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SMART LAB CONCEPT IN MODERN SCIENTIFIC AND LEARNING SPACE OF NANOMATERIALS SCIENCE

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Abstract: *The approaches to the development of the concept of a smart laboratory are described. The structure of the physical and chemical laboratory of nanomaterials was decomposed. The main work blocks and workflows have been highlighted. It is shown that five connected blocks can be distinguished in the laboratory structure, two of which are purely software blocks and three hardware-software blocks. The main block of such a laboratory is the block "chemical synthesis of material". Two internal and one external cycles organize the laboratory workflows. It was shown, that the identified workflow distributions and the modular presentation of physical and chemical laboratory of nanomaterials based on the decomposition of its structure made it possible to develop the Smart Lab concept for its future development. In Smart Lab form, the laboratory is much better suited for use in the educational process, since the visibility of the studied processes themselves and the ability to use the data of experiments.*

Keywords: Smart Lab, nanomaterials, workflow, decomposition of laboratory structure

1. Introduction

Nanomaterials have a wide spectrum of different applications in industry, environmental protection, medicine, energy, and others [1]. Transfer from bulk to nanosized state leads to a significantly changing of characteristics of known materials, so the final properties of such materials are difficult to prognoses [2]. Effective applying of these materials is based on the determined linking between their structures, properties, and working characteristics [3]. Thus, the response between industry and research laboratory should be quick. Training some professional skills is required for work with nanomaterials, their synthesis and characterization [4]. In this connection, the exercise of appropriate specialists has to be close to the tasks of industry technologies that are using nanomaterials. Chemistry, physics, and materials science are specialities that correspond to the training of the appropriate engineers as part of a university program in this direction. Transfer of knowledge acquired by students in university laboratories to real manufacturing or scientific laboratories requires a lot of time and significant investment [5]. It is mainly due to the different principles of planning and controlling the experiment in the laboratory and manufacturing. Thus, the research in the university laboratory is still manual, but the operation in manufacturing is automatic and direct to obtain one final product. Therefore, the corresponding dissonance is between skills of experiment planning and designing acquired students and stagers in the university laboratory and those skills that they will use in manufacturing. In addition, the transfer from large-scale industrial production to small enterprises, in particular, to a pilot line for the production of nanopowders, requires the adjustment of the well-known learning module for the training of engineers, which is focused on traditional types of production. In this regard, the creation of educational platform based on the laboratory of nanomaterials of DIPE NAS of Ukraine, which includes a pilot line for the production of nanopowders, is a significant step for the implementation of such transfer. Also, this approach will accelerate the exchange of knowledge between the university laboratory and production. Restructuring of this physical and chemical laboratory of nanomaterials within the framework of the Smart Lab concept [6-7] can become an effective method for implementing such a platform.

2. Smart Lab conception: developed ways

Smart Lab concept quickly and firmly enters into modern science and begins to be taken into account when creating current scientific, educational, research, and other specialized laboratories [6-7]. Sure, partial automation and computerization of laboratories took place throughout their entire existence. However, discussion about the development trends of modern research or educational laboratory in the 21st century from the traditional (Dark Lab) to the smart (Smart Lab), significantly intensified the development of the concept of Smart Lab [8]. This concept develops in different directions simultaneously:
1) In the context of IoT, it is the creation of a software platform that allows switching on and controlling the devices of laboratory infrastructure [9].
2) In the background “PaperLess” it is a creation of a software platform that allows to redirect significant document flows and digitize laboratory equipment data from paper to computer. This direction refers to the active development and application of a database, storage servers, computing, and software packages for data processing in the laboratory, as well as a creation of a network to coordinate the individual working stages of laboratory processes [10].
3) In the automation context, it is the automation of the individual parts of laboratory processes and the creation of a shared network of controlling laboratory equipment [11]. It is noted that many enterprises offer block research laboratories in which the investigation is carried out in a narrow segment, for example, optics, XRD, biology, others [12].
4) In the context of using multiprogramming calculated packet for data processing and analyzing of experimental data that is obtained in the individual laboratory, it is a unique program - Origin, MatLab, MatCad, HyperChem or other specialized programs [13];
5) In the context GRID technologies it is a creation of an open, standardized network of which provide a flexible, coordinated distribution of computing and storage data resource [14];
6) In the context, the virtual laboratories where the experimental equipment is absent, it is a creation of various simulations that replaced the technical process by virtual [15].

