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**TRIPLET SUPERCONDUCTIVITY AS THE BASIS OF  
SUPERCONDUCTING SPINTRONICS.**

**133.04 – Solid state physics**

**Abstract of the PhD thesis**

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## CONCEPTUAL GUIDELINES OF RESEARCH

### Actuality and importance of the topic

The relentless miniaturization of microelectronic elements are the result of the major use of microelectronics in contemporary life. This is also a reason for the large – scale use of these elements because they have a very low power consumption, which is decisive in the economic context. At the present time the maximum number of elements per unit area has been reached, and already the response, computation, responsiveness and efficiency cannot be increased due to Joule and other interference effects. Spintronics - is a contemporary and current alternative that proposes new principles of utilizing quantum effects and phenomena - such as electron spin. The use of electron spin, as opposed to electron charge used in classical microelectronics, corresponds to a wide range of applications. Elements based on the spin effect are much more effective in terms of electricity consumption, are capable of performing logic operations at colossal speeds, and their use in various types of sensors opens up new areas of application such as artificial intelligence, SMART homes, driverless cars, etc. Elements that utilize electron spin are called spin valves. Spin valves are nanoscale layered structures of superconductors (S) and ferromagnets (F). In a multilayered S/F structure, quantum phenomena such as the proximity effect, wave function oscillation in the ferromagnet, inhomogeneous superconducting state - the LOFF state - occur. The superconducting state and ferromagnetism are mutually exclusive due to having completely different structures of spin configurations. In ferromagnetic the spins are oriented collinear while in superconducting-antiparallel. But notwithstanding this fact the calculations by Larkin and Ovchinnikov iclusiv Fulde and Ferrell show that in S/F structures the inhomogeneous superconducting state arises - when the sum momentum of the Cooper pair is non-zero. But the stable coexistence condition is made more difficult due to the limitation on the size of the exchange energy of the magnetic ordering - superconductivity in the presence of the exchange field  $E_{exc}$ , can be observed only in the range:  $0.75\Delta < E_{exc} < 0.76\Delta$ , where  $\Delta$  - the superconducting gap. On the other hand Buzdin and Radovici propose the idea of the existence of these two orders (superconductivity and ferromagnetism) in a multilayer structure composed of nanometer-thick layers of superconductors and ferromagnets that repeat, and in such a way the pair of elctrons penetrate into the ferromagnetic through the boundary: superconductor/ferromagnetic and form the superconducting par function in the ferromagnetic. Below the critical temperature  $T_c$ , the Cooper pairs from the superconductor due to the proximity effect penetrate into the ferromagnetic where they fall under the action of the exchange field  $E_{exc}$  and as a result these pairs have the sum momentum different from zero. For the nanoscale effects in these structures to be evident it is

necessary that the boundary between any two adjacent layers be atomically smooth. Experimentally it is shown that it is rather tedious to realize atomically smooth boundaries that are subsequently transparent to quantum phenomena.

### **Description of the situation in the research area and identification of the problems**

At the present time the need for memory volume and information processing speed reaches an inevitable maximum. Spin - fan structures as building blocks, based on layered superconductor - ferromagnetic nanostructures, are a firm way to solve this problem. Magnetron deposition of nanostructures presents by itself a very complex methodology that requires materials of the highest quality and contemporary laboratory equipment. One problem that has been solved with the help of mathematical modeling and later demonstrated experimentally is - the quality of adjacent interfaces of neighboring nanostructures. Due to atomically smooth interfaces between nanostructures it was possible to create the basic element - spin valve. Due to the different lattice structures of niobium and cobalt, which cause surface roughness, it is practically impossible to obtain atomically smooth interfaces, but numerical and laboratory experiments have shown that at certain temperatures of the silicon (Si) substrate it is possible to create atomically smooth interfaces with a roughness of only - 0.3 nm. In addition, the development of materials such as nano - layered materials - metamaterials - with specific properties, still allow a wide range of effects that can be used to solve switching problems. A metamaterial consisting of - **[Co(1.5nm)/Nb(8nm)/Co(2.5nm)/Nb(8nm)]<sub>6</sub>** proposes a switching effect at applied magnetic field only of 30 Oe. For this purpose, a spin valve core element was created for the first time, in which the artificial magnetic metamaterial was used.

### **The aim of the research**

The paper proposes a spin valve with memory effects that operates due to triplet superconductivity; and tuning the magnetron coating technology parameters in such a way as to achieve atomically smooth interfaces with minimal mutual material interdiffusion effects - the quality of adjacent interfaces plays a particular role at the quantum level in nanometer-thick structures.

## **The main objectives of the work**

- Optimization of magnetron deposition parameters of superconductor – ferromagnetic nanostructured magnetron with directed and strictly reproducible parameters in a single vacuum cycle,
- Mathematical modeling of the magnetron deposition technology parameters using the LAMMPS package for their adjustment,
- Study of the superconducting properties of nanometric layered structures with spin - valve effects and memory elements,
- Study of the behavior of magnetic states in adjacent ferromagnetic nanostructures using polarized neutron reflectometry - a method for observing spin orientation in magnetic materials.

## **Research hypothesis**

In order to create a new generation of neuromorphic computers with radically reduced power consumption, it is necessary to develop a nonlinear switching element - similar to a transistor, but unlike a transistor, which provides the transition from a state of high electrical resistance to a state of low resistance, the new element must provide the transition from a state of finite electrical resistance to a state of zero resistance, i.e. be a new switching element - a superconducting valve. This hypothesis is to be tested in this paper.

## **Scientific research methodology**

In order to achieve the research aim and objectives, the literature was studied and then the method of nanofilm deposition and characterization was used:

- vacuum machine - magnetron "LEYBOLD Z - 400" magnetron "LEYBOLD Z - 400" was used for the deposition of Nb/Co (superconducting/ferromagnetic) nanostrates,
- the morphological structure of nanostructures was investigated by scanning electron microscopy - SEM,
- transport characteristics in nanofilms were measured by the four-probe method,
- topography and roughness of the superconducting/ferromagnet nanofilms were investigated by MFA - atomic force microscopy,

- FIB (focused ion beam) was used to cut micropunctions at Josephson junctions,
- the special designs were lithographically etched in the Oxford Plasmalab 100,
- In order to determine the magnetron deposition parameters, computer modeling using the Modified Embedded Atom Method ( MEAM ) was used.

### **The scientific novelty and originality of the research**

The magnetron deposition technology of superconductor/ferromagnetic nanostructures with smooth atom – atom interfaces in which triplet-pairing has been recorded due to ferromagnetic nanostructures with nonlinear magnetizations has been optimized. A pseudo spin valve prototype as a novel switching element is proposed, in which the main role plays the triplet superconductivity, consisting of a superconducting superlattice.

**The solved scientific problems** consists in the optimization of magnetron deposition technology with smooth atomar interfaces and the formation of nanostructures for their use as novel memory elements, spin valves.

### **The theoretic significance and the applied value of the work**

- Based on the measurements of the transport characteristics of the superconductor/ferromagnetic, Nb/Co, hybrid structures, the memory element with sufficiently fast switching, parallel (P) and antiparallel (AP) orientations of the ferromagnetic films were realized,
- The spin valve prototype - S/F1/S/F2/AF, in superconductor/ferromagnet heterostructures is realized if at least two ferromagnetic layers (F1, F2) have a noncollinear alignment of their magnetizations - which generates the superconducting odd triplet component,
- In the theoretical field with the help of Molecular Dynamics and the Sunken Atom Model - MEAM, we have tuned the magnetron deposition parameters in order to improve the quality of the interfaces of the nanometric layers,
- Nanostrates magnetron deposition parameters that significantly contribute to the enhancement of adjacent interfaces with the enhancement of quantum effects have been experimentally detected, with the optimized temperature of the silicon substrate ( 300K ).

## Main scientific results submitted for defense

- ❖ The interdiffusivity of nanometer layers increases with increasing Si substrate temperature, which negatively manifests on superconducting quantum phenomena,
- ❖ Modeling using LAMMPS package shows that the optimal temperature for the deposition of superconducting/ferromagnetic nanostructures is 300 K of the Si substrate, in this sense the obtained interface maximally contributes to the amplification of quantum phenomena,
- ❖ Multilayer structure - S/[F1/s/F2/s]<sub>n</sub>/F1/S with reorientation characteristics of ferromagnetic layers, parallel (PA) to antiparallel (APA) in a low external magnetic field, 30 Oe may be used as a novel switching element spin valve.

