

Basic Principles of Decision Making upon Receipt of New NanomaterialVyacheslav Lyashenko¹, Syed Khalid Mustafa², Svitlana Sotnik³, M. Ayaz Ahmad⁴¹ Department of Informatics, Kharkiv National University of RadioElectronics, Ukraine,

lyashenko.vyacheslav@gmail.com

² Department of Chemistry, Faculty of Science, University of Tabuk, Saudi Arabia,

khalid.mustafa938@gmail.com

³ Department of Computer-Integrated Technologies, Automation and Mechatronics, Kharkiv National University of RadioElectronics, Ukraine, svetlana.sotnik@nure.ua⁴ Department of Physics, Faculty of Science, University of Tabuk, Saudi Arabia, mayaz.alig@gmail.com**ABSTRACT**

Review of nanomaterials existing classifications and their preparation methods is carried out. As a result, basic principles of decision-making when obtaining new nanomaterial are determined, which take into account stability, as well as properties when molding products from nanomaterials and directly reproducible properties of materials themselves with check for biocompatibility, biodegradability, and toxicity. It is proposed in decision-making process to pay attention to analysis: nanomaterial behavior in soil (mobility, stability); nanomaterials behavior in water; airborne behavior and photoactivity. It is proposed to classify nanomaterials in terms of their structural components: nanoparticles, carbon nanostructures, thin films. Proposed decision-making algorithm for obtaining new nanomaterial takes into account its safety for human health and environment throughout entire life cycle.

Key words: Nanotechnology, Nanomaterial, Safety, Principles, Decision Making.

1. INTRODUCTION

In recent years, a significant role has been given to innovative development path, basis of which should be determined by nanotechnology [1]– [5].

Nanotechnology (NT) can be called any technology that is implemented on nanoscale and is used in real world. This is technology that every day more and more penetrates into all spheres of human activity at the same time, having an impact

not only on a person, but also on environment. Today, nanotechnology is used in cosmetic products manufacture, medical equipment, and chemical catalysts. For example, nanorobots are capable of moving in liquids and, in future, can become a new round in nanomedicine [6]. Nanoparticles are not only chemically more active than their counterparts, but also able to penetrate into any organism in ways that are inaccessible to larger fragments. However, at present, there are no special standards for safe handling of nanomaterials [6].

Emergence of nanotechnology in oil and gas industry with emphasis on application of silica nanoparticles [7]. Application of nanotechnology in agriculture and food industry. For example, nano-agrochemicals, such as nanopesticides, nanofertilizers or nanosystems, to stimulate plant growth.

Nanotechnology applications can be used for electrical transformers. Nanofluids, nano-isolation, nanostructured insulators are used [8].

Need to create new materials, processes or phenomena at nanoscale, the development of new experimental and theoretical research methods is growing every day due to uniqueness of solutions and becomes a prerequisite for opening new opportunities in science and technology. Nanomaterials have high reactivity, mobility, photo activity and other useful properties [1], [6], [7].

The development of NT depends on nanoproduction, nanomaterials (NM), as well as use of physical, chemical and biological systems on scale from individual atoms or molecules to submicron sizes, as well as integration of resulting nanostructures. All this requires appropriate solutions to obtain new nanomaterials.

In other words, analysis of main stages in making decisions for obtaining a new nanomaterial will allow affecting on solution of nanotechnology safety problem and is one of key values for development of nanotechnology industry.

2. A REVIEW OF LITERATURE ON RESEARCH TOPIC

Nanotechnology has become a new challenge to modern society, advent of new nanomaterials every day expands nanoindustry, therefore a whole series of works is devoted to this area.

In [9], theoretical and experimental studies of coal use and its pyrolysis products for obtaining carbon nanomaterials and seizing man-made carbon nanoparticles. Methods for using carbon nanoparticle suspensions in many industrial sectors are described. Influence of carbon nanomaterials on social and environmental aspects of human life is considered, and possibility of producing carbon nanomaterials from renewable raw materials is also shown.

[10] is devoted to collected traditional measures of nanomaterials control in order to potential risk minimize to human health and environment as a result of exposure to materials. Focus is on "engineering" nanomaterials and selection of most appropriate risk management measures. Issues related to production, use and disposal of engineering nanomaterials (ENM), which lead to release of ENM into environment, are also disclosed. The work also deals with methods for quantitative monitoring of ENM emissions in environment.

The methods of synthesis of nanomaterials are the subject of [11]. The advantages and disadvantages of the basic methods for producing nanomaterials are determined.