The parts of each of these directions often are an integral part of the development of modern laboratories. However, the main task of any research laboratory is the formation of knowledge about the nature of the object and the development of skills necessary for working and analyzing the data obtained. According to [8], the work of the laboratory is the realization of the process of knowledge cycle by the implementation of many methods such as analysis of known scientific and specialized literature, planning of the experiment, experimental data obtaining, analytical processing, and analyzing of acquired data. The articles, books, conference materials, or other types of knowledge dissemination are the finish of this knowledges cycle, and the obtained knowledge is coming to a new spiral.

Thus, the structure of the research laboratory or learning laboratory should be based on specific laboratory tasks. The research laboratories are strictly classified according to the types of particular laboratory tasks, in particular, analytical and measuring laboratory, biological and biosafety laboratory, cleanrooms, incubations laboratory, medical and clinical laboratory, pilot line, research laboratory, others.

3. Analysis of Workflows of Physical-Chemical Laboratories of Nanomaterials

The physical and chemical laboratory of nanomaterials includes a whole complex of equipment for materials synthesis, characterization, and measuring of their properties [16]. How to mention above, in modern material science, the synthesis and investigation of nanomaterials require a quick response to market demand. It leads needing a rapid change of synthesis conditions, chemical, phase, the granulometric composition of synthesized materials, and it puts forward requirements to the speed of the planning and controlling of the experiment, as well as for the qualifications of engineers. The synthesis of nanomaterials is based on an understanding of the relationship between their structure, characteristics and functional properties. Fig. 1 shows the scheme of main blocks and distribution of workflows in the laboratory of the synthesis of nanomaterials. They are marked based on an analysis of the work of a laboratory in Donetsk Institute for Physics and Engineering named after O.O.Galkin NAS of Ukraine.

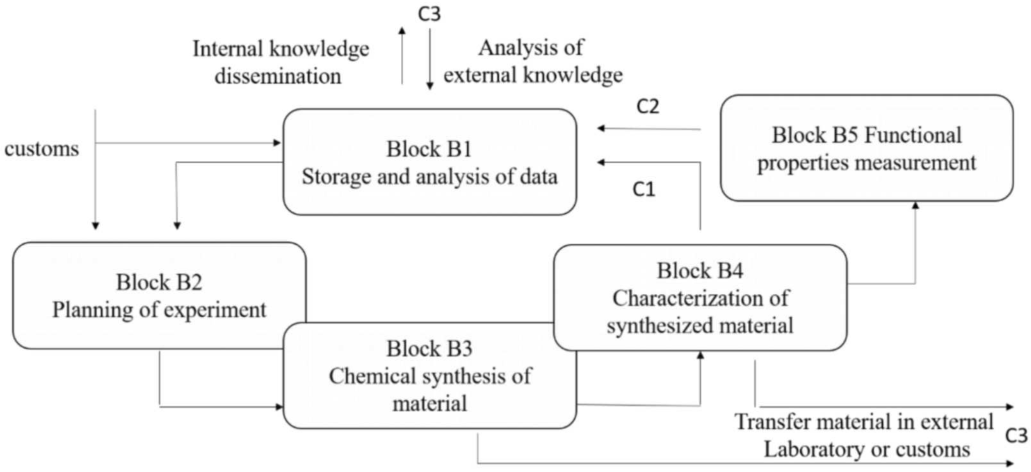

Fig. 1. Scheme of main blocks and distribution of workflows in the laboratory of nanomaterials

According to presented information (Fig.1) the main workflows in the physical and chemical laboratory of nanomaterials occur between the next main blocks:

- Block B1 – Storage and analysis of data;
- Block B2 – Planning of experiment;
- Block B3 – Chemical synthesis of material;
- Block B4 – Characterization of synthesized of material;
- Block B5 – Functional properties measurement.

The distribution of workflows can be described by two inner closed cycles (small cycle C1 and big cycle C2) of workflows and workflows directly related to other laboratories, databases, and open scientific space (conference, articles, different types of dissemination). The outer workflows may be open or include in external cycle C3. The last includes the transfer materials or some results from Block B2, Block B3, or Block B4 to external laboratories for study materials or data process and return the data and results from outside to Block B1. It is noted that the computerization of such a laboratory should provide for full support of all processes in it. These processes are necessary calculations, the work with database and data storage, visualization, analysis program, chemical process control including automation, sensors, others, and also the creation and support of a fast exchange of information inside marked Blocks and between them.