## Approval of the scientific results

Research results have been presented at the following international and national conferences, and exhibitions:

1. National scientific conference " **Contemporary trends of science development: visions of young researchers** ", IX edition , Chisinau, Moldova, June 15, 2020,
2. International scientific conference " **8th International Conference on Functional Nanomaterials and High-Purity Substances** " FNM 2020, Suzdal, Russia, October 5 – 9, 2020,
3. International scientific conference " **The 12th international conference on intrinsic Josephson effect and horizons of superconducting spintronics** ", Chisinau, Moldova, October 22 – 25, 2021,
4. The international scientific conference " **Electronics, Communications and Computing** ", 12th Chisinau, Moldova, October 20 – 21, 2022,
5. National scientific conference " **Technical – scientific conference of students, master and PhD students** ", Chisinau, Moldova, IEN, April 5 – 7, 2023,
6. International Symposium XXIV, "Нанофизика и Наноэлектроника", April 26, 2022,
7. International Scientific Conference: NANO – 2024: " **Quo Vadis - Ethics of the Scientific Research** ", Chisinau. Moldova, April 15 – 18.

## Publications on the thesis topic

The basic research and studies in this thesis has been summarized in **15** scientific papers published in journals on the topic of the thesis; **5** articles in journals in SCOPUS and Web of



Science databases; **7** publications at national and international conferences; **4** single – authored articles, the list is presented at the end of this Abstract.

**The volume and structure of the thesis**

The thesis consists of an introduction, five chapters, general conclusions and bibliographical references consisting of **161** headings, presented on **112** pages of basic text, containing **56** figures, **6** tables.

**Keywords:** nanotechnologies, triplet superconductivity, spin valve, metamaterial, magnetron deposition, mathematical modeling.

## THESIS CONTENT

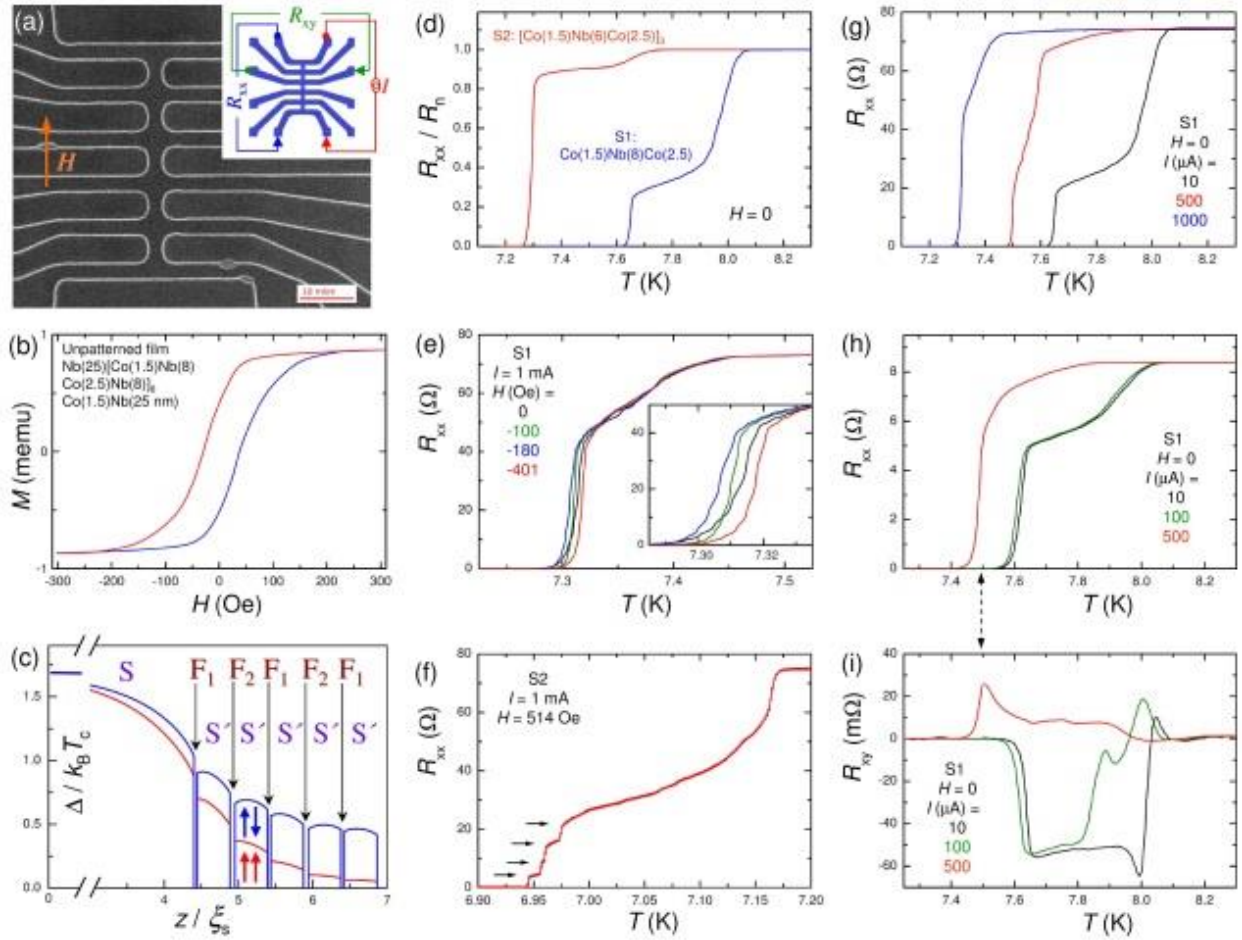
In the introduction, the research topic, the purpose and objectives of the thesis, the methodology of the scientific research, the scientific novelty and the results obtained, the scientific problem solved, the theoretical and applied significance of the thesis, the main scientific results submitted for defense, the approval of the scientific results, as well as the volume and structure of the thesis are presented.

**Chapter I:** consists of study and literature review of the field such as: Behavior of some materials at liquid helium temperatures and lower, basic properties of superconductors - zero resistance and magnetic field expulsion from the superconductor volume (Meissner effect), microscopic theory of Bardeen - Cooper - Schrieffer superconductivity, homogeneous singlet superconductivity, superconductor - normal metal proximity effect with superconducting singlet superconductivity intertwining in normal metal, Andreev reflection process.

**Chapter II:** experimental technique as well as technological methods of magnetron deposition of superconducting/ferromagnetic nanostructures, methods of measuring magnetic and transport characteristics, and morphological investigation of superconducting hybrid structures are presented. To achieve the basic objectives were used - the fundamentals of solid state physics, the basics of superconductivity. For the physical realization of spin valves and memory elements in a single high-vacuum cycle in Ar atmosphere, the vacuum machine - magnetron "LEYBOLD Z - 400" was used. The results were taken with LabView package and processed with PyMca, Origin, wolfram mathematica.

**Chapter III:** The Chapter III is focused on research directly related to: the superconducting-ferromagnetic proximity effect with the penetration of singlet superconductivity into ferromagnetic metal (described by the pioneering theoretical work Efetov - Volkov - Bergeret - Golubov, with the prediction of the possibility of the occurrence of non-uniform triplet superconductivity in superconducting/ferromagnetic structures), the experimental detection of the triplet superconductivity and the triplet spin valve effect; The main goal being the proposal of a prototype spin valve with subsequent use as a memory element, based on superconducting/ferromagnetic nanostructures. The competition between ferromagnetism and spin-singlet superconductivity leads to a variety of interesting phenomena, including the possible generation of odd frequency, the spin-triplet order parameter. In recent years, this exotic state has been extensively studied both theoretically [1-4] and experimentally [5-8] in various superconductor/ferromagnet (S/F) heterostructures. This phenomenon can be used to create new superconducting devices, in which the overcurrent ( $I_c$ ) is determined and controlled by the

