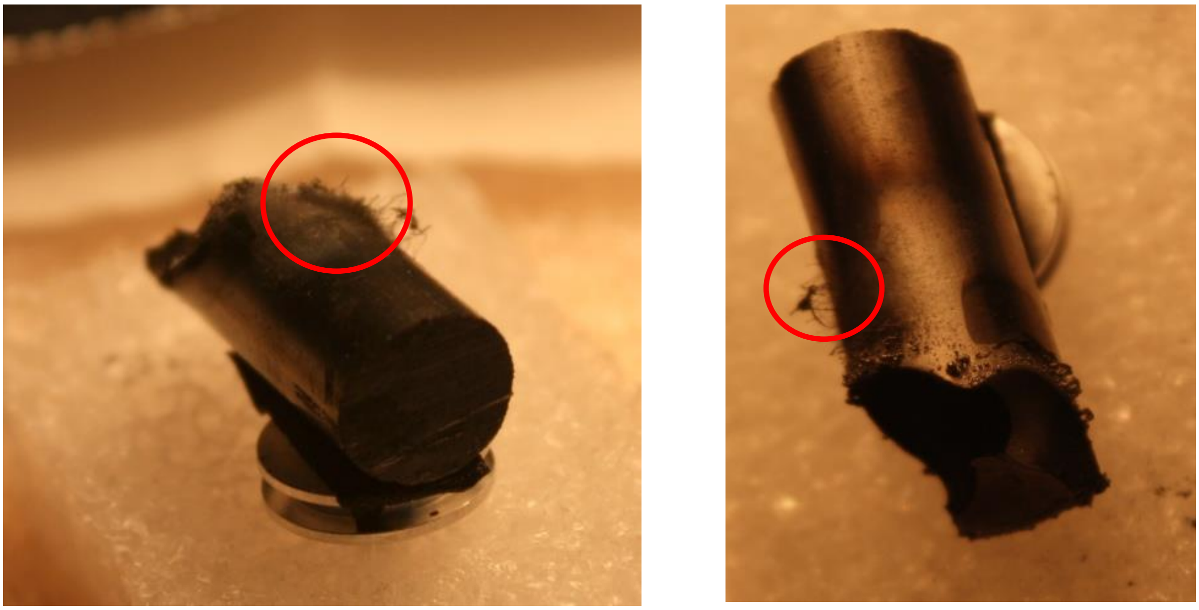
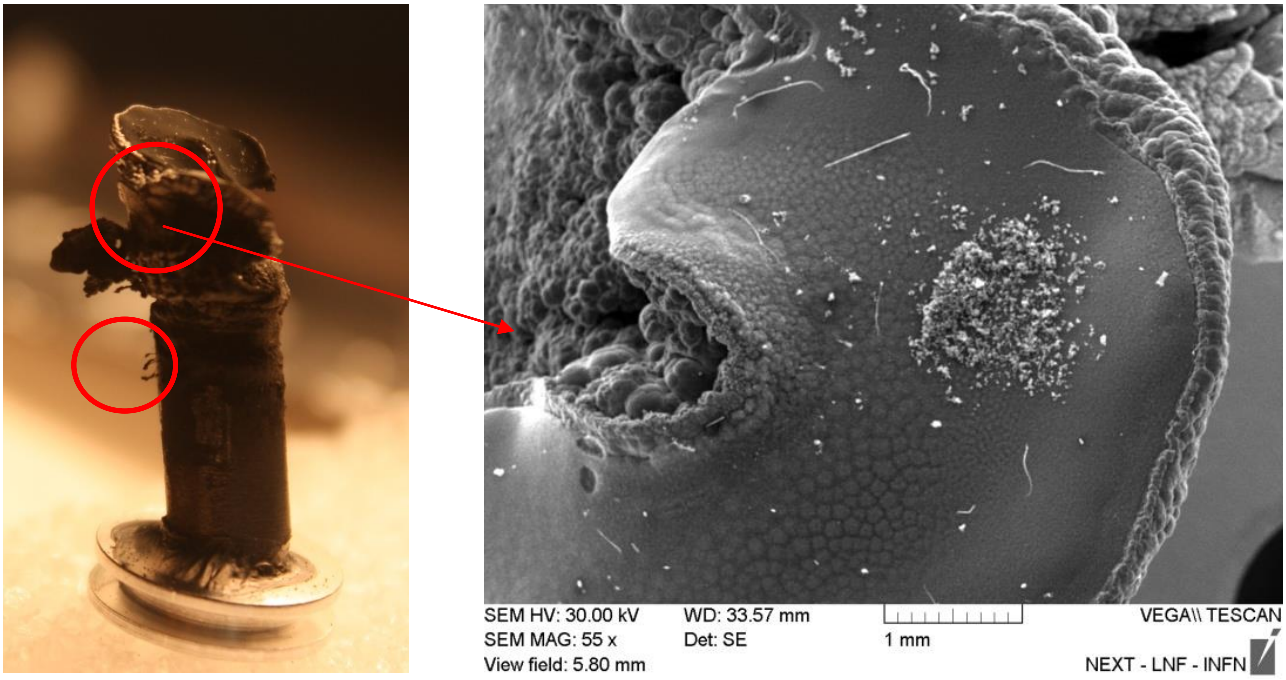

a) b)

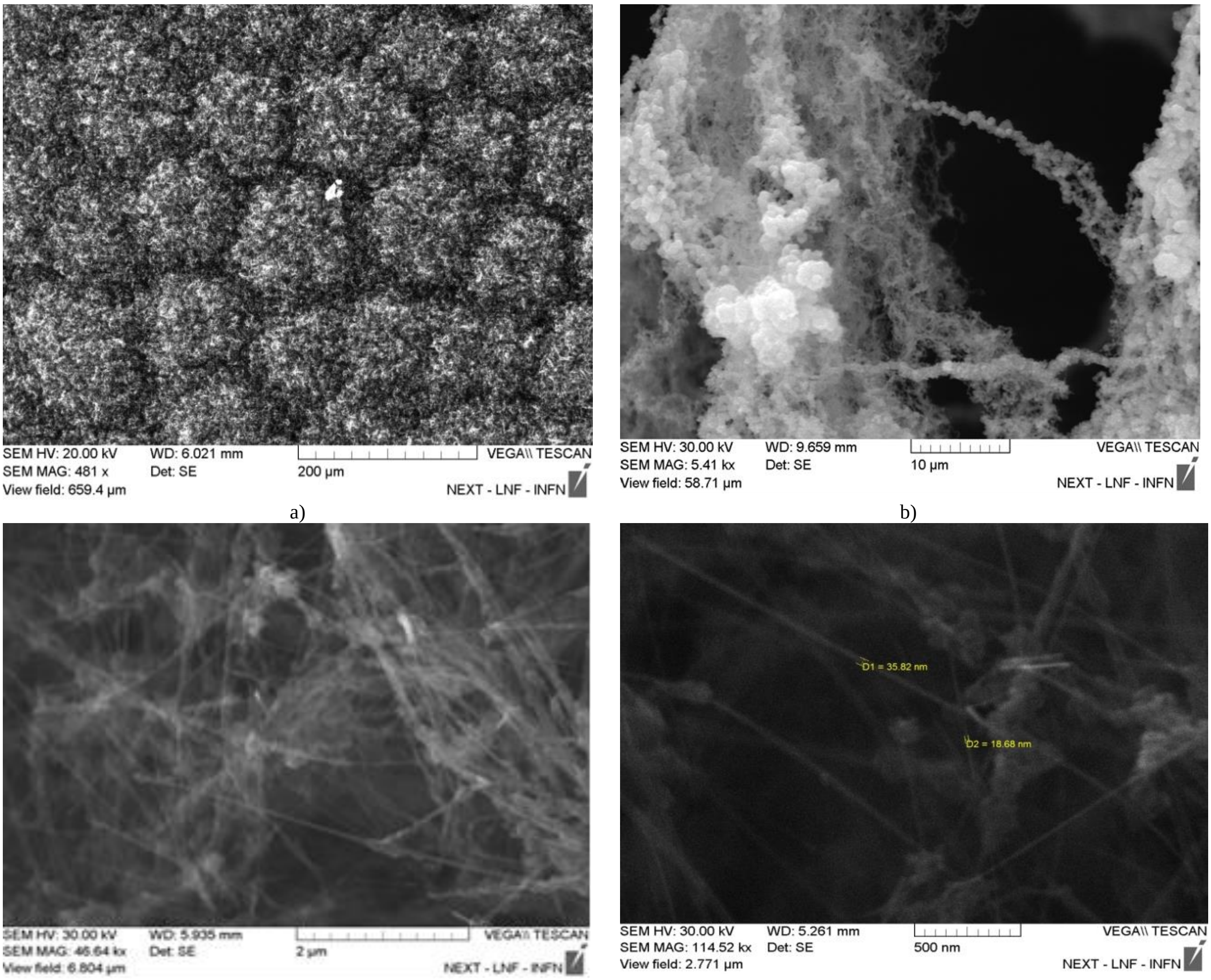
FIGURE 2 Two views of the anode with filaments after exiting out of the synthesis: a); b)

Some filaments also exit from the outer wall of the cathode but in smaller quantities than found on the anode. The residue of the deposit formed on the upper part of the synthesis chamber was collected. It appeared to be quite little compared to other discharges with other catalyst.



a) b)

FIGURE 3 a) Photo of the cathode filaments exiting out after the synthesis, b) SEM photo of the cathode surface



a) b)

c) d)

FIGURE 4 Evolution view of filaments in the arc discharge process (Bellucci-Capobianchi): a),b),c),d) [60-63].

The figure 4 shows that filaments are of different nature - some formats are created from these spheres and others have very fine structures of a few nanometers, probably single-walled nanotubes, covered by these spheres, partly or totally. The question is: What percentage of nanoparticles was originally made or how much iron and platinum and how this underwent a change, during the arc discharge process?