4. Block functionality and structure

The task of Block B1 is a collection, storage, and analysis of internal and external data and knowledge, and also the exchange of this knowledge in open scientific and industry space. Fig.2 shows the decomposition of the Block B1 structure.

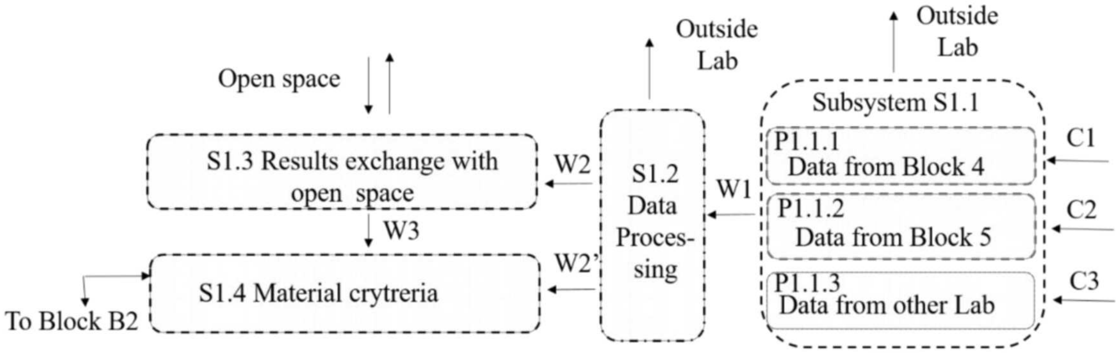

Fig. 2. Decomposition of the structure of Block B1 «Storage and analysis of data»

Block B1 basis on the database (DB1). This database obtains and storages information. Input data of Block B1 are providing:
- Block B4 provides a characterization of the material that is synthesized in Block B3. Information comes in part P1.1.1 of subsystem S1.1 «Data collecting and storage»;
- Block B5 provides information about the functional properties of synthesized materials. Materials are manufactured in Block 3 and characterized in Block 4. Information comes in part P1.1.2 of subsystem S1.1.
- Cycle C3 provides information from external laboratories (Fig. 1). Information comes in part 1.1.3 of subsystem S1.1 «Information collecting and storage» and subsystem S1.2 «Data processing»;
- it is information from open space. It comes in subsystem S1.3 «Data collecting and storage».

Information is coming as output digital signal of the equipment of laboratories (for example, IR, UV-vis spectrometers, XRD analyzer, others). These signals reflect physical parameters that are special for particular equipment (time, voltage, current, wavelength, others). If the equipment has its data processing program, then the data can be sent in block B1 as converted to secondary data. This conversion is obtained by converting digital data within a mathematical model inside a programmed hardware package. Workflows inside Block B1 are:

- Workflow W1 sends collected primary digital and secondary data from subsystem S1.1 «Data collecting and storage» to subsystem S1.2 «Data processing» in which the analysis, mathematical processing, data comprise, finding of dependencies between particular data at using specialized programs. These programs can be specialized programs of laboratory such as licensed programs, for example, Microsoft, Origin, and et all. Results are obtained in subsystem S1.2 and stored in it.
- Workflow W2 sends results are obtaining in subsystem S1.2 in subsystem S1.3 «Exchange with open space». Based on these data, the criteria for material synthesis with known structure characteristics and functional properties are creating.
- Workflow W2' sends results are obtaining in subsystem S1.2 in subsystem S1.4 «Material criteria». Based on these data, the criteria for material synthesis with known structure characteristics and functional properties are forming.
- Workflow W3 sends information that is obtaining in subsystem S1.3 for storage in subsystem S1.4 «Material criteria». This subsystem S1.4 issues the recommendations in Block B2 (subsystem S2.1).

Block B1 interrelates with Block B2. The subsystem S1.3 (Block B1) controls access to data and exchange between inner personals of the laboratory, and in the crucial case, it provides the accessing to external users. Block B1 is a software block.

Block B2 is also a software block. Fig. 3 shows the decomposition of Block B2.