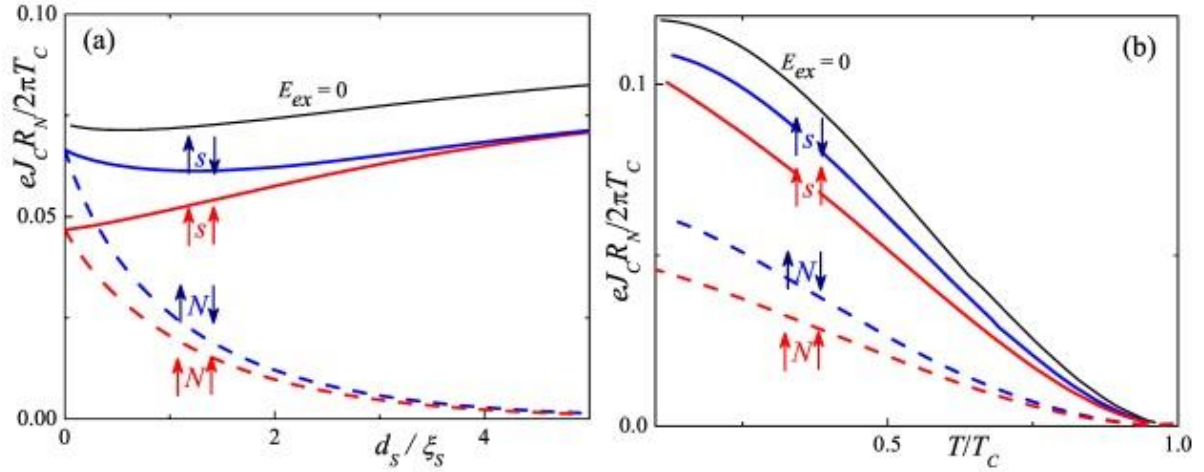
magnetic state of the heterostructure, i.e. by the relative orientation of the magnetizations in the several F – layers [5]. The situation is complicated by a variety of coexisting phenomena: **(a)** both singlet and triplet currents can flow through S/F heterostructures [9], **(b)** the overcurrent strongly depends on the usually unknown domain structure in F and the flux quantization in S, both influenced by the heterostructure size and geometry, **(c)** the spin – triplet overcurrent only occurs in the noncollinear magnetic state. Therefore, the utilization of this phenomenon for device applications requires the precise determination and control of the micromagnetic state of devices at the micro – or nanoscale. Similar control is required for the operations of a large number of superconducting spintronic devices, including memory elements and spin valves [10,11,12]. Figure 1.(c) shows a numerical simulation of the superconducting order parameter,  $\Delta$ , in an S/F heterostructure. This provides a qualitative understanding of the modulation of the proximity effect in heterostructures in the P (red) and AP (blue) states. A thick lower S layer, Nb (50 nm), acts as a Cooper pair reservoir and is only modestly affected by the magnetic orientation of the F layer. However, thin S' spacers, Nb (6 and 8 nm), with a thickness comparable to the superconducting coherence length,  $\xi_S \approx 10$  nm, are strongly affected. Superconductivity in the S' layers is strongest in the AP state and is nearly quenched in the outermost S' layer in the P state. This is caused by the subtractive (in the AP state) and additive (in the P state) influences of the exchange field in the neighboring ferromagnetic - F layers, which are detrimental to the spin-singlet order in S' [13,14]. The simulations in Fig. 1.(c) demonstrate the tunability of superconductivity in such S/F structures by changing the magnetic state. Due to the lower S layer, there is a  $\Delta$  gradient in the S' layers, implying that the S' layers have different superconducting properties. In all cases, the magnetic field is applied parallel to the planar film as shown in Fig. 1.(a). The multi – terminal geometry of the probes allows the simultaneous use of four probes measuring at different segments of the probe in both longitudinal directions,  $R_{xx}$ ,  $R_{xy}$ . When the current is sent through the central vertical bridge as sketched in Fig. 1.(a), the measurements correspond to the magnetization orientation in the direction of the long side of the vertical line. Alternatively, we can send current through the horizontal bridges, which corresponds to the magnetization orientation perpendicular to the long side of the bridge. In the latter case, the resistance the entire electrode is measured with four probes - a mode using two wires connected to each contact.



**Fig. 1. (a) SEM image of an Nb/Co multilayer with microdots. The sample contains twelve contacts, six horizontal and one vertical with widths of several micrometers (4 $\mu$ m).**

Fig. 1.(d) shows the dependences  $R_{xx}(T)$ , normalized by the normal – state resistance  $R_n(T \geq T_c)$ , for micropunctions at S1 (blue) and S2 (red) of the structures at  $H = 0$ . The resistances are measured at the intensity  $-I_{ac} = 10 \mu\text{A}$  for S1 and  $20 \mu\text{A}$  for S2, which correspond to approximately equal small current densities in both structures. Both structures show a double transition, which could be attributed to different critical temperatures in the S and S' layers,  $T'_c(S') < T_c(S)$ . Consistent with this assumption, the  $T'_c$  of S2 with layer  $S' = 6 \text{ nm}$  is lower than that of S1 with  $S' = 8 \text{ nm}$ . Figure 1.(e) shows the  $R_{xx}(T)$  curves for a horizontal bridge of sample S1 at four magnetic field strengths increasing sequentially with  $I_{ac} = 1 \text{ mA}$ . It is seen that the onset of resistivity at  $T \approx 7.3 \text{ K}$  is affected by the field. Digital superconductor devices have attracted increasing attention due to their unique energy efficiency and performance, as well as due to their compatibility in quantum computers and neuromorphic computers under development [15,16]. However, the lack of cryogenic memory elements (including synapses) with sufficiently fast switching between stable states and sufficiently low energy dissipation is still the main obstacle in this field. By utilizing competition and coexistence of superconducting (S) and ferromagnetic (F)

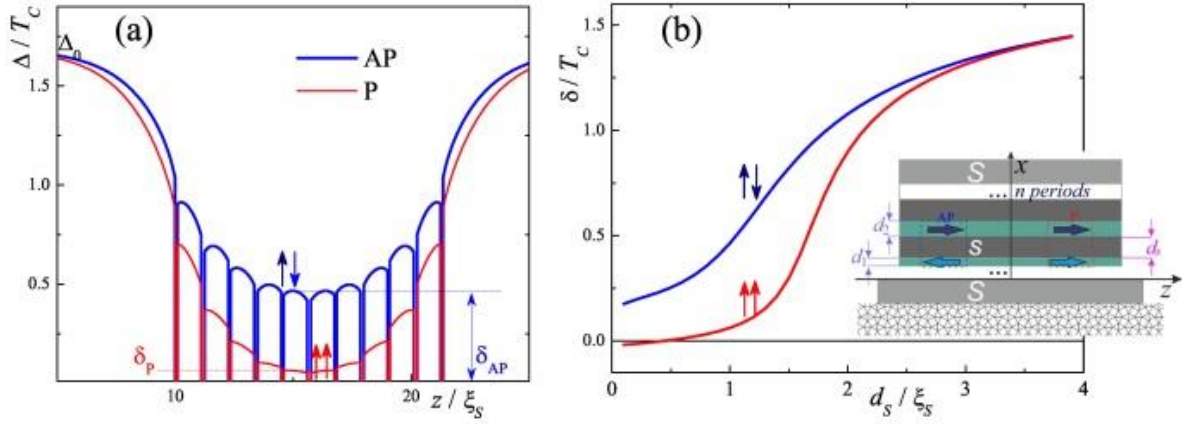
correlations we could provide an increase in performance and degree of integration for cryogenic memory storage devices and cryogenic memory and synaptic elements. These ideas can be implemented using a Josephson contact with two stable states: a high value of the critical current,  $I_c$ , corresponds to the "open" state and a low value - to the "closed" state. Such a device can be assembled if the "weak link" is a composite F/N/F tristructure (N is a normal metal) whose magnetic state can be switched between parallel and antiparallel directions of the magnetization vectors of the F layers. In contrast, the use of a thin superconducting layer as a spacer instead of a normal metal N layer can lead to an enhancement of the spin valve effect due to the proximity effect of thick superconductor layers and thin superconducting spacers [17]. To verify this hypothesis, we calculated the critical current of the Josephson junctions S/F/s/F/S and S/F/N/F/F/S (Fig. 2).



**Fig. 2. (a) Normalized critical current of S/F/s/F/F/S (solid lines) and S/F/N/F/F/S (broken lines) structures as a function of the thickness of the spacer layer between ferromagnets, and (b). Dimensionless temperature magnitude. The red lines are for the case where the exchange energies in both layers of the ferromagnet are equal in magnitude, and the magnetization vectors lying in the plane of the magnetic layers are parallel (P). The blue lines are for the case where the exchange energies -  $E_{exc}$ , in both layers F are equal in magnitude, and the magnetization vectors described are antiparallel (AP). The black curves correspond to the case where  $E_{exc} = 0$ .**

Moreover, for the AP orientation of the magnetization vectors of the F-layers, an additional mechanism for renormalization of the effective exchange energy arises, which leads to further decrease of the effective exchange energy. To confirm these claims, we generalized a S/[F/N] $n$  structure according to the model [18], in the case of the existence of superconductivity in its nonferromagnetic parts. In order to make the model more realistic, we consider a periodic spin -

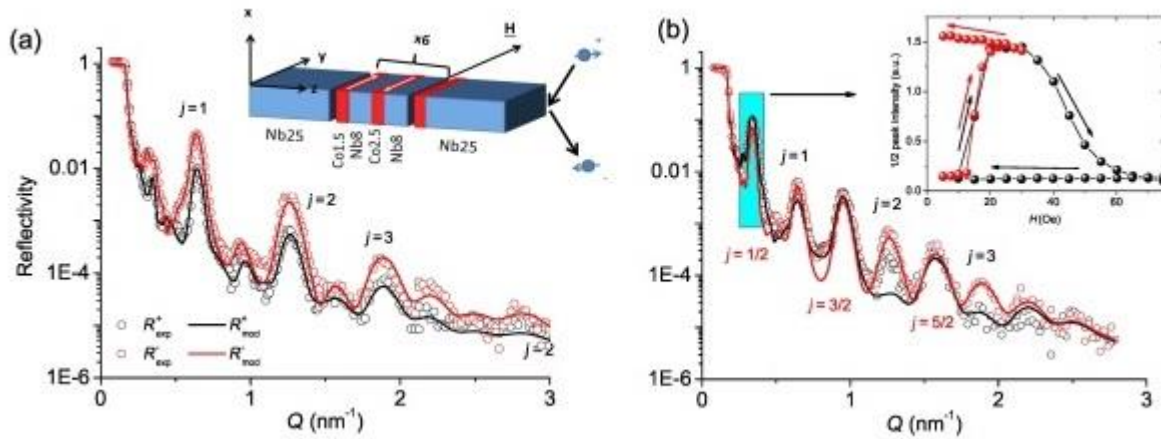
wave structure, in which two neighboring ferromagnetic layers have slightly different thicknesses  $d_1$  and  $d_2$  (inset in Fig. 3.(b)).