We also take into account the extremely marginal parameters of the Pt-Fe system: Pt has the melting point at T = 2041.4 K (1768.2° C) and the boiling point at T = 4098 K (3825° C);

There are four major crystal structure modifications for Fe: below 769° C (Curie temperature) it is α-Fe (α-ferrite) with a body-centered cubic crystal structure and ferromagnetic properties. Ferrite above the critical temperature (769-917° C) is beta-ferrite (β-Fe) where it is paramagnetic rather than ferromagnetic and it is crystallographically identical to α-Fe. Within the interval of 917-1394°C it is γ-Fe (austenite) with acicular cubic crystal structure. At temperatures between 1394 °C and 1538 °C, the body-centered cubic crystal structure is the more stable form of delta-ferrite (δ-Fe), the melting point 1538°C (1811 K), and the boiling point at T = 3273 K (3000 ° C).

Our earlier research proved that close to the arc the temperature ranges between 4000 – 6000 K and there is a subsequent rapid temperature gradient decrease with the distance from it. Filaments are found nearby the arc itself, more precisely, upstream of it. Taking into account the essentially non-steady character of the **arc discharge** process and very high working temperatures, the CNT growth control is practically impossible and CNT morphologies are non-predictable.

3 CNTs growth in the chemical vapor deposition process based on metal nanoparticles

3.1 CVD PROCESS ANALYSIS

The Chemical Vapour Deposition (CVD) is a highly versatile approach to producing nanotubes and is, perhaps, the most commonly published technique for nanotube growth often used to synthesize CNTs for commercial applications. The process involves decomposition of a carbonaceous precursor at high temperatures under oxygen-free conditions and reduced atmosphere to produce nanotubes.

The carbonaceous precursor may be a carbon gas, methane or ethylene for instance, or it can be in the form of a volatile hydrocarbon solvent such as ethanol, which is generally fed into the reactor with some inert carrier gas. In the reaction chamber, the precursor is decomposed in the presence of a catalyst –usually a transition metal such as iron, cobalt or some similar combination of metals. The catalyst can be introduced in a number of different ways.

The substrate needs to have catalyst nanoparticles providing the growth of CNTs where nanoparticles present the place from which nanotubes start growing. Nanoparticles can be composed of lots of different substances (usually, a metal like Fe, Co, Ni Co, Mo, Mn, Pd etc) [9].

The substrate is then heated to the temperature of about 700-800°C under H_2. As the nanoparticles heat up, the hydrogen pulls oxygen out from the nanoparticles, leaving behind metallic nanoparticles. At the target temperature, a carbon-containing gas such as ethylene (or some others, e.g., alcohol vapor) is introduced. At these temperatures, the gas partly decomposes, giving carbon-containing fragments and other molecules. These fragments and molecules then work their way onto the catalyst nanoparticles, where they stick and then break down into carbon. The carbon dissolves with some probability into or on the nanoparticle. When a critical concentration of carbon is reached in the nanoparticle, the addition of just a little bit more carbon from the vapor causes carbon to precipitate as a crystal.

When carbon crystallizes under the atmospheric pressure (like in CVD), it crystallizes into flat sheets of hexagonally-patterned carbon. However, because the nanoparticle is so small and has such a high curvature, when the carbon crystallizes out, it is constrained into a cylindrical shape in the form of a carbon nanotube. Additional carbon atoms on the nanoparticle provide further nanotube growth, which stops when the carbon-containing gas is turned off if the substrates cool down, or for a number of other reasons that can influence the nanotube or catalyst nanoparticles.

Tuning the appropriated parameters, it is possible to obtain a huge amount of CNTs in a cheap and quick way. In addition, it is the technique enabling the growth of CNTs with specific characteristics: particular diameter, length and orientation (alignment), and family (Multi or Single Wall). It has been well known for a long time that carbon nanotubes are synthesized by catalytic decomposition of hydrocarbon [10] in the reactor, where metal nanoparticles are presented as a catalyst on a substrate. Catalyst metals mostly used for these purposes are listed in the following Table 1 [11, 12].

TABLE 1 Most commonly used catalyst metals for the CVD method [11].

Catalyst			**Temperature, ^{0}C**	**Carbon source**
Metal	***Catalyst type***	***Preparation method***		
Fe	Ultra fine particle	Decomposition of metallocene	1060	Benzene
	Silica support	Pore impregnation	700	Acetylene
	Zeolite or Clay support	Ion exchange	700	Acetylene
	Graphite support	Impregnation	700	Acetylene
	Ultra fine particle	Decomposition metal of carbonyl	800	Acetylene
	Silica support	Sol-gel process	700	Acetylene
Co	Ultra fine particle	Laser etching of Co thin film	1000	Triazine
	Ultra fine particle	Decomposition metal of carbonyl	800	Acetylene
	Silica support	Pore impregnation	700	Acetylene
	Zeolite or Clay support	Ion exchange	700	Acetylene
	Graphite support	Impregnation	700	Acetylene
Ni	Graphite support	Impregnation	700	Acetylene
	Ultra fine particle	Decomposition of $Ni(C_8H_{12})_2$	800	Acetylene
Mo	Ultra fine particle	Decomposition of Mo*[1]	800	Acetylene
Mn	Ultra fine particle	Decomposition metal of carbonyl	800	Acetylene
Pd	Ultra fine particle	Decomposition metal of carbonyl	800	Acetylene

[1] $Mo^* = (NH_4)_{25\pm5}[Mo_{154}(NO)_{14}O_{420}(OH)_{28}(H_2O)_{70}]$ $350H_2O$.

Hydrocarbon, such as methane, adsorbed on the catalytic particle surface, releases carbon during decomposition, which dissolves and diffuses into a metal particle. When a supersaturated state is reached, carbon precipitates in a crystalline tubular form.

It is necessary to emphasize that it will be possible to grow CNTs using a gas, both as a catalyst and as hydrocarbon. If a stream of catalyst particles can be injected into the flowing feedstock, it is possible to produce nanotubes in the gas phase. This approach is amenable for scale-up to large-scale production. Sen et al. [13] first reported such a possibility when they used ferrocene or nickolecene as a source of the transition metal and benzene as a carbon source. This approach yielded MWNTs, whereas their later work [14] with gas-phase pyrolysis of acetylene using a metallocene yielded

SWNTs with diameters around 1 nm [15]. CVD-produced CNTs are curved and have high amount of defects, mainly after the purification in the acid bath; it is needed to remove metal nanoparticles inside of tubes.

The main interests related to iron-containing nanoparticles are focused on their potential applications as high-quality magnetic materials. Thus, a new generation of iron–metal nanoparticles is studied to be used as a catalyst in growing CNTs, with a magnetic nanomaterial inside, making it possible to design a precise carbon nanomagnetic device for drug delivery diagnostics.

For example, iron nanoparticles have been widely used as a catalyst for CVD synthesis of multiwalled carbon nanotubes, [16] while iron-molybdenum can act as a very efficient catalyst for the synthesis of either single-walled or multiwalled carbon nanotubes with the CVD method [17-22].

To prevent the magnetic behaviour of these iron – nano-compounds, it is necessary to grow carbon nanotubes of nanocompounds below the Curie temperature. Typically, the growth temperature is around 600 – 700°C at the atmospheric pressure [23].

The potential applications of carbon nanotubes grown for semiconductor and sensor devices are presented for CMOS industrial applications [24]. The low-temperature growth of vertically aligned carbon nanotubes (CNTs) at high growth rates by a photo-thermal chemical vapour deposition (PTCVD) technique using a Ti/Fe bilayer film as a catalyst is presented in [25]. The bulk growth temperature of the substrate is as low as 370 °C and the growth rate is up to 1.3 μmmin−1, at least eight times faster than the values reported by traditional thermal CVD methods.

It should be recognized that the mechanism of CNTs growth is not obvious enough. Technological growth characteristics may differ in detail, although the concept remains the same. The mechanism of carbon atoms deposition on metal catalyst nanoparticles with the subsequent nucleation of CNTs can be considered one of the most effective and practically important. Crystal (eg. Si) nanoparticles with a set diameter created on a substrate give a high probability of producing CNTs with the regulated diameter. However, the problem of controlling the chirality of CNTs remains a pressing one. Among more effective catalysts, it is possible to distinguish Pt, Pd, Cu, Ag, Au, Si, SiC, Ge, Al_2O_3 [26] in addition to the earlier investigated Mg, Ti, Cr, Mn, Fe, Co, Ni, Sn, Pb [27-29].

TABLE 2 Comparison of catalysts for SWCNTs growth [27-29]

Type	State	Size for SWCNT growth	Catalysis for cracking	Carbon solubility	Growth temperature for ethanol (°C)	Growth rate
Fe, Co, Ni	Liquid/ solid	<10 nm	Yes	High	600-950	High
Pt, Pd	Liguid/ solid	<5 nm	No?	High	850-950	High
Au, Ag, Cu	Liquid/ solid	<5 nm	No	Low	850-950	High
Ge	Liquid/ solid	<5 nm	No	Low?	850-950	Low?
Si, SiC	Solid	<5 nm	No	No?	850-950	Low
Al_2O_3	Solid	<5 nm	No	No	850-950	Low

3.2 ADVANTAGES OF CVD

Compared to the discharge and laser-ablation methods, CVD is a simple and economic technique for synthesizing CNTs at low temperatures and ambient pressures. Arc- and laser-grown CNTs are superior to the CVD-grown ones. In yield and purity, CVD has advantages over the arc and laser methods. Considering CNTs in relation to structure or architecture control, CVD is the only answer. CVD is versatile in the sense that it offers harnessing plenty of hydrocarbons in any state (solid, liquid or gas), enables the use of various substrates, and allows CNT growth in a variety of forms, such as powder, thin or thick films, aligned or entangled, straight or coiled nanotubes, or a desired architecture of nanotubes on predefined sites of a patterned substrate. It also offers better control over the growth parameters zone, while carbon crystallization (being an endothermic process) absorbs some heat from the metal precipitation zone. This precise thermal gradient inside the metal particle keeps the process going on. This last advantage is the most essential one [26].Taking only two main CNT parameters, namely, CNT diameter and chirality, the problem cannot be solved well enough. There are two marginal cases of CVD growth.