Nevertheless, little attention has been paid to decision-making problem in development of new nanomaterials. In this case, special attention should be paid to principles of making such decisions. This in turn makes it necessary to consider, in particular, methods for producing nanomaterials.

3. OBTAINING NANOMATERIALS AS A BASIS FOR FORMATION OF PRINCIPLES FOR MAKING APPROPRIATE DECISIONS

Obtaining nanomaterials requires various experimental methods and often (but not always) very high-tech and expensive equipment, and all of them are based on various principles, which are subsequently reflected in methods of obtaining nanomaterials. So, for example, there are two

general principles for synthesis of nanoobjects – "bottom up" and "top down", shown in Fig. 1 [12]. In first of them, nano-objects are obtained from atoms, molecules and other tiny building blocks, usually due to self-organization and self-assembly. In second of them, substance is "disassembled," as they say, dispersed due to high-energy mechanical, physical, chemical influe. Another important principle can be attributed to safety of NM for human health and environment.

Therefore, there is a whole knowledge infrastructure supporting assessment of nanomaterials in field of environment, health and safety Fig. 2 [13].

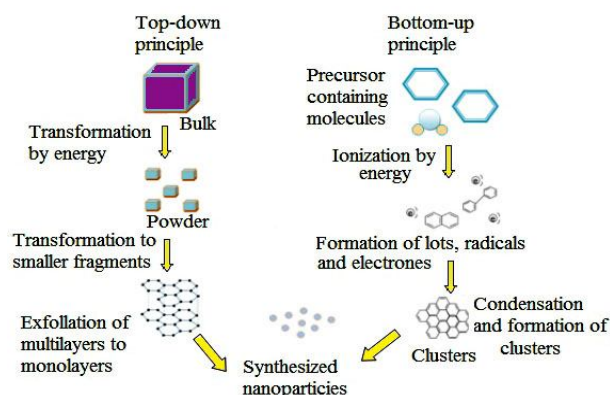


Figure 1: General principles for synthesis of nanoobjects

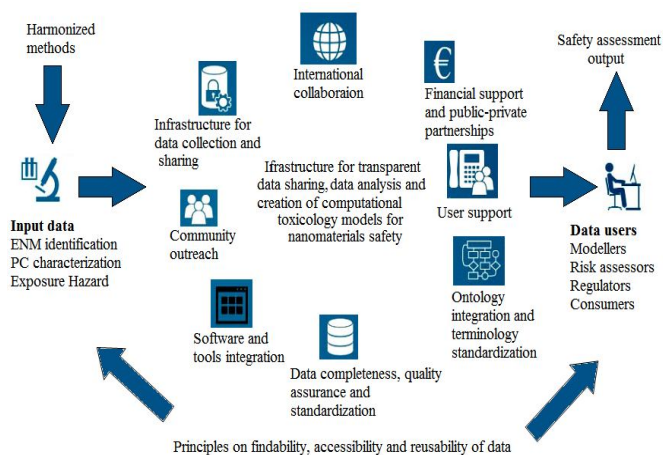


Figure 2: Knowledge infrastructure supporting assessment of nanomaterials in field of environment, health and safety

Success in development of nanotechnology is largely dependent on success in initial NM creating.

The class of nanomaterials includes materials containing structural elements whose geometric dimensions in at least one dimension do not exceed 100 nm, and have qualitatively new properties, functional and operational characteristics [14].

Currently, there are several approaches to classification of nanomaterials: according to geometric parameters of their structure; by composition, distribution and form of structural components; by physical principle; by origin and topology etc. It should be borne in mind that classification features and boundaries between individual groups of nanomaterials are very arbitrary.

For example, according to geometric characteristics, these elements are usually classified into:

- zero-dimensional atomic clusters and particles;
- one and two-dimensional layers, coatings and laminar structures;
- three-dimensional bulk nanocrystalline and nanophase materials.

Often proposed following classification of NM:

1. Nano-products (size not exceeding 100 nm): nanopowders, nanowires, nanofibres, thin films, nanotubes;
2. Micro products (size no more than 1 ... 2 mm): wire, tape, foil;
3. Massive NM (size over 1 ... 2 mm):
 - 3.1 Single-phase (microstructurally homogeneous): glasses, gels, supersaturated solid solutions.
 - 3.2 Multiphase (microstructurally heterogeneous): complex alloys and ceramics.
4. Composites with components from NM.

However, after reviewing features of NM, it is proposed to classify them according to structural components:

- nanoparticles;
- carbon nanostructures;
- thin films.