**Fig. 3. (a) Depth profile of the superconducting pair amplitude of the S/[F1/s/F2/s]n/F1/S structure in the P and AP cases. (b). Amplitudes of the superconducting pair amplitudes in the middle of the weak – bond for the P and AP alignments.**

The difference in thicknesses of the  $F_1$  and  $F_2$  layers gives a difference in their coercive fields  $H_{c1} \neq H_{c2}$  that allows an AP organization in the magnetic field diapason -  $H$ ,  $\max(H_{c1}, H_{c2}) > H > \min(H_{c1}, H_{c2})$  after saturation with negative-going magnetization. Using the concept of pseudo – spin – valve allows us to organize the AP alignment without exchange or magnetostatic coupling of neighboring F – layers. Figure 3.(a) shows the spatial distribution of Cooper pair amplitudes in the S/[F1/s/F2/s]n/F1/S structure for P and AP orientations. From Fig. 3.(a) shows that the structure considered is a series connection of Josephson s/F1/s and s/F2/s junctions with the weakest bond located in the middle of the structure. Figure 3.(b) shows the amplitudes of the Cooper pair potential,  $\delta_P$  and  $\delta_{AP}$ , ( $\delta_P$  and  $\delta_{AP}$  from Fig. 3.(a)) in the middle of the weak bond as a function of layer thickness  $s$ . It can be seen that the amplitudes for the AP and P configurations are significantly different for  $d_s \sim \xi_s$ . As soon as  $I_c$  is proportional to the product of the Cooper pair amplitude of the outer thick superconductors, it can be estimated that the ratio of  $I_c$  for the AP orientation and the P orientations is of order  $(\delta_{AP}/\delta_P)^2 \approx 25$ . From Fig. 3.(b) it follows that this enhancement depends on the ratio  $d_s/\xi_s$  and is maximum in the vicinity of  $d_s = \xi_s$ . The realization of the S/[F1/s/F2/s]n/F1/S structure as a Josephson device requires the development of a technology for fabricating multilayer structures that satisfies the following conditions: a) the presence of superconductivity in the s-layers at  $T_c \geq 4.2$  K, b) the in – plane orientation of the magnetization vector in the F films, and c) the ability of coherent switching between the P and AP configuration throughout the structure. These requirements can be met when using a combination of Nb and Co

as superlattice materials. To do this, we fabricated the structure – Nb(25 nm)/[Co(1.5 nm)/Nb(8 nm)/Co(2.5 nm)/Nb(8 nm)]<sub>6</sub>/Co(1.5 nm)/Nb(25 nm). Niobium was chosen as the superconducting material because it has the highest  $T_c = 9.25$  K of all elemental superconductors and forms stable structures with cobalt as the ferromagnet. The thickness of the Nb superconductor was chosen to be close to  $\xi_S \approx 6 - 10$  nm, the value found in previous studies. The thickness of the Co layers was in the range  $\xi_F \approx 1$  nm [19], which is sufficient to form a homogeneous and magnetic layer. For the structural characterization and magnetic ordering of the Nb/Co superlattice we used polarized neutron reflectometry (PNR). The measurements were performed at the NREX neutron reflectometer at the FRM – 2 research reactor (Munich, Germany). The neutron reflectance coefficients were measured using a polarized neutron flux of wavelength  $\lambda = 0.43$  nm at temperature  $T = 13$  K in the presence of the magnetic field, applied parallel to the plane of the nanostrate as well as perpendicular to the scattering plane Figure 4.a:



**Fig. 4. (a) Experimental reflectivity of specular neutrons (dots) measured at  $T = 13$  K in magnetic fields  $H = 300$  Oe and (b)  $H = 30$  Oe. The solid lines show the model curves for the magnetization depth profiles shown in Fig. 4.a. The numbers above show the corresponding order of the Bragg reflection from the periodic-superlattice structure [Co(2nm)/Nb(8nm)]<sub>12</sub>. The inset in (b) shows the field dependence of the  $j = 1/2$  peak shown by the blue rectangle in (b) – switching from P to AP alignment of cobalt layers magnetization appears at 30 Oe.**

**Chapter IV:** In this chapter I propose – mathematical model building and theoretical calculations of superconducting niobium – cobalt, cobalt – iron – niobium nanostructures using molecular dynamics - mathematical modeling of adjacent interfaces between two nanometric layers with the aim of improving the quality of their interface. The molecular dynamics method is based on the concept of potential, which is responsible for the nature and character of the interactions of

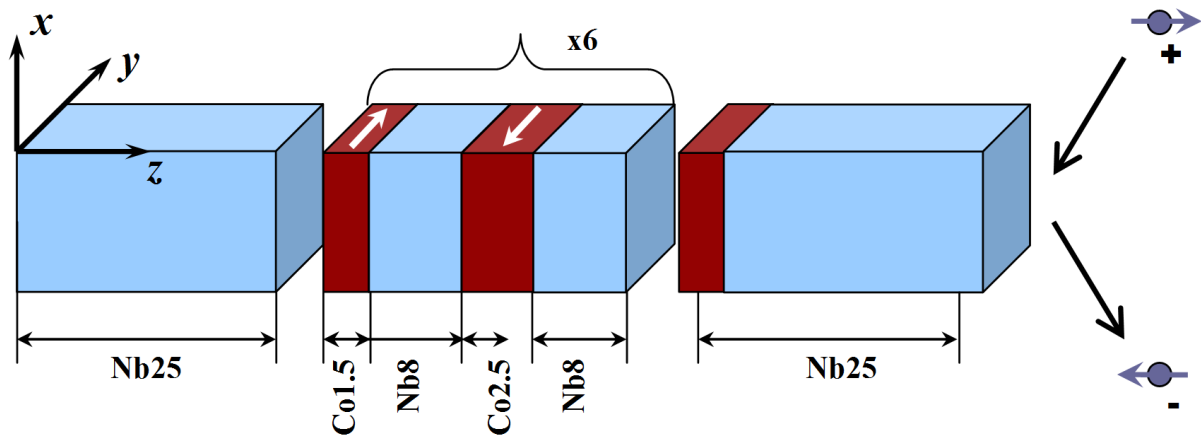
nanosystem atoms. We used the potential of the **Modified Embedded Atom Method – MEAM**. The modified embedded atom method is based on the Density Functional Theory (DFT). In this method, the resulting potential of the nanosystem is represented as the sum of the energy contributions of individual atoms, and the contributions of pairwise and multi-element interactions are considered separately. The **LAMMPS (Large – scale Atomic/Molecular Massively Parallel Simulator)** computational complex was used as the computational module of the program for theoretical research. The results were visualized using the **VMD (Visual Molecular Dynamics)** and **OVITO (Open Visualization Tool)** software packages, which provide images of atomic and molecular nano-object structures, as well as construct profiles and spatial distributions by target parameter such as height or coordination number. The resulting potential of the nanosystem is represented as the sum of the energy contributions of individual atoms, and the contributions of pairwise and multi-element interactions are considered separately.

$$U(r) = \sum_i U_i(r) = \sum_i \left( F_i(\bar{\rho}_i) + \frac{1}{2} \sum_{j \neq i} \phi_{ij}(r_{ij}) \right), \quad i = 1, 2, \dots, N, \quad (1)$$

where  $U_i(r)$  - is a potential of an individual atom, which influences the type and degree of interaction in the equations of motion (1);  $F_i$  - is the atomic immersion function, dependent on the electron background density;  $\bar{\rho}_i$ ;  $\phi_{ij}(r_{ij})$  - is a contribution of the pair potential to the total energy, which varies with distance.