- ***Tip-growth model*** – the catalyst–substrate interaction is weak (metal has an acute contact angle with the substrate); hydrocarbon decomposes on the top surface of the metal; carbon diffuses down through the metal, and CNT precipitates out across the metal bottom, pushing the whole metal particle off the substrate; as long as the top of the metal is open for fresh hydrocarbon decomposition, CNT continues to grow longer and longer; the metal is fully covered with the excess carbon and its catalytic activity ceases and the CNT growth stops.
- ***Base-growth model*** - the catalyst–substrate interaction is strong; initial hydrocarbon decomposition and carbon diffusion take place similar to that in the tip-growth case; the CNT precipitation fails to push the metal particle up, so the precipitation is compelled to emerge out of the metal apex; carbon

crystallizes out as a hemispherical dome, which then extends up in the form of seamless graphitic cylinder; subsequent hydrocarbon deposition takes place on the lower peripheral surface of the metal, and a dissolved carbon diffuses upward; CNT grows up on the catalyst nanoparticle base.

3.3 CNT PRECURSORS

Most commonly used CNT precursors are methane [30-31], ethylene [14, 17] acetylene [32], benzene [13] xylene [33] and carbon monoxide [34].

SWCNTs were first produced from the disproportionation of carbon monoxide at 1200 °C, in the presence of molybdenum nanoparticles [35], and later they were produced from benzene [36] acetylene [14], ethylene [37], methane [38], cyclohexane [39], fullerene [40] by using various catalysts.

It means that the working temperature and pressure of the CVD process can be changed in a wide range of ways and the kinetics of carbon atoms deposition can also be widely varied.

In 2002, the low-temperature synthesis of high-purity SWCNTs from alcohol on Fe–Co-impregnated zeolite support was carried out [41] and since then, ethanol has become the most popular CNT precursor in the CVD method worldwide [42-44].

A special interest in binary catalysts becomes principal now. The unique feature of ethanol is explained by the fact that ethanol-grown CNTs are almost free from amorphous carbon, owing to the etching effect of OH radical [45]. Later, vertically-aligned SWCNTs were also grown on Mo-Co-coated quartz and silicon substrates [46-47]. It has been shown that intermittent supply of acetylene in ethanol CVD significantly assists ethanol in preserving the catalyst activity, thus, enhancing the CNT growth rate [48].

Generally, low-temperature CVD (600-900^{o} C) yields MWCNTs, whereas high-temperature (900–1200 °C) reaction favours SWCNTs growth. It means that SWCNTs have a higher energy of formation (presumably owing to small diameters and the fact that high curvature bears high strain energy). Probably, this is the reason that MWCNTs are easier to grow than SWCNTs.

Recent developments in the nanomaterials synthesis and characterization have enabled many new catalysts for the CNTs growth. Apart from popularly used transition metals (Fe, Co, Ni), a range of other metals (Cu, Pt, Pd, Mn, Mo, Cr, Sn, Au, Mg, Al) have also been successfully used for horizontally-aligned SWCNT growth on quartz substrates [49]. It has been also proposed that the active catalyst is Au–Si alloy with about 80 at% Au [50].

3.4 CNT GROWTH CONTROL

It is a general experience that the catalyst-particle size dictates the tube diameter. The particle size dependence and a model for iron-catalysed growth of CNTs has been reported in [51]. Metal nanoparticles of the controlled size, pre-synthesized by other reliable techniques, can be used to grow CNTs of the controlled diameter [52].

3.4.1 Influence of a catalyst material and concentration

The additional advantage of using the bimetallic catalyst is that CNTs can be grown at a much lower temperature - 550°C. E.g., the melting point of the mixture of Fe and Co is lower than their individual melting points. Moreover, alloys are known to be better catalysts than pure metals. These trends suggest that tri-metallic catalysts should also give interesting results, though the interpretation of the results would be more complicated.

3.4.2 Influence of temperature

There are investigations of the temperature effect on camphor CVD in a wide range of temperatures 500-1000°C [53]. It was noticed that camphor did not decompose below 500 °C. At 550 °C very short-length tubes emerged from the zeolite pores suggesting that the catalyst activity, and hence the CNT growth rate, was quite low at 550°C. However, the CNT growth abruptly increased at 600 °C, and a profound growth was observed all around the zeolite pores. At 650°C and above, the growth rate was so enormous that hardly a zeolite particle could be located amid nanotubes. The CNT diameter is increased with the growth temperature increase. Very pure CNTs, almost free from metallic impurity, were produced up to 750°C. From 750°C onward, both the diameter and the diameter-distribution range increased drastically. It is supposed that at high temperature, the metal atoms agglomerate into bigger clusters leading to thick CNTs. At 850°C and above, SWCNTs began to take shape alongside with MWCNTs and the volume of SWCNTs increased with the increasing temperature. For instance, at 900 °C, samples of large bundles of SWNTs can be observed. The CVD temperature plays the central role in CNT growth. For a fixed metal concentration, the increasing CVD temperature enlarges the diameter distribution. It should also be noted that MWCNTs and SWCNTs can be selectively grown as a function of CVD temperature if the catalyst concentration is properly optimized [53, 54].

3.4.3 Influence of pressure

For the controlled growth of CNTs by CVD, the vapor pressure of the hydrocarbon in the reaction zone is another very important parameter. For gaseous hydrocarbons, a desired vapor pressure in the CVD reactor can be maintained by a limited gas-flow rate and the controlled suction with a rotary pump [55]. In the case of a liquid hydrocarbon, its vapor pressure is controlled by its heating temperature before it enters the reactor

[56]. However, for a solid hydrocarbon such as camphor, it is quite problematic to control its vapor pressure. It becomes a function of three parameters: camphor mass, its vaporization temperature, and the flow rate of argon—the carrier gas. By proper optimization of these three parameters, the influx of camphor vapor to the zeolite bed and its decomposition rate were balanced to a great extent, and a record growth of MWCNTs was achieved at atmospheric pressure by CVD [9]. Pure SWCNTs (free from MWCNTs) have been selectively obtained from camphor CVD at low pressures (10–40 torr) where the camphor vapor pressure is quite in tune with the low metal concentration [53]. It is important to note that the melting point of nanoparticles below 10 nm falls abruptly .E.g., a 5-nm Fe and Co particles can melt at about 850 °C and 640 °C, respectively [9]. It leads to essential limitations in the CVD process of small diameter (< 5nm) CNTs growth.

Schematic representation of the basic steps of SWCNT growth on a metal catalyst is usually simulated in three steps [58]:

1) the diffusion of single C atoms on the surface of a catalyst;
2) the formation of an sp^2 graphene sheet floating on the catalyst surface with edge atoms covalently bonded to the metal;
3) the root incorporation of diffusing single C atoms. It has been shown that carbon atoms diffuse only on the outer surface of the metal cluster. At first, a graphene cap is formed which floats over the metal, while the border atoms of the cap remain anchored to the metal. Subsequently, more C atoms join the border atoms pushing the cap up and, thus, constituting a cylindrical wall.

4 Magnetically stimulated CNTs CVD growth on Fe-Pt catalysts

4.1 EFFECTIVE BONDS MODEL FOR CNT-Pt-Fe INTERCONNECTS ELECTROMAGNETIC PROPERTIES

We have developed structural models for CNT-Me and GNR-Me junctions, based on their precise atomistic structures - clusters, which take into account the CNT chirality effect and its influence on the interconnect resistance for Me (= Fe, Ni, Cu, Ag, Pd, Pt, Au) as well as the pre-defined CNT (or GNR) geometry. These atomistic structures are in compliance with the proposed ‘effective bonds’ model. The ‘effective bonds’ are responsible for mechanical, electronic, magnetic and electrical properties of interconnects. The common consideration of two marginal carbon structures (CNTs and GNRs) is induced by the similar technological problems in respect of these materials for the modern nanoelectronics.

Our main interest in this particular case is focused entirely on CNT-Me interconnects, when the modelling of CNTs growth on metal surfaces is combined with the controlled electromagnetic properties in the interconnect area. To ensure a predictable interconnect morphology, the permanent magnetic field is used that accompanies the growth, and magnetic drops are used as growth catalysts that provide for the special composition of Fe-Pt with unique magnetic properties.

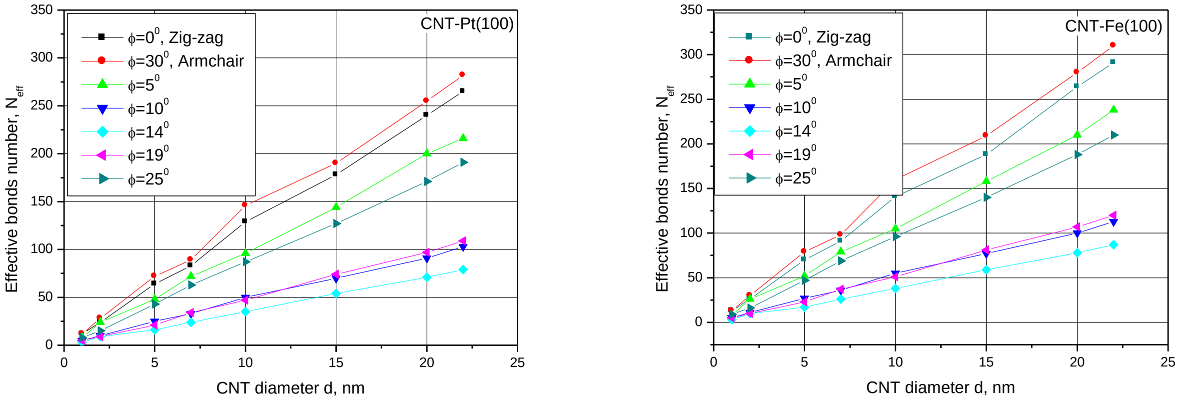
The results of our simulations show that interconnects resistance and the number of effective bonds can be considered as indicators of chirality.