At the same time, methods that result in nanoparticles are:

1. Mechanical methods: methods of grinding materials mechanically in mills of various types; type of mechanical grinding is mechanosynthesis, or mechanical alloying; intensive plastic deformation (torsion under pressure, angular pressing, rolling, forging) – essence of methods is multichannel intense plastic shear deformation of processed materials [15];
2. Physical methods: methods of evaporation (condensation), or gas-phase synthesis of obtaining metals nanopowders; by an electric explosion of a metal wire from which it is planned to obtain a nanopowder; ion-plasma methods are used to obtain non-porous nanocrystalline materials (amorphous alloys and nanocrystalline materials); method of controlled recrystallization from a solid amorphous state; high-frequency induction heating [8],[15].

3. Chemical methods: co-precipitation; sol gel method; recovery and thermal decomposition; hydrolysis; thermolysis; pulsed laser; pulsed sonoelectrochemistry [15], [16].

Nanoparticles can also be obtained in liquid media, which excludes their contact with air. However, in this case, solvent molecules may bind to surface of nanoparticle, or surfactant may be added.

Methods that result in carbon nanostructures include [16]:

1. Methods for synthesis of fullerenes: laser evaporation of graphite; synthesis using vacuum; synthesis at atmospheric pressure.
2. Methods for synthesis of nanotubes: laser evaporation; using a carbon arc; chemical vapor deposition.
3. Methods for isolation and purification of carbon nanoparticles: isolation and purification of fullerenes; extraction and purification of carbon nanotubes.

Methods that result in thin films include [8], [16]:

1. Langmuir-Blodgett method;
2. Method of molecular beam epitaxy.
3. Ion plasma spraying.
4. Electron beam evaporation.
5. Ion beam spraying.
6. Method of thermal evaporation in vacuum.

Thus, existence of all these methods is due to diversity of composition and nanomaterials properties, which must be taken into account when forming basic principles for obtaining nanomaterials in order to avoid spontaneous degradation. Fundamentally new properties of nanomaterials are provided at micro (but not macro) level. This is basis for formation of decision-making principles upon receipt of new nanomaterials.

4. BASIC PRINCIPLES OF DECISION MAKING UPON RECEIPT OF NEW NANOMATERIAL

Currently, there is no method that fully complies with all principles of obtaining NM, however, it is necessary to adhere to basic ones.

There are number of principles, for example, maximum filling of space with matter or principle of “building blocks”, fundamental configurations from which structural elements of any nanoparticles type are created.

Some principles of obtaining nanomaterials suggest an integrated approach to creation of nanotechnologies, including processes of steelmaking complex, intense plastic deformation, and heat treatment [17].

It was determined that upon receipt of NM it is necessary to adhere to following principles:

- temporary stability of nanomaterials properties, which provides particles surface protection from spontaneous oxidation and sintering in manufacturing process;
- nanomaterial with specific particle or grain size, and their size distribution should, if necessary, be sufficiently narrow;
- material with reproducible properties;
- material of controlled composition with verification for biocompatibility, biodegradability, toxicity.

By making decisions on obtaining new nanomaterial in future we will mean solving problems of material safety for human health and environment, since artificial nanoparticles and nanomaterials entering environment represent a special unprecedented class of industrial pollution. Their particular harm may be due to unusual properties of substances, including their mobility and stability in soil, water, air; bioaccumulation, unpredictable interaction with chemical and biological materials.

As a result, taking into account principles indicated above and generalized classification of nanomaterials, in which all nanomaterials can be divided into: nanoparticles, carbon nanostructures and thin films, as well as a review of methods for their preparation, we will present decision-making process for obtaining a new nanomaterial in form of an algorithm:

Stage 1 – expected use of NM (scope).

Stage 2 – determination of product type (nano-product, micro-product, etc.).

2.1 If you intend to use new NM for "products from nanoparticles", then you must:

- Determination of geometric structure of nanoparticles;
- Determination of electronic structure of nanoparticles;
- Determination of reactivity and stability of material (as well as temporary stability of properties of nanomaterials upon receipt);
- Definition of fluctuations.

2.2 If you intend to use new NM for "products with a carbon nanostructure", then you must:

- Determination of vibrational properties;
- Determination of electrical conductivity;
- Determination of adsorption properties;
- Determination of reactivity and stability of material (as well as temporary stability of properties of nanomaterials upon receipt).

2.3 If you intend to use new material for "products from thin films", then you must:

- Determination of crystal structure;
- Determination of film thickness;

Determination of reactivity and stability of film (as well as temporary stability of properties of film upon receipt);

Stage 3 – determination of operating conditions for product from NM.