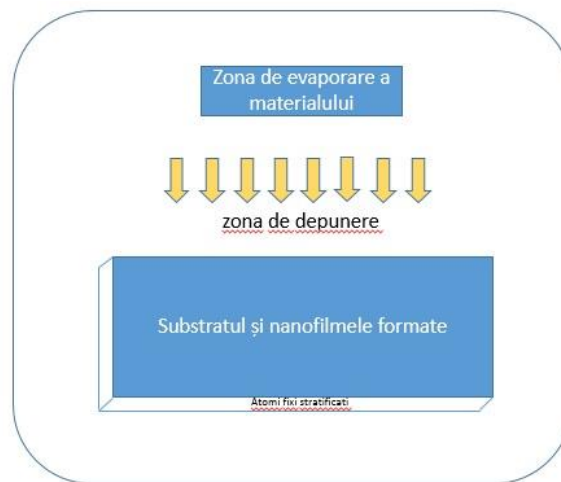
The influence of the parameters of the "superconducting/ferromagnetic" formation processes of the hybrid structures of the spin valve system is studied for a multilayer nanosystem based on cobalt and niobium. This system is a functional material that has demonstrated a gigantic spin valve effect. A new design was proposed and the calculation was carried out of a spin valve consisting of superconducting plates and an artificial magnetic metamaterial placed between them, formed by the periodic alternation of thin and thick layers of a ferromagnetic metal. The thickness of the layers affects the magnetic exchange interaction between the ferromagnetic layers, which offers the possibility of designing artificial magnetic metamaterials with tunable properties. The choice of niobium and cobalt as nanolayer forming metals is due to the wide potential of using these elements in spintronics.





**Fig. 5. Sketch of a Nb/Co spin valve nanosystem (Nb25nm/[Co1.5nm/Nb8nm/Co2.5nm/Nb8nm]<sub>6</sub>/Nb25nm ) modeled on the computer.**

The numbers in figure 5 next to the elements in the layers show their thickness in nanometers. The production of samples is carried out by the magnetron deposition method of vacuum materials. In general, a nanosystem contains about 20 layers. In this modeling, we consider the deposition of only the first four layers of cobalt and niobium. The general formulation of the problem of modeling the processes of formation of multilayer nanosystems is presented in figure 6. The first material layer formed by single – crystal niobium atoms serves as a substrate and basis for the vacuum deposition of subsequent nanofilms.



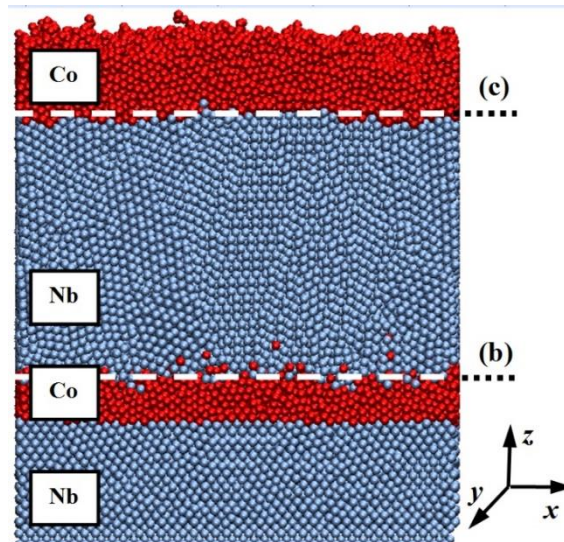
**Fig. 6. Schematic of the modeling processes of the formation of multilayer nanosystems. The nanosystem contains a material evaporation zone, an atom deposition zone, a substrate with a fixed lower layer of atoms.**

The substrate is placed in the lower region of the computing cell; its extreme layer is fixed to prevent chaotic movement of the sample during the simulation. In horizontal directions, periodic boundary conditions are imposed on the computational cell, which reduce the computational time.

In the upper region, boundary reflection conditions are present so that the deposited atoms do not leave the modeling system. The deposition process is simulated by the appearance of atoms in the evaporation zone above the substrate. In this case, the deposited atoms gained speed towards the substrate. The layers are sprayed in stages. During the formation of all layers, the magnetic field in the nanosystem was absent. The temperature and pressure for the deposited atoms are regulated. The deposited atoms are imprinted with an initial velocity of about  $0.1 \text{ \AA/ps}$  or toward the substrate surface. Subsequently, the speed of these atoms gradually decreases due to the energy exchange with the surface atoms of the substrate and the upper atom layers of the formed nanolayers. The substrate temperature in each calculation is held constant. The concentration of deposited atoms was about 5 atoms per cubic nanometer. The upper limit of the calculation cell was shifted during the transition to the deposition of the next nanolayer by its thickness value. Thus, the deposition region above the substrate was found to be approximately the same for each nanosystem layer. The regulatory parameters of the process, which affect the properties of the resulting nanomaterials, were: the deposition rate, controlled by the number of atoms deposited per unit of time; substrate temperature; the spray flux density, which was determined by the area of the evaporation zone. As the calculation mode of the program for theoretical research, the **LAMMPS** (**L**arge – **s**cale **A**tomic/**M**olecular **M**assively **P**arallel **S**imulator) calculation complex was used [158]. This software and tools package is freely distributed, contains the ability to perform parallel calculations, and supports multilevel mathematical models, including molecular dynamics. Algorithms for analyzing the results were described in TCL and C++. Based on LAMMPS, scripts and algorithms were developed and implemented for a detailed study of the structure of superconducting–ferromagnetic materials and the determination of its spatial profile. The results were visualized using the software packages **VMD** (**V**isual **M**olecular **D**ynamics) [20] and **OVITO** (**O**pen **V**isualization **T**ool) [21], which not only provide images of the atomic and molecular structures of nano-objects, but also construct profiles and spatial distributions through target parameter, eg height or coordination number.

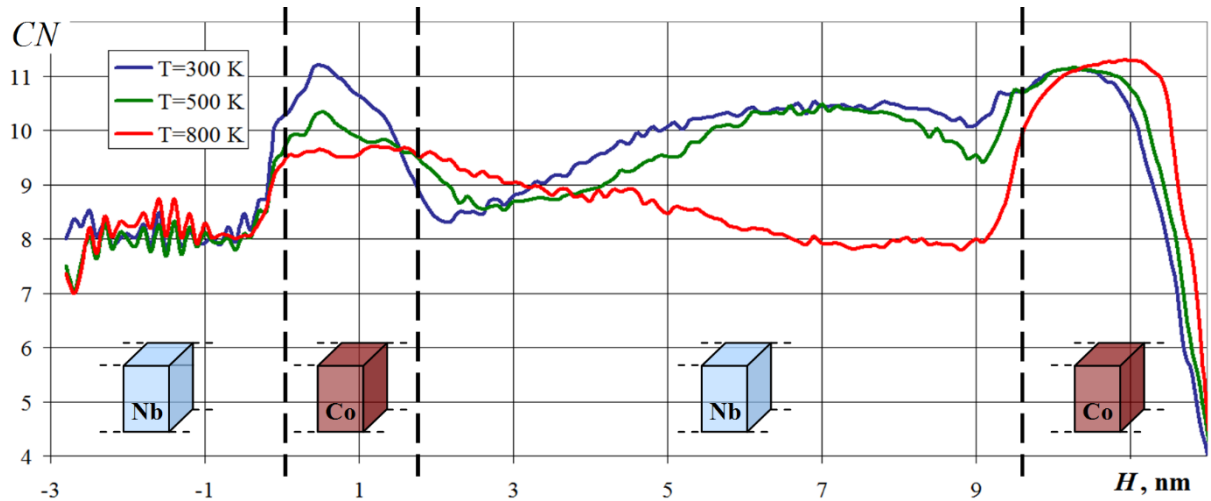
**Chapter V:** a series of numerical experiments were performed on the modeling of the formation processes of the multilayer hybrid structure based on cobalt, iron and niobium. The variable elements in the numerical experiments were the technological parameters of the material fabrication, including the substrate temperature, the intensity and the area of the deposition flow. The influence of the technological modes was evaluated in comparison with the basic version of the formation of nanosystems. As a basic variant, the growth processes were considered at the normal temperature, 300 K (substrate temperature), and the deposition was performed by a

uniform flow over the entire surface of the substrate. The temperature in the nanosystem was controlled using a Nose – Hoover thermostat. Another series of numerical experiments was performed on an MRAM memory element. The formed nanofilm is deposited, with height differences of a few angstroms. This effect can be explained by stronger interaction forces that occur between niobium atoms compared to other types of atoms considered. The analysis of the system shows that the Co – Fe layers did not undergo significant restructuring and their structure remained predominantly crystalline. S – performed a series of numerical experiments on the modeling of the formation processes of the multilayer hybrid structure based on Co and Nb. In the first step, Co was deposited on a substrate consisting of Nb atoms. The substrate had a crystalline structure with a height of 3.7 nm and a width of 13.2 nm in horizontal directions. For the zero height landmark, from which the layers of deposited material began to form, the surface of the substrate was chosen. The number of Nb atoms in the substrate was 33600. To match the simulation results and experimental data, as well as the formation of nanolayers of the required thickness, 18000 Co atoms were deposited on the substrate in the first step, 70000 Nb atoms were deposited in the second and 30000 Co atoms were deposited in the third step. As a result, three nanofilms with the thickness of 1.5 nm, 8 nm and 2.5 nm were formed. The duration of all three-layer deposition steps for the basic version of the sample preparation under normal conditions was chosen according to their thickness and was 0.2 ns, 0.6 nm 0.4 ns. The image of a multilayer nanosystem formed as a result of mathematical modeling is presented in fig. 7:



**Fig. 7. Nb/Co multilayer nanosystem. The contact points of the nanofilms are indicated by the letters (b) and (c). At the indicated contact points, the distribution of coordination numbers will be plotted below. The substrate temperature is fixed at 300 K.**

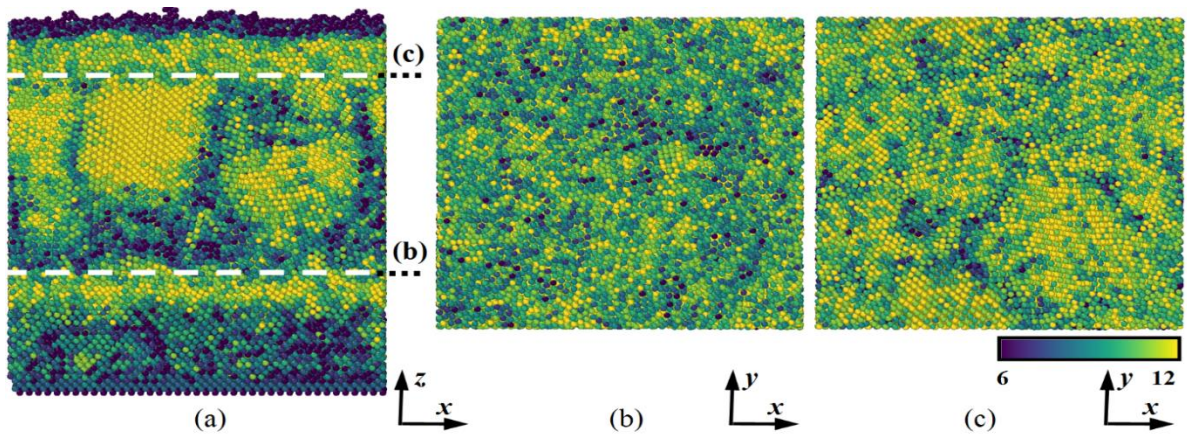
The image in fig. 7 clearly demonstrates the formation processes of the Nb and Co layered nanosystem and the structure of the layers: the layers formed by Nb and Co atoms have a polycrystalline structure. In this case, groups of atoms are combined into domains with different spatial orientations. Blurring of the contact area between the layers and a less uniform surface profile compared to Nb is observed. A quantitative characteristic of the spatial structure of the material can be obtained by calculating the coordination number. The coordination number reflects the number of close atoms of the same type in the crystal lattice. The number of nearest neighbors determines the packing density of the material. For different types of crystal lattices, the coordination number will be different. The centered cubic lattice (characteristic Nb) has a coordination number equal to 8, the compact hexagonal lattice (corresponds to Co) – 12. For the nanosystem formed, the change in the average value of the coordination number in the layers were calculated - fig. 8. The Nb substrate has a parameter value close to 8, which indicates its crystalline structure. Co nanofilms are characterized by – an increased coordination number in the range of 10 – 11. This value does not reach 12, which corresponds to the ideal crystalline state of a hexagonal network, which indicates an amorphous structure of Co nanofilms. Variations of the coordination number in the layer intermediate of Nb are more significant. When we approach the contact regions with Co, an increase in this parameter is observed, fig. 8:



**Fig. 8. Coordination number (CN) change along the Z-axis (shown in Fig. 7) in the Nb and Co layers of the nanostructure. The contact points of the nanofilms are shown by vertical lines. The distribution is plotted for the cases of deposition on substrates at temperatures of 300, 500 and 800 K.**

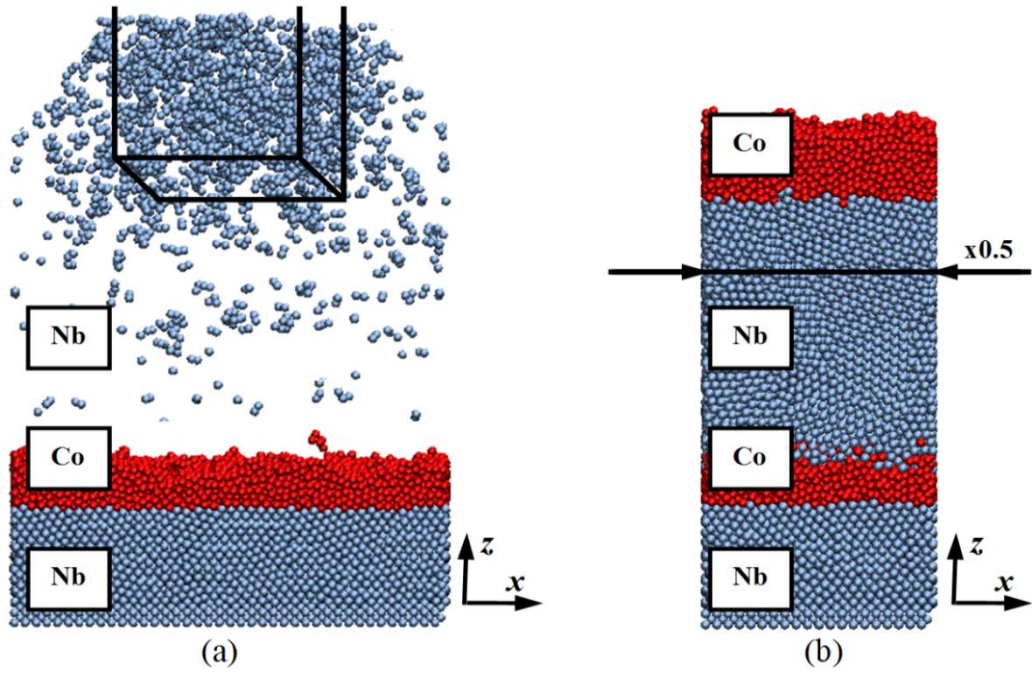
Thus, it was shown that the structure of the nanomaterial depends not only on the actual characteristics of the layer, but also on the structural characteristics of the regions adjacent to it. In addition, temperature has a clear effect on the number of nearest neighbors in a nanosystem and therefore on its structure and properties. A significant decrease in the coordination number in the

outer layers of the last nanofilm is associated with surface effects and the occurrence of boundary phenomena in that region. The distribution of this parameter in space is shown in fig. 9:



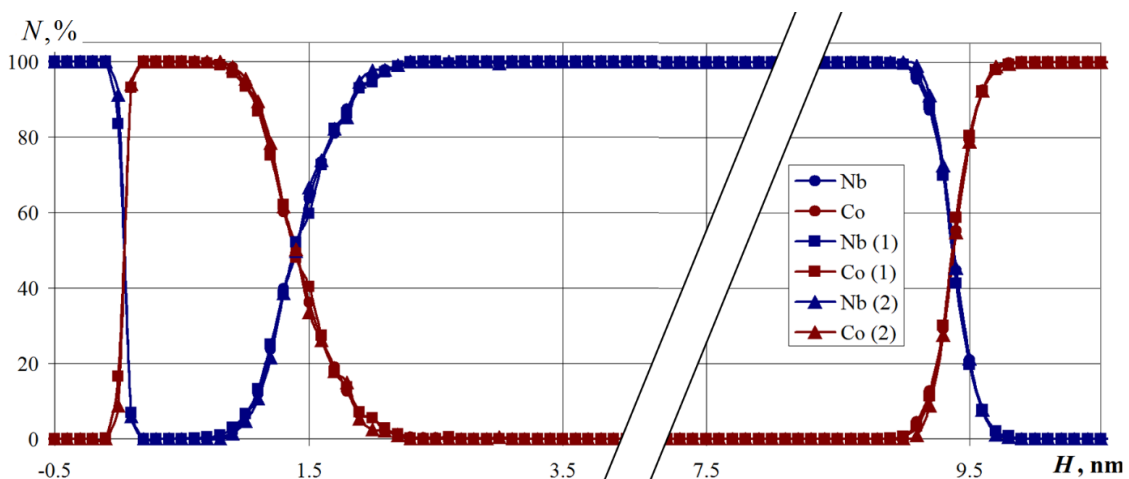
**Fig. 9. (a) Spatial distribution of the coordination number in the formed Nb – Co multilayer system (a) and in its parallel sections (b) and (c). Substrate temperature 300 K.**