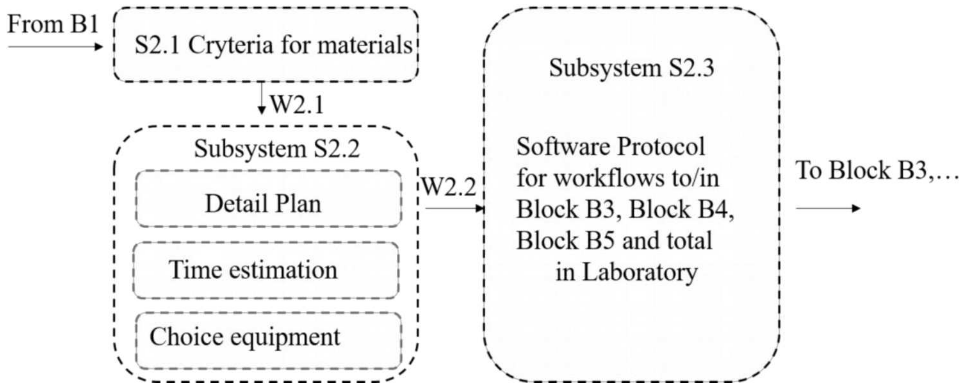

Fig.3. Decomposition of the structure of Block B2 «Planning of experiment»

Input data for this block is an internal laboratory database (Block B1, subsystem S1.4) or an external order. Block B2 use the next algorithm:

-in subsystem S2.1 the criteria of material are described;

-the workflow W2.1 transfers criteria to subsystem S2.2;

- in subsystem S2.2 the detailed plan of experiment with a sequence of stages is described and the necessary resource and experiment time is also calculated;
- the workflow W2.2 transfer information from S2.2 to subsystem S2.3;
- in subsystem S2.3 based on criteria the protocol distribution of workflows in Block B3, Block B4, Block B5, and workflows of the launch of the programs of particular blocks, transfer of materials, and sending of the database is formed. The information exchange between the block management program is carried out through the created protocol of the distribution of workflows. Data protocol (S2.3) sends data in subsystem PD3.1 of Block B3 (fig.4).

The main task of Block B3 «Chemical synthesis of material» starts the synthesis equipment according to the special regime and the controlling apparatus. Fig. 4 shows the decomposition of the structure of block B3.

The structure of Block B3 is a hardware and software solution. It contains two hardware subsystems S3.1 and S3.2.

- The first hardware subsystem S3.1 includes the main components of the equipment of the pilot line, in particular, motors, mixers, mills, vacuum and peristaltic pumps, water supply, washing system (CIP), others.
- The second hardware S3.2 subsystem includes different sensors of chemical processing, namely, pH sensor, a sensor on chloride ions, levels, others.

Input data of Block B3 is data of Protocol (Block B2). The protocol PD3.1 sets parameters of protocol «Part for Synthesis». Block B3 use the next algorithm:

- The workflow W3.1 transfers the control signal to the starting of S3.4 subsystem.
- The workflow W3.2 transfers control signal to the starting of software of S3.5 «Sensors».
- The individual interrelation software subsystems S3.3 «Automatic» and S3.4 «Sensors» start the hardware S3.1 and S3.2 subsystems through workflows W3.4 and W3.3 accordingly.
- The S3.2 subsystems are starting and controlling through exchange data/control signals with S3.4 subsystem (workflows W3.3 and W3.3’).
- The workflow W3.5 coordinates the data of S3.5 and 3.4. This coordination controls the work of S3.1 subsystem through workflow W3.4.

After the stop of work of mention above subsystems (synthesis stop), the synthesized material is accommodated and packed in storage (individual box), stage of S3.5 of Block B3. Then the material is transferred to follow investigation in the laboratory or customers accordingly to requirements of protocol from S.2.3 (fig.3).