Stage 4 – determination of NM profiles:

4.1 Determination of properties of nanomaterial:

Chemical properties:

Definition of category of nanoparticles of which NM will consist of: natural (volcanic ash, magnetotactic bacteria of ocean, minerals, etc.), associated (waste from the industrial process) and produced (metal, semiconductors, quantum dots, metal oxides, etc.);

Definition: percent solubility in acids; temperature behavior of chemical reactions; the presence / absence of "induction" period.

Mechanical properties – hardness, rigidity and elasticity of material, impact strength, strength, ductility, yield strength, tensile strength, fatigue strength. A unique feature of nanomaterials is optimal combination of strength and ductility, due to implementation of special non-dislocation ductility mechanisms.

Magnetic properties – paramagnetism, coercive force, magnetoresistance.

Thermal properties – debye temperature; melting; phase transitions; sintering; coefficient of thermal expansion and heat capacity.

Electrical properties – dimensional dependence of electron work function and electrical resistance.

Optical properties – change in electromagnetic spectra of radiation and absorption; scattering; ability to "black body" implement.

4.2 Determination of NM properties affecting human health, not only for a long time, but throughout its entire life cycle;

4.3 Determination of NM properties affecting environment, not only for a long time, but throughout its life cycle.

Analysis of NM behavior in soil (mobility);

Analysis of NM behavior in water;

Analysis of NM behavior in air;

Analysis of NM photoactivity, since it is a prerequisite for possible adverse environmental consequences.

Stage 5 – clarification. Determining nature operating process of product from NM, that is, how properties of a new NM can change over time and under what conditions;

Stage 6 – assessment of NM for biocompatibility, biodegradability, toxicity [8], [11], [16].

Stage 7 – assessment of NM in terms reproducibility of properties.

Stage 8 – decision making. At this stage, question is decided whether to continue development / production of this nanomaterial.

Stage 9 – obtaining a new alternative to NM, taking into account all factors.

5. DISCUSSION OF THE RESULTS

In [18], risk associated with created nanomaterials is described: various tools for different control methods. The paper assesses nanomaterials, which wins due to proposed multicriteria assessment of environmental impact hazard. However, in contrast to material presented above, reactivity of materials is not taken into account in [18].

Proposed principles in above study, unlike [19], are designed for entire class of nanomaterials, starting from those obtained from nanoparticles of nanomaterials and ending with thin films, and here a narrowly focused profile, since we are only talking about silicon. The work [19] is also devoted to problem of assessing risks of manufactured nanomaterials. At the same time, main idea of material presented by us is need to develop grouping and intelligent strategies for testing nanomaterials. Therefore, we focus on physicochemical characteristics and toxicity protocols, which in turn will affect safety of materials obtained.

A distinguishing feature of presented study from [20] is that it takes into account principle of material properties reproducibility, although paper covers all relevant aspects of life cycle and biological paths of a nanomaterial: internal material properties and system-dependent properties (which depend on corresponding environment of nanomaterial), biological stability, absorption and biodistribution, as well as cellular and apical toxic effects. In [20], general principles of assessing safety of nanomaterials using advanced decision-making system, DF4nanoGrouping, are considered. Principles of this study are appointment of nanomaterials in four main groups with a possible further subgroup to clarify specific information needs.

6. CONCLUSION

Review of methods for producing nanomaterials is carried out according to well-known classifications of nanomaterials in order to select the most significant parameters that must be taken into account in technological process of obtaining nanomaterials.

In course of review of methods for obtaining NM, it was determined that physical and chemical methods are extremely expensive. The mechanical methods are simple, do not

require expensive equipment and, provided that coarse raw material powder can be obtained, powder can be processed.

Based on a review of existing classifications of nanomaterials and their methods of preparation, it is proposed to divide all nanomaterials by structural components into: nanoparticles, carbon nanostructures, thin films.

As a result, taking into account basic principles when deciding to obtain a new nanomaterial, an algorithm is presented that takes into account safety features of new NM for human health and environment throughout life cycle. Proposed algorithm differs from existing ones in that it takes into account:

- determination of HMs properties affecting human health not only for a long time, but throughout its entire life cycle, but in future, cases of changes in properties of new HM for a long period will be clarified;
- analysis of NM behavior in soil in order to take into account situation of getting product from new NM into soil and ensure environmental safety of materials;
- analysis of NM behavior in water and air also ensuring safety of materials.

Thus, key parameters from point of view of NM safety are: biocompatibility, biodegradability, toxicity, reactivity.

Basic principles of decision-making upon receipt of a new nanomaterial, which will ensure stability of properties during molding of products from NM, as well as their reproducibility, are highlighted.

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