The spatial distribution of the coordination number in the multilayer nanocomposite, illustrated in fig. 9, characterizes its structure in detail. The dotted lines in fig. 9 indicates the locations of the parallel sections shown in fig. 9.(b) and 9.(c). The sections correspond to the contact areas of the nanolayers and are also marked in fig. 7. The color profile of the coordination number confirms its increased value for Co layers. The value of the parameter in these layers is variable, with a spread in a certain range of values. The Nb substrate has a lower coordination number. The structure of this region was initially crystalline and changed insignificantly during modeling and deposition. An interesting effect is observed in the intermediate niobium nanolayer, where distinct crystallization zones have appeared. Crystallization zones have a higher coordination number and are characterized by a denser pack of atoms. The described regions appear in sufficiently thick films, mainly near the Co layers. The mismatch of the crystal lattices in the initial metals causes mutual rearrangements of the atoms and the transformation of the structure inside the material. The next series of experiments addressed the influence of the deposition flow area and patterning region size on the structure and morphology of the simulated layered nanosystem. Fig. 10 shows these parameters of the nanosystem:



**Fig. 10. Deposition flow area (a) and simulation area size (b). The deposition flow area is shown at the top of figure (a) with black lines. The reduction of the computational domain in figure (b) is illustrated by the factor  $x0.5$  in the horizontal directions.**

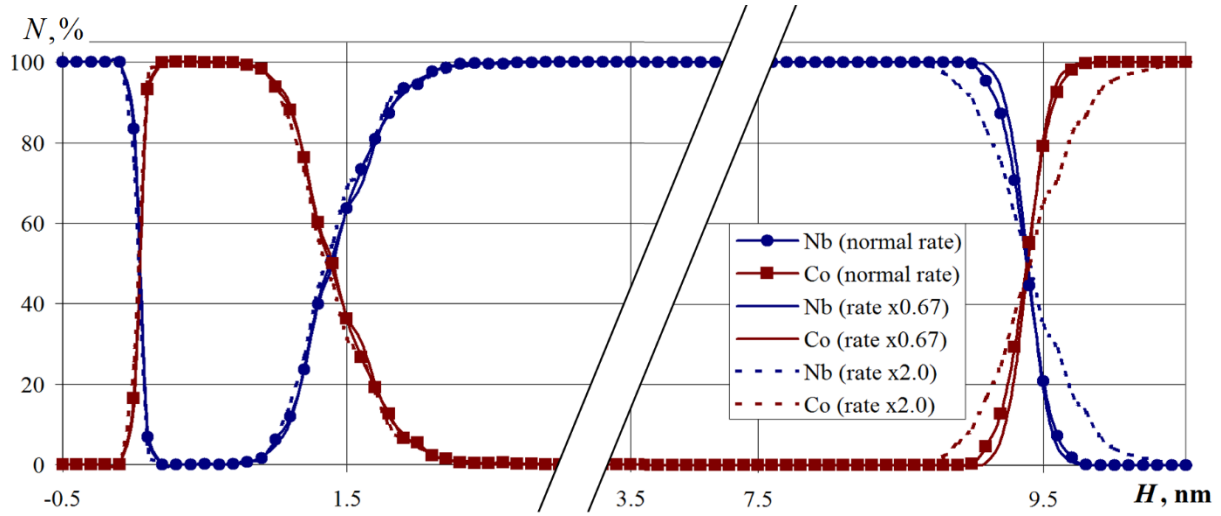
The modification of the deposition flow area, illustrated in fig. 10.(a), was performed by reducing the evaporation area of the raw materials shown in the upper region of this figure. The spray flow area was reduced four times from the original value. Also, the modeling of nanocomposite formation processes was carried out on a 4-fold reduced scale. In this case, the number of atoms deposited in each layer was proportionally reduced, so that the thickness of the formed nanofilms did not change.



**Fig. 11. Relative layer-by-layer composition of the Nb–Co nanosystem for the 4-fold reduced deposition flux (1) and the 4-fold reduced patterning area (2). The parameter N is the percentage of Co and Nb in the horizontal nanofilm layers. The substrate temperature is 300 K.**

The influence of the deposition flow area and patterning region size on the relative composition of the layer-by-layer nanosystem is shown in Fig. 11. Dependencies without index in parentheses correspond to the basic mode of nanosystem formation. Analysis of the graphs shows that the change in the studied range of a decrease in evaporated metals and a decrease in the calculated region, do not lead to rearrangements of the active atoms and to the change in the composition of the nanolayers. A decrease in the deposition flow area only led to the appearance of the area of increased atomic density in the upper region above the substrate. Leaving the evaporation zone, the deposited atoms tend to occupy an energetically more favorable state and are spread over a uniformly distributed layer over the entire free volume. When the deposited atoms reach the surface of the substrate, the flux reduction effect is leveled off. A decrease in the transverse dimension of the nanosystem by a factor of 4 also did not affect the composition of the nanosystem layers, which can be seen in fig. 11. The dependences of the Nb and Co fractions differ slightly from the basic version of the nanosystem formation. Changing the size of the simulation area allows us to analyze the representativeness of the computational cell. Small computational domains can lead to wrong simulation results due to the appearance of boundary effects. As results from the calculations, a four-fold decrease in the volume of the nanosystem did not affect the composition of the nanocomposite layers. The layers are connected in the same places, and the dependences of the proportions of Nb and Co differ slightly from the main variant of the sample formation. The obtained data indicate that the initially selected modeling area fully meets the requirement of representativeness, and the research results appropriately reproduce the properties of the modeled nanosystem. The following series of computational experiments was aimed at elucidating the degree of dependence of the structure of the multilayer nanosystem on the flux density of the deposited atoms. This value is controlled by an increase or decrease in the number of deposited atoms per unit time introduced into the system from the evaporation zone. Here, variants of the numerical experiments on the formation of nanofilms with a 2 – fold increase and a 1.5 – fold reduction of the flux density of the deposited atoms are calculated. The relative layered composition of the nanocomposite for calculations is shown in fig. 11. Here, the fraction of elements in the composition during the formation of nanolayers with a 1.5 – fold reduced deposition rate is shown by solid lines without markers, with increased intensity with dots, lines without markers, and the intensity of the base atom deposition by solid lines with markers. The

dependence analysis in fig. 12 shows that a decrease in the metal deposition rate did not significantly affect the compositional distribution in the layers of a multilayer nanosystem.

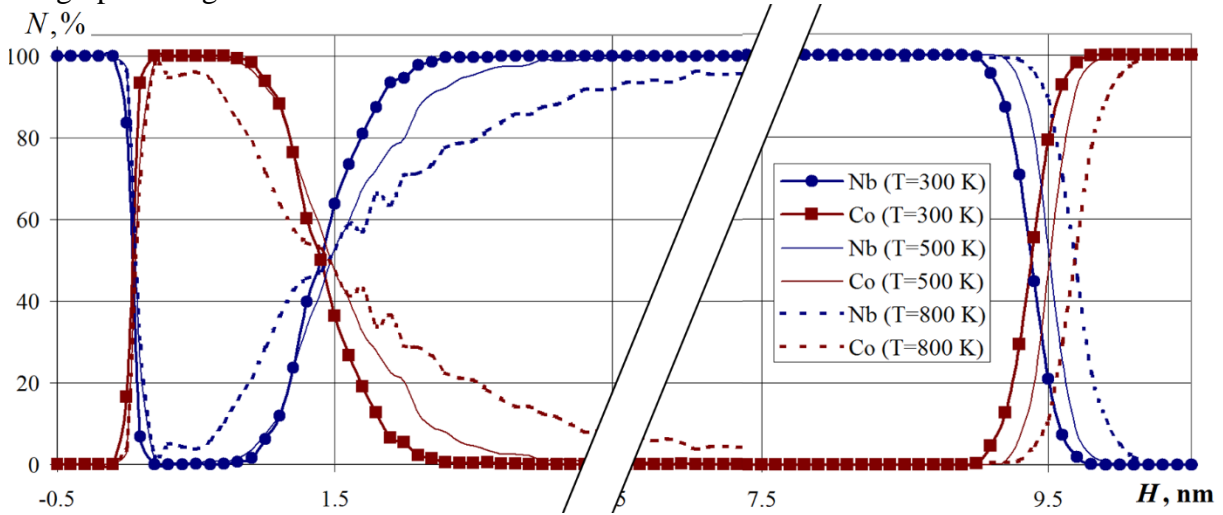


**Fig. 12. Layered relative composition of the Nb – Co nanosystem for different deposition rates. The parameter N is the percentage of Co and Nb in the horizontal nanofilm layers. The substrate temperature is 300 K.**

An increase in speed led to a deviation of the composition from the data obtained in the basic version of the calculation. A significant increase in flux intensity leads to the fact that metal atoms begin to agglomerate into nanoparticles above the surface of the substrate. The structure of the resulting nanofilms directly depends on the size of the deposited clusters and does not always have time to rebuild upon direct contact with the surface. Due to these effects, inhomogeneities, dislocations and voids may appear in the material. The deviation in the compositional dependencies built in the upper layers of the nanocomposite, where due to a more rarefied structure, the additional mixing of the contact regions with the nanofilms is especially noticeable. The studies conducted indicate the presence of a certain critical rate of deposition, the excess of which leads to a different structure of the nanomaterials. Since in real technological processes the deposition is carried out with a sufficiently low intensity (about 1000 nm per hour), in order to obtain physically appropriate research results, the deposition processes must be simulated at a speed that does not exceed this critical value. On the other hand, it is not necessary to increase the duration of the nanofilm growth stages, approximating as much as possible its real value, since, according to the graphs in fig. 4.5, the structure and composition in this case are similar. A series of computer experiments was carried out in which the formation of Nb – Co multilayer nanosystems was studied in the temperature range 300 – 800 K, for substrate temperatures of 300, 500 and 800 K, respectively. The simulation results are presented in fig. 12 in the form of a



percentage compositional graph of this nanosystem. The calculations showed that the temperature of the substrate significantly affects the formation of the nanosystem structure. An increase in temperature leads to an increase in the total thickness of the nanosystem (at 800 K, this value increased by 0.3 nm compared to a temperature of 300 K). The region of mutual penetration of Nb atoms into the layers of the Co system, and vice versa, is also increasing, which is clearly seen in the graphs in fig. 13:



**Fig. 13.** Percentage composition of the Nb–Co multilayer nanosystem formed at a substrate temperature of 300, 500, and 800 K, respectively. The parameter  $N$  is the percentage of Co and Nb in the horizontal nanofilm layers.