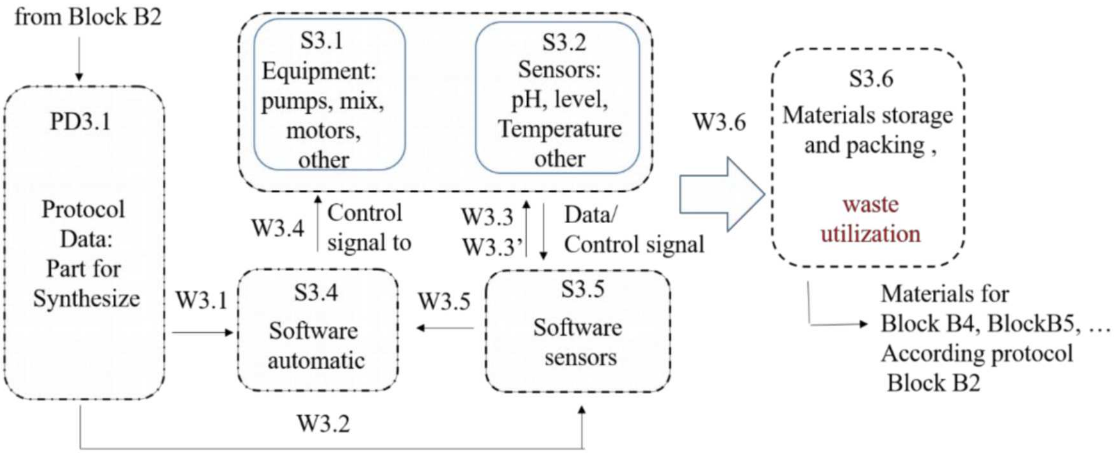

Fig. 4. Structure and distribution of workflows in Block B3

The development of elements of the material synthesis block involves combining both existing equipment that works offline and the development of new hardware and software solutions that allow connecting all equipment into a single controlled system.

Block B4 «Characterization of the synthesized material» is based on a set of physicochemical methods for characterizing the finished product, collecting and transmitting digital signals from equipment to the database of Block B1 through cycle C1 for their storage and subsequent analysis. The input data for this block are generated based on the Block B2 protocol S.2.3. Features of the hardware-software solution of this block consist of combining old devices with analogue output data and tools with digital output data into one network. Data obtained in Block B4 are sent according to the protocol of Block B2 by the corresponding workflows (Fig. 1).

Block B5 - "Investigation of the functional properties of the material" is based on a set of physicochemical methods for studying the properties of synthesized material, collecting and transmitting digital signals or secondary data from the equipment used to the Block1 database through cycle C2 for storage and subsequent analysis. The input data for this block are formed based on the Block B2 protocol. Features of the hardware-software solution of this unit consist of combining devices with an analogue output and devices with a digital output in one network.. Data obtained in Block B5 are sent by the requirements of the Protocol of Block B2 for the corresponding workflows (Fig. 1).

5. Conclusion

The considerations explained in this contribution show that the physicochemical laboratory of nanomaterials could be described as a modular system of interconnected blocks. Blocks are distinguished by the nature of the processes performed within the given block. Blocks can be as a pure software solution. For example, it is a B1 «data storage and analysis», as well as an B2 «Planning of experiment». The B1 and B2 blocks are interrelated. They are based on the analysis of the input data in these blocks, formed criteria that link the characteristics and properties of the synthesized material with the protocol data. Protocol data describes the work process and generated the number and sequence of workflows in the laboratory. A task of these blocks is the formation of a protocol of synthesis criteria and a protocol of the working process in the laboratory. Blocks built as a hardware-software solution; for our case, they are blocks B3 "Chemical synthesis of material", B4 "material characterization", and B5 "functional properties research". In terms of their tasks, the Block B3 "material synthesis" and the Block B4 "material characterization" and Block B5 "functional properties research" differ not only in their goals but also differ in hardware and software solutions. The block B3 is the most complex in structure since it contains at least two dedicated hardware subsystems S3.1 and S3.2, which at first glance can be controlled independently within two different software subsystems S3.3 and S3.4, accordingly. However, for effective control of the synthesis process, data exchange between these software subsystems S3.3 and S3.4 must take place. It is noted that the structure of the block B3 "material synthesis" requires further more detailed decomposition to create an effectively integrated scheme to control the operation of this block. It is shown that the identified workflow distributions and the modular presentation of this physical and chemical laboratory of nanomaterials based on the decomposition of its structure made it possible to develop the Smart Lab concept for its future development. Smart Lab concept includes not only automation of individual processes, creation of software subsystems integrated into a single network, different IoT elements, tools for perfect data collection, data analysis and processing, Paperless technologies, but also the launch of an educational and scientific platform on its basis. The educational and scientific platform needs for fast transfer and exchange of knowledge between research laboratory and industry. In this form, the laboratory is much better suited for use in the educational process. Since the visibility of studied processes themselves and the ability to use the data of experiments in training are increasing. It should also be noted that this approach provides a field of activity not only for specialists in the field of chemistry, physics, and materials science but also allows computer specialists to improve and develop their skills.

6. References

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