Figures 5, 6, 7 and 8 demonstrate the numbers of effective bonds via CNT diameters, chirality angles, CNT-Me interconnects resistances and impedances..

It means that resistances and the number of effective bonds in the interconnect space are indicators of CNTs morphology.

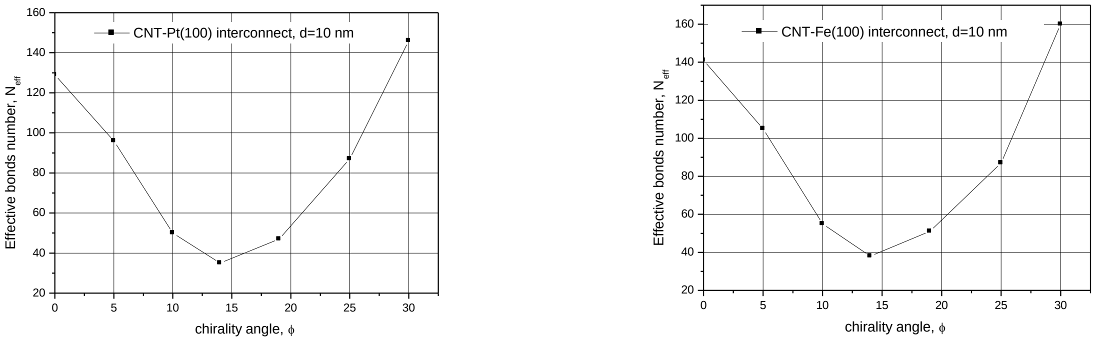
4.2 CNT-Fe_xPt_{1-x} INTERCONNECT FORMATION

There is a relation between the use of magnetic catalysts and the CVD growth of CNTs determining the most commonly used materials for the CNT growth - Fe, Co and Ni. The nanoparticles of the latter catalysts are magnetically isotropic. Magnetism of the particles-catalysts brings order into the process of CVD growth. Additional possibilities in controlling the process of CVD growth open up the ways to use magnetically anisotropic nanoparticles such as those in the alloys with a different substitutional disorder (*e.g.*, Fe_xPt_{1-x}), to manage the CVD process with the formation of the predefined CNT chiralities. Besides, the stimulation of the process by means of the external magnetic field activates magnetic moments of the catalyst and the deposited carbon atoms. This also means that we can control the number of effective bonds inside interconnects. We pay a special attention to Pt and Fe substrates as possible elements for nanoelectronic and nanomagnetic devices considering interconnects fundamental properties and magnetically stimulated nanoprocesses on Fe-Pt $L1_0$ nanoparticles [59].



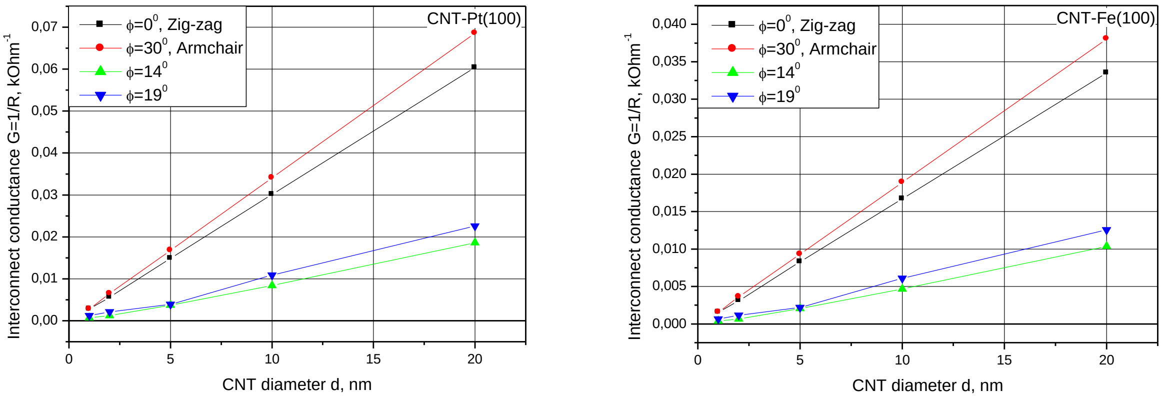
a) b)

FIGURE 5 Effective bonds number via CNT diameter: a) CNT-Pt; b) CNT-Fe.



a) b)

FIGURE 6 Effective bonds number via CNT chirality for the diameter d=10 nm: a) CNT-Pt; b) CNT-Fe.



a) b)

FIGURE 7 Interconnect conductance via CNT diameter: a) CNT-Pt; b) CNT-Fe.

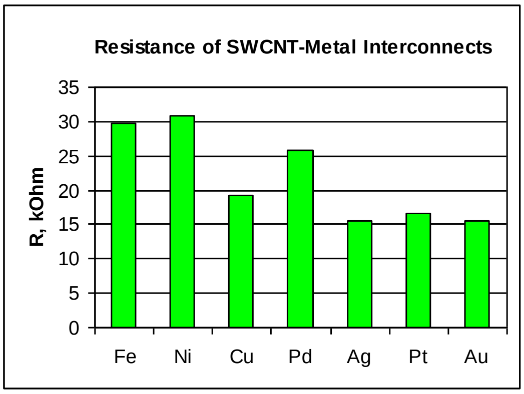


FIGURE 8 Resistances of zig-zag SWCNT-Metal interconnects in comparison.

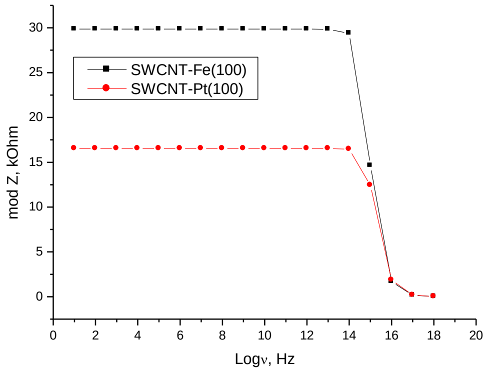


FIGURE 9 Impedances of SWCNT-Fe and -Pt interconnects in comparison.

It means that resistances and the number of effective bonds in the interconnect space are indicators of CNTs morphology.

4.2 CNT-Fe_xPt_{1-x} INTERCONNECT FORMATION

There is a relation between the use of magnetic catalysts and the CVD growth of CNTs determining the most commonly used materials for the CNT growth - Fe, Co and Ni. The nanoparticles of the latter catalysts are magnetically isotropic. Magnetism of the particles-catalysts brings order into the process of CVD growth. Additional possibilities in controlling the process of CVD growth open up the ways to use magnetically anisotropic nanoparticles such as those in the alloys with a different substitutional disorder (*e.g.*, Fe_xPt_{1-x}), to manage the CVD process with the formation of the predefined CNT chiralities. Besides, the stimulation of the process by means of the external magnetic field activates magnetic moments of the catalyst and the deposited carbon atoms. This also means that we can control the number of effective bonds inside interconnects. We pay a special attention to Pt and Fe substrates as possible elements for nanoelectronic and nanomagnetic devices considering interconnects fundamental properties and magnetically stimulated nanoprocesses on Fe-Pt $L1_0$ nanoparticles [59].

4.2.1 Magnetic properties of Fe-Pt alloys.

The unique magnetic properties of Fe-Pt alloys - is an open field for research to correlate different CNT techniques in terms of the catalyst role in entirely different range of temperatures and pressures. Carbon nanotubes grow using bimetallic nanoparticles Fe-Pt as a catalyst [64-67]. Since the mid-1930s Fe-Pt alloys have been known to exhibit high coercivities due to high magnetocrystalline anisotropy of the $L1_0$ FePt phase but their high cost prevented these alloys from widespread applications in the past. In Fe-Pt alloys, both Fe and Pt atoms carry a magnetic moment: The induced magnetic moment on the Pt sites and the enhanced magnetic moment on the Fe sites. A wide variety of the magnetic structure types in the Fe-Pt alloys is evidently the consequence of various atomic configurations around Fe atoms, which, in turn, has a considerable effect on the electronic structure of these alloys (see, Figure 10, and Table 3)

TABLE 3 Specific magnetic structures of Pt-Fe systems

Magnetic Structure	**Behaviour**	**Curie Temperature**
$L1_2$ Fe_3Pt	**Ferromagnetic**	**410K**
$L1_0$ FePt	**Ferromagnetic**	**750K**
$L1_2$ $FePt_3$	**Paramagnetic**	**273K**

To obtain the Fe-Pt alloy in $L1_0$ phase we use a new chemical synthesis strategy reported in details in our previous works [60-63]. By planetary ball milling of the nanocrystals of a particular precursor $[Fe(H_2O)_6]PtCl_6$ and NaCl were grounded and then annealing at 400 °C (300 °C less than typical used temperature) in reductive atmosphere, After washing we obtain FePt $L1_0$ NPs with selected size as function of fraction of $[Fe(H_2O)_6]PtCl_6$ and NaCl used. By varying the precursor ratio we are able to avoid the coalescence phenomena and obtain single crystal NPs with the size around 6 nm, not agglomerated.

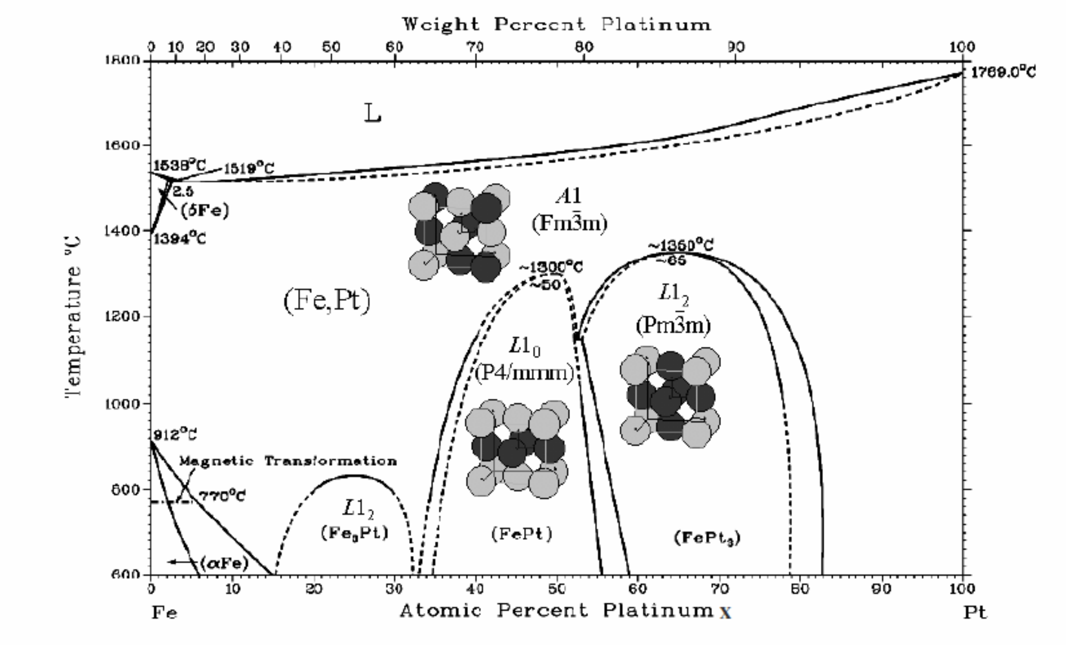


FIGURE 10 Eutetic Phase Diagram of Fe-Pt alloy (http://www.himikatus.ru/art/phase-diagr1/Fe-Pt.php)

4.2.2 Magnetically stimulated CNTs growth with the probabilistically pre-defined morphology

The formation of the initial optimal perimeter for C-Metal (Fe-Pt) bonds is a synergetic process with a minimal free energy (see Figure 11).

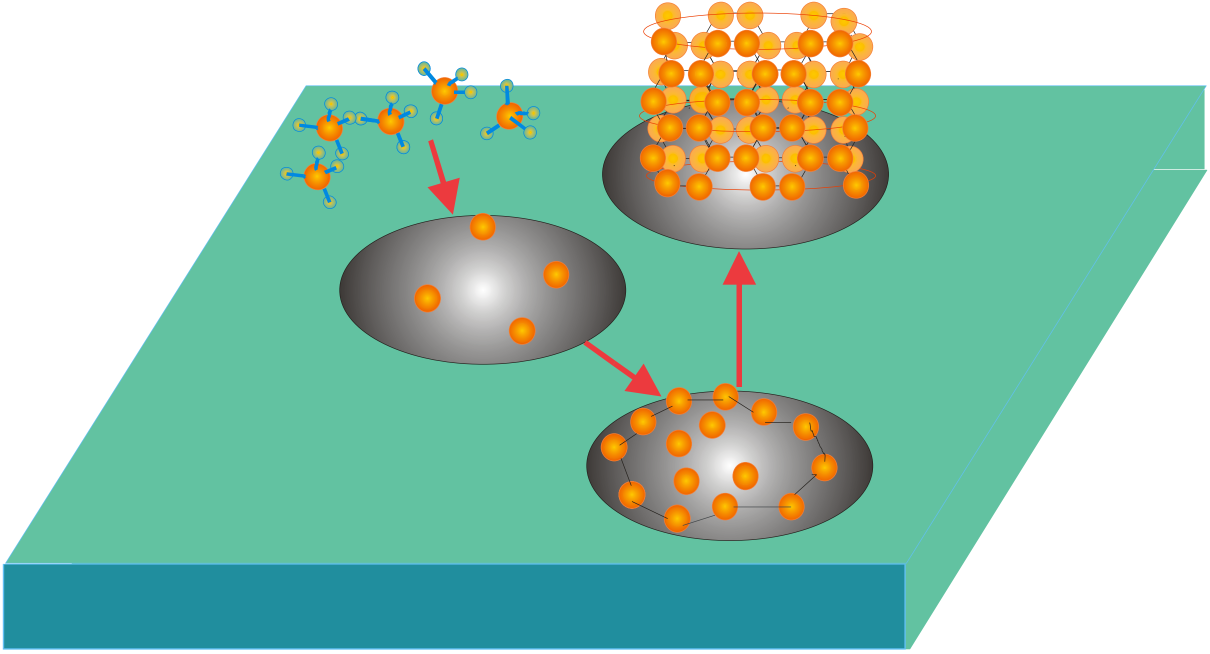
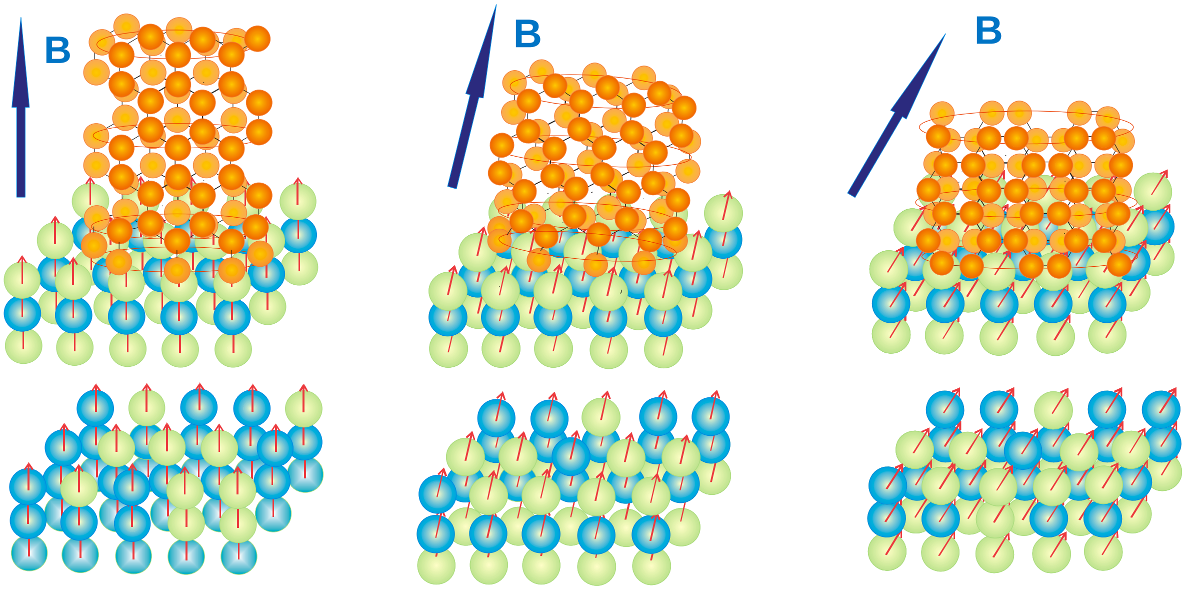


FIGURE 11 A fragment of the CNT CVD process growth on nanoparticle surfaces

The nanoparticle diameter determines with a certain error the diameter of a CNT. The number of effective bonds defines the morphology of the future CNT (See Fig.12, arm-chair, chiral, zig-zag CNTs,) in terms of chirality. Obviously, there is a considerable uncertainty in the morphology of the future CNTs, owing to sporadic thermal dynamics of the deposited carbon atoms.



a) b) c)

FIGURE 12 Magnetically stimulated orientation of magnetic moments of atoms in model interconnects during the CNTs controlled growth with the expected chiralities under the directed mag $\phi = \Theta_B$: a) arm-chair CNT, netic field B with the orientation angle Θ_B , where **B** is the magnetic induction and the chirality angle is $\phi = 0^\circ$; b) chiral CNT, $0^\circ < \phi < 30^\circ$; c) zig-zag CNT, $\phi = 30^\circ$

According to our model, the process can be considerably streamlined using even minor diamagnetic properties of carbon atoms at the expense of magnetic field and strong induced ferromagnetism of the nanoparticle. It becomes evident that the nanoparticle composition Fe-Pt and its atomic structure (including the short-range order) play a primary role in the process of CNT growth stimulated by the magnetic field of CVD.

Nucleation in the process of CNT growth in cases of the ordered Fe-Pt nanoparticles is more stable and has principal advantages in relation to the controlled CNTs growth compared with the cases of any kind of anisotropic Fe-Pt nanocatalysts [68].

The availability of substitutional disorder and anisotropy in Fe-Pt nanodrops used for CNT CVD controlled growth is a negative factor for the production of CNTs with predictable morphologies. There are some essential negative features of disorder in Fe-Pt nanodrops for the CVD process:

1) C atoms chemical binding preferences (C-Fe bonds are stronger than C-Pt ones),
2) A higher structural anisotropy leads to higher relaxation times of a nanodrop structure [69]
3) Disordering effects in Fe-Pt lead to sporadic magnetization phenomena

Thus, it is important to control the process of formation of nanodrop structures corresponding to $L1_0$ (Fe-Pt) and $L1_2$ (Fe_3Pt) systems with reliable magnetism and adequate cooling rates, when relaxation processes in nanodrops are accomplished.

4.2.3. Model of CVD CNT growth

Magnetically stimulated CNT CVD model formulation looks as follows (see Figs.11, 12):

- Effective bonds are responsible for the future chirality of CNT in the CVD processes.
- The permanent magnetic field provides the alignment of CVD growth.
- The binding with the Fe-Pt nanoparticle has a probabilistic character; the probability of binding of C atoms with Fe atoms is preferable as compared to Pt atoms.
- The composition of Fe-Pt atoms in a nanoparticle and the atomic structure ordering are essential for chirality of the obtained CNTs.
- The diameter of the future CNT is correlated with the nanoparticle size.
- The direction of the magnetic field stabilizes the direction of CNT forest growth and is a tool of the growth control.
- The ordering of a nanoparticle atomic structure, as well as a substitutional disorder or arbitrary disorder of a nanoparticle, is responsible for the magnetic state of the nanoparticle, which is essential for the possible future nanomemory devices.

Even a very strong magnetic field is not able to suppress thermal fluctuations of magnetic moments in carbon atoms. It is a different thing, when carbon diamagnetic atoms appear on the surface of a catalyst in the ferromagnetic condition where magnetism induced by the external field can be very strong and is able to correct the behaviour of carbon atoms by suppressing thermal fluctuations.

At the same time, the growth control over chiral and non-chiral nanotubes essentially depends on stoichiometric composition of Pt-Fe nanoparticles. The beginning of the nucleation process with the growth of nanotubes might be connected with stochastic fluctuations of the magnetic moment in a carbon atom relative to the direction of the local magnetic field in a nanoparticle. Distribution of the fluctuation angle obeys the Gaussian law: $f(\theta)=\frac{1}{\sigma\sqrt{2\pi}}\cdot\exp\left(-\frac{(\theta-\theta_B)^2}{2\sigma^2}\right)$, where σ^2 is the angular dispersion of thermal fluctuations of the magnetic moment angle of a carbon atom. To evaluate this dispersion, the potential energy change of the magnetic moment under the influence of the thermal energy should be evaluated: $\mu_C B(1-\cos\theta_T)\approx k_B T_{CVD}$, where μ_C is the induced magnetic moment of a carbon atom $\mu_C=1.25\mu_B$ (see evaluations in [65], $\mu_B=5.788\cdot 10^{-5}\,eV/T$, **B** is the magnetic induction of the catalyst surface, $\theta_T=\theta-\theta_B$ T_{CVD} - is the operating temperature of the CVD process, k_B =8,617 3324(78)·10^{-5} *eV/K*- is the Boltzmann constant. Hence $2\sin^2\frac{\theta_T}{2}\approx\frac{k_B T_{CVD}}{\mu_C B}$. Taking into consideration one of the main problems of the nanotubes growth control – the chirality control – it is necessary to seek for the small fluctuation angle θ. Then $\sigma^2=\theta_T^2=\frac{2k_B T_{CVD}}{\mu_C B}$.

The condition of the small fluctuation angle (e.g., $<10^\circ$) at a certain temperature of the CVD process imposes limitations on the values of the demanded magnetic induction ***B***.

Taking into account the ratio between the chirality angle and the direction of the magnetic field $\phi=\theta_B$, Figure 13 displays the predictable scattering of chiralities for nanotubes of approximately the same diameter.

We are also able to evaluate the necessary value of the magnetic field **B** providing the expected chirality angles scattering, e.g. $\sigma=0.2$ (approximately 12°) leads to the **B** evaluation for the CVD process temperature $T_{CVD}=700^\circ C$ as $B=\frac{2k_B T_{CVD}}{\sigma^2\mu_C}\approx\frac{16755}{\sigma^2\mu_C}\approx 57895\approx 6\cdot 10^4\ T$. For small angle dispersions $\sigma^2=\theta_T^2=\frac{2k_B T_{CVD}}{\mu_C B}$ the high local magnetic field on the nanoparticle surface is necessary. The result also strongly depends on the carbon atom magnetic moment μ_C.

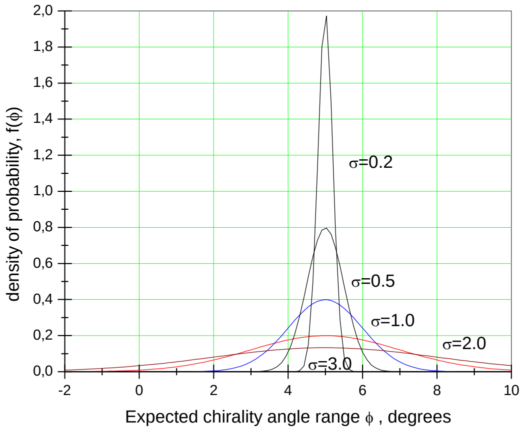


FIGURE 13 The predictable scattering of chiralities for nanotubes of approximately similar diameters

Speaking about the possible errors in diameters of growing nanotubes, their evaluation from beneath is defined by the minimal variations in parameters of the chirality vector $\vec{c}=(n,m)$ Δn and Δm, which are equal 1.

Taking into consideration the formula for calculating the diameter of CNT: $d=\frac{\sqrt{3}a}{\pi}\sqrt{m^2+n^2+mn}$, where α = 0,142 nm is the distance between the neighbouring carbon atoms in the graphite plane.

The relationship between chirality indices (*n* and *m*) and the angle ϕ is given by the ratio: $\sin\phi=\frac{m\sqrt{3}}{2\sqrt{m^2+n^2+mn}}$.

Then the minimum relative error in the diameter of CNT is possible to define as: $\varepsilon_d=\frac{\Delta d}{d}\approx\frac{\sqrt{5m^2+5n^2+8mn}}{2(n^2+m^2+mn)}$.

Particularly, in the case of arm-chair CNT (*m=0*) $\varepsilon_d\approx\frac{\sqrt{5}}{2n}$, in the case of zig-zag CNT (*m=n*) $\varepsilon_d\approx\frac{1}{2\sqrt{2n}}$.

Thus, the errors in the diameter of growing CNTs are incorporated in discrete morphological properties. However, these minimum estimates are only reinforced, given the obvious errors in the size of catalyst nanoparticles are taken into consideration.

The perfect picture of the magnetically stimulated CVD process for growing CNTs can be presented as a CNT forest (see Figure 14). Such a system of nanotubes can also be considered as a prototype of the magnetic memory, where ferromagnetic nanoparticles serve as cells of the magnetic memory – that is, ferromagnetic contacts are controlled by spin pulses, the transport of which is provided by nanotubes.

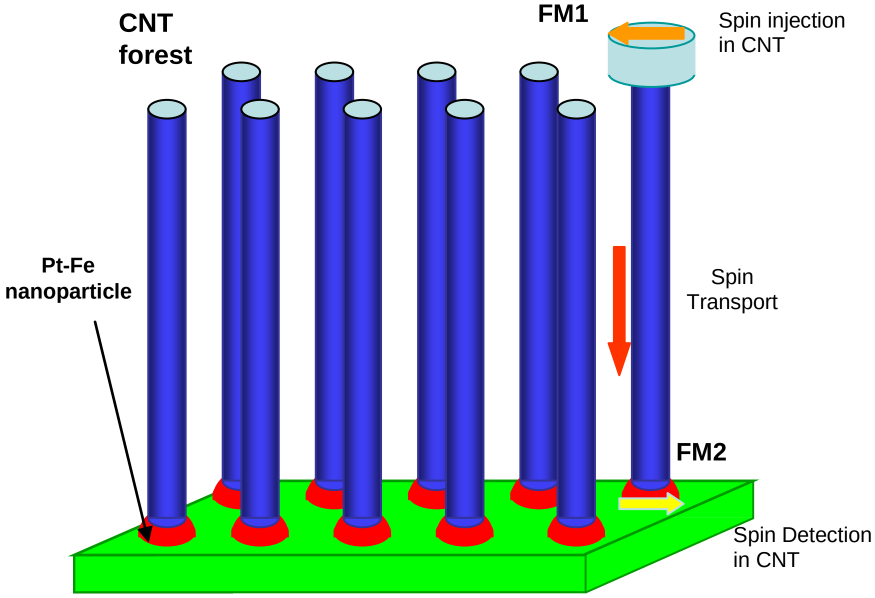


FIGURE 14 CNTs forest is grown on the Fe-Pt nanoparticles of the predefined radius as a fragment of magnetic nanomemory device, which can be realized if spin injection, spin transport and spin detection (spin recording) are provided

5 Conclusions

Electromagnetic properties of Pt- and Fe-CNT interconnects are considered from the point of view of mechanical stability and electrical efficiency. CNT-Fe interconnects are stronger mechanically. However, CNT-Pt interconnects having smaller resistances are more suitable electrically and more effective for various electronic nanodevices.

The use of Pt-Fe nanoclusters during the CVD magnetically stimulated growth allows controlling with some limitation the diameter and chirality of growing CNTs. The diameter of nanoclusters defines the diameter of CNTs, while the angles of chiralities are correlated with the orientation of external permanent magnetic field.

Pt-Fe nanoclusters and CNTs composition is the prototype of the magnetic nanomemory devices. The magnetic efficiency depends on the stoichiometry coefficient ‘x’ and the ordering of Pt-Fe atomic structure.

Chemically ordered Fe-Pt nanoparticles, where we meet the sequence of Pt and Fe layers, allows us to provide all possible predicted magnetic properties. In case of substitutional disorder, this advantage disappears and we should talk about the percolation phenomenon of Fe_xPt_{1-x} ferromagnetism via ‘x’ alteration.

The CVD process of CNTs growth with the presence of Fe-Pt nanoparticles in the conditions of a strong magnetic field is a more orderly process.

Statistical dispersion of CNTs output according to the diameter is determined by a discrete number of effective bonds (especially in the case of small diameters of growing CNTs).

Here with, the dependence of the number of the effective bonds, formed on the nanoparticle perimeter, on the chirality angle is the essential tool for the morphology control of the future CNT.

The balance factor of the thermal energy and magnetic energy in deposited nanoparticles of carbon atoms plays the decisive role in evaluating the dispersion of chirality angles in CNTs.

The morphology of the forthcoming growing CNT stimulated by the magnetic field is set when forming the perimeter of the CNT base and the character of the magnetic orientation in effective bonds.

We can consider CNT forest magnetically stimulated by the CVD process as a fragment of the magnetic nanomemory. CNT chirality in this case defines the efficiency of magnetic cells access (rates of exchange).

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References

[1] Shunin Yu, Kiv A, ed 2012 *Nanodevices and Nanomaterials for Ecological Security. Series: Nato Science for Peace Series B - Physics and Biophysics* Hiedelberg: Springer Verlag 363p
[2] Shunin Yu N, Zhukovskii Yu F, Burlutskaya N Yu, Gopejenko V I, Bellucci S 2012 In: *Nanodevices and Nanomaterials for Ecological Security, Series: Nato Science for Peace Series B - Physics and Biophysics*, ed Yu Shunin and A Kiv Hiedelberg: Springer Verlag 237-262
[3] Shunin Yu N, Zhukovskii Yu F, Gopejenko V I, Burlutskaya N, Lobanova-Shunina T and Bellucci S 2012 *Journal of Nanophotonics* **6**(1), 061706-1-16
[4] Shunin Yu N, Schwartz K K 1997 *Computer Modelling of Electronic and Atomic Processes in Solids* ed R C Tennyson and A E Kiv Dodrecht/Boston/London: Kluwer Acad. Publisher 241-257
[5] Shunin Yu N 1991 *Dr.Sc.Habil. Thesis (Phys&Math)* Riga-Salaspils: Institute of Physics
[6] Economou E L (2006) *Green's Functions in Quantum Physics Solid State Ser.* **7** (3rd edition) Berlin/Heidelberg: Springer Verlag
[7] Ziman J M 1979 *Models of Disorder* New York-London: Cambridge Univ. Press Ch 10
[8] Shunin Yu N, Zhukovskii Yu F, Burlutskaya N, Bellucci S 2012 *Journal of Nanoelectronics and Optoelectronics* **7**(1) 3-11
[9] Moisala A, Nasibulin A G, Kauppinen E I 2003 *J. Phys. Condens. Mater.* **15**, S3011-35
[10] Baker R T K, Hams P S 1978 *Chemistry and Physics of Carbon* **14** ed P L Walker Jr and P A Thrower New York: Marcel Dekker 83p
[11] Muller T E, Reid D G, Hsu W K, Hare J P, Kroto H W, Walton D R M 1997*Carbon* **35** 951
[12] *The Science and Technology of Carbon Nanotubes* 1999 ed K Tanaka, T Yamabe, K Fukui Amsterdam: Elsevier Science Ltd
[13] Sen R, Govindaraj A, Rao C N R 1997 *Chem.Phys.Lett.* **267** 276
[14] Satishkumar B C, Govindraj A, Sen R, Rao C N R 1998 *Chem.Phys.Lett.* **293** 47
[15] *Carbon Nanotubes Science and Applications* 2005 ed M Meyyappan Florida:CRC Press LLC Google e-Book
[16] Xie S, Chang B, Li W, Pan Z, Sun L, Mao J, Chen X, Qian L, Zhou W 1999 *Adv.Mater.* **11** 1135
[17] Cassell A M, Raymakers J A, Kong J, Dai H J 1999 *Phys.Chem.* B **103** 6484
[18] Su M, Zheng B, Liu J 2000 *Chem.Phys.Lett.* **322** 32
[19] Su M, Li Y, Maynor B, Buldam A, Lu J P, Liu J J, *Phys.Chem.* B **104** 6505
[20] Fan S S , Chapline M G, Franklin N R, Tombler T W, Cassell A M, Dai H 1999 *Science* **283** 512
[21] Cheng H M, Li F, Su G, Pan H Y, He L L, Sun X , Dresselhaus M S 1998 *Appl.Phys.Lett.* **72** 3282
[22] Li Y, Liu J 2001 *Chem. Mater.* **13**, 1008-14
[23] Lee D C, Mikulec F V, Korgel B A 2004 *Amer. Chem. Soc.* **126** 4951
[24] Chen G Y, Jensen B, Stolojan V, Silva S R P 2011 *Carbon* **49**(1) 280-5
[25] Shang N G, Tan Y Y , Stolojan, V, Papakonstantinou P, Silva S R P 2010 *Nanotechnology* **21**, 505604
[26] Kumar M, Ando Yo 2010 *Journal of Nanoscience and Nanotechnology* **10** 3739
[27] Takagi D, Hibino H, Suzuki S, Kobayashi Y, Homma Y 2007 *Nano Lett.* **7** 2272
[28] Takagi D, Homma Y, Hibino H, Suzuki S, Kobayashi Y 2006 *Nano Lett.* **6** 2642
[29] Liu H, Takagi D, Ohno H, Chiashi Sh, Chokan T, Yo. Homma Yo 2008 *Appl.Phys.Express* **1** 014001
[30] Hernadi K, Fonseca A, Nagy J B, Bernaerts D, Lucas A A, 1996 *Carbon* **34** 1249
[31] Kong J, Cassell A M, Dai H 1998 *Chem. Phys. Lett.* **292** 567
[32] Li W Z, Xie S, Qian L X, Chang B H, Zou B S, Zhou W Y, Zhao R A, Wang G 1996 *Science* **274** 1701
[33] Wei B Q, Vajtai R, Jung Y, Ward J, Zhang R, Ramanath G, Ajayan P M 2002 *Nature* **416** 495
[34] Nikolaev P, Bronikowski M J, Bradley R K, Rohmund F, Colbert D T, Smith K A, Smalley R E 1999 *Chem. Phys. Lett.* **313** 91
[35] Dai H, Rinzler A G, Nikolaev P, Thess A, Colbert D T, Smalley R E 1996 *Chem. Phys. Lett.* **260** 471
[36] Cheng H M, Li F, Sun X., Brown S D M., Pimenta M A, Marucci A, Dresselhaus G, Dresselhaus M S 1998 *Chem. Phys. Lett.* **289** 602
[37] Hafner J H, Bronikowski M J, Azamian B R, Nikolaev P, Rinzler A G, Colbert D T, Smith K A, Smalley R E 1998 *Chem. Phys. Lett.* **296** 195
[38] Flahaut E, Govindaraj A, Peigney A, Laurent C, Rao C N R 1999 *Chem. Phys. Lett.* **300** 236
[39] Gruneis A, Rummeli M H, Kramberger C, Grimm D, Gemming T, Barreiro A, Ayala P, Pichler T, Kuzmany H, Schamann C, Pfeiffer R, Schumann J, Buchner B 2006 *Physica Status Solidi* B **243** 3054
[40] Maruyama S, Miyauchi Y, Edamura T, Igarashi Y, Chiashi S and Murakami Y 2003 *Chem. Phys. Lett.* **375** 553
[41] Maruyama S, Kojima R, Miyauchi Y, Chiashi S, and Kohno M, 2002 *Chem.Phys.Lett.* **360** 229
[42] Okubo S, Sekine T, Suzuki S, Achiba Y, Tsukagoshi K, Aoyagi Y and Kataura H, 2004 *Jpn. J. Appl. Phys.* **43** L396
[43] Gruneis A, Rummeli M H, Kramberger C, Barreiro A, Pichler T, Pfeiffer R, Kuzmany H, Gemming T, Buchner B 2006 *Carbon* **44** 3177
[44] Nasibulin A G, Moisala A, Jiang H, Kauppinen E I 2006 *J. Nanopart. Res.* **8** 465
[45] Murakami Y, Miyauchi Y, Chiashi S, Maruyama S 2003 *Chem. Phys. Lett.* **377** 49
[46] Murakami Y, Chiashi S, Miyauchi Y, Hu M, Ogura M, Okubo T and Maruyama S 2004 *Chem. Phys. Lett.* **385** 298
[47] Maruyama S, Einarsson E, Murakami Y, Edamura T 2005 *Chem. Phys. Lett.* **403** 320
[48] Xiang R, Einarsson E, Okawa J, Miyauchi Y and Maruyama S. 2009 *J.Phys.Chem.C* **113** 7511
[49] Yuan D, Ding L, Chu H, Feng Y, McNicholas T P, Liu J 2008 *Nano Lett.* **8** 2576
[50] Ward J, Wei B Q, Ajayan P M 2003 *Chem.Phys.Lett***.** **376** 717
[51] Morjan R E, Nerushev O A, Sveningsson M, Rohmund F, Falk L K L, Campbell E E B 2004 *Appl. Phys.* A **78** 253
[52] Ago H, Komatsu T, Ohshima S, Kuriki Y, Yumura M 2000 *Appl.Phys.Lett.* **77** 79
[53] Kumar M, Ando Y 2005 *Carbon* **43** 533
[54] Li W Z, Wen J G, Ren Z F 2002 *Appl. Phys.* A **74** 397
[55] Li W Z, Wen J G, Tu Y, Ren Z F 2001 *Appl. Phys.* A **73** 259
[56] Maruyama S, Murakami Y, Shibata Y, Miyauchi Y, Chiashi S 2004 *J. Nanosci. Nanotechnol.* **4** 360
[57] Kumar M, Ando Y 2008 *Defence Sci. Journal* **58** 496
[58] Raty J-Y, Gygi F, Galli G 2005 *Phys.Rev.Lett.* **95** 096103
[59] Bellucci S, Zhukovskii Yu F, Gopejenko V I, Burlutskaya N, Shunin Yu N 2012 *CIMTEC2012 Theses*, June 10-14 Montecatini, Terme, Tuscany, Italy, 78
[60] Capobianchi A, Colapietro M, Fiorani D, Foglia S, Imperatori P, Laureti S, Palange E 2009 *Chem. Mater.* **21**(10) 2007
[61] Capobianchi A, Campi G, Camalli M, Veroli C 2009 *Z. Kristallogr.* **224** 384
[62] Faustini M, Capobianchi A, Varvaro G, Grosso D 2012 *Chem. Mater.* **24** 1072
[63] Bellucci S. 2005 *physica status solidi* (c) **2**(1) 34
[64] Sun A C, Kuo P C, Chen S C, Chou C Y, Huang H L, Hsu J H 2004 *J. Appl. Phys.* **95**(11) 7264
[65] Elkins K, Li D, Poudyal N, Nandwana V, Jin Zh, Chen K, Liu J P 2005 *J. Phys.* D **38** 2306
[66] Yan M L, Sabirianov R F, Xu Y F, Li X Z, Sellmyer D J 2004 *IEEE Trans. on Magnetics* **40**(4) 2470
[67] Kim Y-H, Choi J, Chang K J 2003 *Phys. Rev*. B **68** 125420
[68] Medwal R, Sehdev N, Annapoorni S 2012 *J. Phys. D Appl. Phys.***45** 055001
[69] Arabshahi H, Hematabadi A, Bakhshayeshi A, Ghazi M 2012 *World Applied Programming* **2** (8) 415-20

Authors

Yuri N Shunin

Current position, grades: Professor and Vice-Rector on academic issues at Information Systems Management University and a leading researcher at the Institute of Solid State Physics, University of Latvia.
University studies: PhD (physics and maths, solid state physics, 1982) at the Physics Institute of Latvian Academy of Sciences and Dr. Sc. Habil. (physics and maths, solid state physics, 1992) at Saint-Petersburg Physical Technical Institute (Russia).
Scientific interest: His current research activities concern nanophysics, nanoelectronics, nanodevices, nanomaterials, nanotechnologies, nanorisks, nanoeducation, and nanothinking
Publications: over 470, 1 book with Springer
Experience: director of NATO ARW "Nanodevices and Nanomaterials for Ecological Security" Riga, Latvia, 2011, a visiting researcher at Gesellschaft für Schwerionenforschung mbH, Darmstadt, Germany (1995), INFN—Laboratori Nazionali di Frascati, Frascati-Roma, Italy (2010 to 2014), participation in EU FP7 Projects CATHERINE (2008 to 2011) and CACOMEL (2010 to 2014), experience in Higher Education from 1975 till nowadays

Stefano Bellucci

Current position, grades: PhD, Professor, currently coordinates all theoretical physics activities at INFN Laboratori Nazionali di Frascati (Italy).
Universisty studies: April 1982: Laurea in Physics (Magna cum Laude), University of Rome "La Sapienza" July 1984: Master in Physics of Elementary Particles, SISSA and University of Trieste, PhD in physics of elementary particles in 1986 at SISSA, Trieste, Italy.
Publications: over 400 papers in peer-reviewed journals (with h = 40), and more than 10 invited book chapters, the editor of ten books with Springer
Scientific interest: research interests include theoretical physics, condensed matter, nanoscience and nanotechnology, nanocarbon-based composites, and biomedical applications.
Experience: He worked as a visiting researcher at the
Brandeis University, Waltham, MA, USA (1983 to 1985); at the M.I.T., Cambridge, MA, USA (1985 to 1986); the University of Maryland, USA (1986 to 1987); at the University of California at Davis, USA (1987 to 1988). He is an editorial board member of the Springer Lecture Notes in Nanoscale Science and Technology, as well as the editorial board member of the Global Journal of Physics Express and the Journal of Physics & Astronomy

Yuri Zhukovskii

Current position, grades: Dr.Chem, Head of Laboratory of Computer Modelling of Electronic Structure of Solids, Institute of Solid State Physics (University of Latvia).
Publications: He is the author of over 120 regular and review papers in international scientific journals. His Hirsch index is 16.
Experience: From 1977 until 1995 he was a researcher at the Institute of Inorganic Chemistry, Latvian Academy of Sciences. Since 1995 he has been a leading researcher at the Institute of Solid State Physics, University of Latvia. Within the last 20 years he has been granted several fellowships for collaboration, visiting activities and positions at seven universities and scientific centres of Canada, Finland, Germany, United Kingdom, and the United States. He has also been actively engaged in developing active collaboration with some scientific groups in Belarus, Italy, Russia, and Sweden. Simultaneously, he has been a contact person and participant in a number of collaboration projects under support of European Commission. His current research activities concern theoretical simulations on the atomic and electronic structure of crystalline solids (with 3D, 2D and 1D dimensionalities).

Victor Gopeyenko

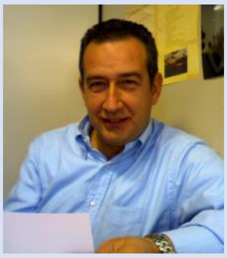
Current position, grades: professor, Dr.Sc.Eng Vice-Rector on scientific issues at Information System Management University and the director of ISMU Computer Technologies Institute.
University studies: Riga Civil Aviation Engineering Institute (Latvia), obtained his doctor's degree (Dr. Sc. Eng., 1987) at Riga Civil Aviation Engineering Institute (Latvia).
Scientific interest: current research activities concern nanophysics, nanoelectronics, nanodevices, and nanotechnologies in the EU FP7 Project CACOMEL (2010 to 2014). His special interests concern carbon nanotubes and graphene systems applications and modelling.
Publications: 80 regular papers in international scientific journals
Experience: he was the member of local organizing committee of NATO ARW "Nanodevices and Nanomaterials for Ecological Security," Riga, Latvia, 2011, he is the editor-in-chief of the journal Information Technologies, Management and Society and editorial board member of the journal Innovative Information Technologies.

Nataly Burlutskaya

Current position, grades: a researcher at the Information Systems Management University and the Institute of Solid State Physics, University of Latvia
University studies: Master degree in computer systems (2011) at Information Systems Management University, Riga, Latvia.
Scientific interest: current research activities concern theoretical simulations of the electronic and electrical properties of carbon nanotubes and graphene nanoribbons in the EU FP7 Project CACOMEL (2010 to 2014).
Publications: 30 regular papers
Experience: Nataly Burlutskaya was the secretary of organizing committee of NATO ARW "Nanodevices and Nanomaterials for Ecological Security," Riga, Latvia, 2011.

Tamara Lobanova-Shunina

Current position, grades: Associate Professor at Riga Technical University, PhD, Dr.edu
University studies: University of Latvia, She obtained her PhD (2009) on innovative education at South-Ukrainian National University
Scientific interest: current research activities concern nanotechnologies, nanomanagement, nanoeducation, nanorisks, and nanothinking in the EU FP7 Project CACOMEL (2010 to 2014), special interests concern the systemic approach to nanosystems applications.
Publications: 55 regular papers
Experience: She was a member of the NATO ARW Local Organizing Committee 'Nanodevices and Nanomaterials for Ecological Security', Riga, Latvia, 2011. Her She has been working as a visiting researcher at INFN-Laboratori Nazionali di Frascati, Frascati-Roma, Italy (2010 to 2014). She was the Head of International Business Communications Department, Director of the study programme 'International Business Communications' at Information Systems Management University (till 2013). She is the Editorial Board member of the journal 'Innovative Information Technologies'. She is the author of over 53 scientific papers in international scientific journals.



Aldo Capobianchi

Current position, grades: Istituto di Struttura della Materia ISM, Dr chem.
University studies: Dr Degree in Chemistry (Rome , 1996) taken at CNR Consiglio Nazionale delle Ricerche since 1989, http://www.ism.cnr.it
Scientific interest:
Inorganic Chemistry,Mechanical Engineering,Material Science
Publications: about 30
Experience: Extensive experience in summary: Sitesi and characterization of organometallic compounds to the charge transfer as phthalocyanines and porphyrins. Synthesis and characterization of nanostructured hybrid materials (nanocomposite) based on carbon nanotubes and nanoparticles. (a patent) Synthesis and characterization of nanostructured magnetic materials for magnetic recording. Application experience in various fields: Growth of thin films of organic and inorganic substances with different devices (LB, thermal evaporation, etc.), for applications in the fields of chemical sensors and organic photovoltaics. Chemical gas sensors for environmental pollutants (a patent). Construction and testing of organic solar cells based on phthalocyanines.

Federico Micciulla

Current position, grades: Contrator Research at Frascati National Laboratories - National Institute of Nuclear Physics
University studies:
Università degli Studi di Roma 'La Sapienza'Aerospace Engineer, Postdoctoral Research Fellow presso Università degli studi di Cassino e del Lazio Meriodinale Roma, Italia
Scientific interest: Nanotechnology, Polymers, Carbon Nanotubes, Graphene
Publications: about 40
Experience: Synthesis of Carbon Nanotubes (CNTs) by Arc Discharge method. Growth of Graphene Nano - Plates (GNPs) by Microwave assistance.
Development and project of nano composites as shielding coating against electromagnetic interference, using several Carbon Materials: CNTs, GNPs, Graphene, Carbon Black, Exfogliated Graphite, Activated Graphite.
Growth of Carbon Nanotubes inside pores of alumina membrane for novel high speed interconnections for electronics
Characterization of nano materials by scanning electron and atom force microscope.
Responsible for analysis service and maintenance of s Scanning Electron Microscopes and Atomic Force Microscopes. Interpretation of data, problem resolution