## GENERAL CONCLUZIONI AND RECOMMENDATIONS

1. The Nb/Co, Co/Fe/Nb superconducting structures must not be formed of immiscible metals to avoid island – like growth of film nanolayers due to their mutual non-wetting at the interface.
2. Following the optimization of the technological parameters of magnetron deposition, it was possible to deposit nanolayers with atomically smooth interfaces, in a single vacuum cycle, in an Ar atmosphere.
3. X – ray analysis of the superconducting/ferromagnetic structures interfaces showed the high quality of the interfaces with roughness up to 0.3 nm.
4. An analysis of the coordination number distribution in the material showed that the layers have a different structure when multilayer nanofilms are formed under normal conditions. Co nanofilms are characterized by an amorphous structure. The mismatch of the networks of the initial metals causes mutual rearrangements of the atoms and the transformation of the structure inside the nanosystem.
5. A decrease of the deposition flow area and the simulation region by 75 % of the initial values does not lead to atom rearrangements and a change in the composition of the nanofilms. A decrease in the deposition flow area caused the appearance of the area of increased atomic density in the upper region above the substrate.
6. A significant increase in the intensity of the deposition flow leads to the appearance of inhomogeneities, dislocations and voids inside the formed nanosystem, due to the preliminary grouping of free atoms.
7. As the main result, the basic element was proposed - the spin valve with artificial magnetic metamaterial in which triplet superconductivity plays the main role.

## RECOMMENDATION

1. With the help of molecular dynamics and the immersed atom model – MEAM, the magnetron deposition parameters were adjusted in order to improve the quality of the interfaces of the adjacent nanometer layers, which significantly contributes to the improvement of the adjacent interfaces with the enhancement of quantum effects, so it is recommended to deposit the structures at temperature of 300 K of the silicon substrate.
2. It is recommended to apply the artificial metamaterial composed of the nanolayers: [Co(1.5 nm)/Nb (8 nm)/Co (2.5 nm)/Nb (8 nm)]<sub>6</sub> as the weak link of the spin-valve base element .
3. The configuration of superconducting/ferromagnetic nanolayers that makes up the weak link of the basic spin-valve element provides the difference of the superconducting pair amplitude up to  $\Delta/T_c = 0.5$  at P and AP alignments of the neighboring ferromagnetic layers magnetization.
4. A weakly coupled Josephson junction composed of an artificial magnetic metamaterial can be switched between the parallel and antiparallel magnetic states by applying a small field of 30 Oe, which gives the closed or open state of this base element.

## BIBLIOGRAPHY

1. GORKOV, L.P. *Microscopic Derivation of the Ginzburg – Landau Equations in the Theory of Superconductivity*. În: Soviet Journal of Experimental and Theoretical Physics, 1959, 36, 1364.
2. FROLICH, H. *Theory of the Superconducting State. The Ground State at the Absolute Zero of Temperature*. În: Physical Review, 1950, vol. 79, 845.
3. COOPER, L. N. *Bound Electron Pairs in a Degenerate Fermi Gas*. În: Physical Review, 1956, 104, 1189–1190. <https://doi.org/10.1103/PhysRev.104.1189>.
4. De GENNES, P. G. *Boundary Effects in Superconductors*. În: Reviews of Modern Physics, 1964, vol. 36, p. 225–237. <https://doi.org/10.1103/RevModPhys.36.225>.
5. BELL, C., BURNELL, G., LEUNG, C. W., TARTE, E. J., KANG, D.J., BLAMAIRE, M. G. Controllable Josephson current through a pseudospin–valve structure. În: Applied Physics Letters, 2004, vol. 84, p. 1153–1155. doi:10.1063/1.1646217.
6. ROBINSON, J. W. A., HALASZ, G. B., BUZDIN, A. I., BLAMIRE, M. G. Enhanced Supercurrents in Josephson Junction Containing Nonparallel Ferromagnet Domains. În: Physical Review Letters, 2010, vol. 104, 207001. doi:10.1103/physrevlett.104.207001.
7. LEKSIN, P. V., GARIFIANOV, N. N., GARIFULLIN, I. A., SCHUMANN, J., KATAEV, V., SCHMIDT, O. G., BUCHNER, B. Manifestation of New Interference Effects in a Superconductor–Ferromagnet Spin Valve. În: Physical Review Letters, 2011, vol. 106, 067005. doi:10.1103/physrevlett.106.067005.
8. ZDRAVKOV, V. I., KEHRLE, J., OBERMEIER, G., LENK, D., KRUG von NIDDA, H. A., MULLER, C., KUPRIYANOV, M. Y., SIDORENKO, A. S., HORN, S., TIDECKS, R., TAGIROV, L. R. Experimental observation of the triplet spin–valve effect in a superconductor–ferromagnet heterostructure. În: Physical Review B, 2013, vol. 87, 144507. doi:10.1103/physrevb.87.144507.
9. SOSNIN, I., CHO, H., PETRASHOV, V. T., VOLKOV, A. F. Superconducting Phase Coherent Electron Transport in Proximity Conical Ferromagnets. În: Physical Review Letters, 2001, vol. 96, 570026. DOI: [10.1038/srep00699](https://doi.org/10.1038/srep00699).
10. BAEK, B., RIPPARD, W. H., BENZ, S. P., RUSSEK, S. E., DRESSELHAUS, P. D. Hybrid superconducting–magnetic memory device using competing order parameters. În: Nature Communication, 2014, vol. 5, 3888. doi:10.1038/ncomms4888.

11. GLICK, J. A. AGUILAR, V., GOUGAM, A. B., NIEDZIELSKI, B. M., GINGRICH, E. C., LOLOEE, R., PRATT, W. P., BIRGE, N. O. Phase control in a spin – triplet SQUID. *În: Science Advances*, 2018, vol. 4, p.1-7. doi:10.1126/sciadv.aat9457.
12. KAPRAN, O. M., IOVAN, A., GOLOD, T., KRASNOV, V. M. Observation of the dominant spin–triplet supercurrent in Josephson spin valve with strong Ni ferromagnets. *În: Physical Review Research*, 2020, vol. 2, 013167. doi:10.1103/physrevresearch.2.013167.
13. BUZDIN, A. I., VEDYAYEV, A. V., RYZHANOVA, N. V. Spin–orientation–dependent superconductivity in F/S/F structures. *În: Europhysics Letters*, 1999, vol. 48, p. 686–691. doi:10.1209/epl/i1999-00539-0.
14. ESCHRIG, M. Spin–polarized supercurrents for spintronics: a review of current progress. *În: Reports on Progress in Physics*. 2015, vol. 78, 104501. doi:10.1088/0034-4885/78/10/104501.
15. SCHNEIDER, M. L., DONNELLY, C. A., RUSSEK, S. E. Tutorial: High–speed low–power neuromorphic systems based on magnetic Josephson junction. *În: Journal of Applied Physics*, 2018, vol. 124, 161102. doi:10.1063/1.5042425.
16. SCHEGOLEV, A. E., KLENOV, N. V., SOLOVIEV, I. I., TERESHONOK, M. V. Adiabatic superconducting cells for ultra–low–power artificial neural networks. *În: Beilstein Journal of Nanotechnology*, 2016, vol. 7, p. 1397–1403. doi:10.3762/bjnano.7.130.
17. BAKURSKY, S. V., KLENOV, N. V., SOLOVIEV, I. I., KUPRIYANOV, M. Y., GOLUBOV, A. A. Superconducting phase domains for memory applicatons. *În: Applied Physics Letters*, 2016, vol. 108, 042602. doi:10.1063/1.4940440.
18. BAKURSKIY, S. V., KUPRIYANOV, M. Y., BARANOV, A. A., GOLUBOV, A. A., KLENOV, N. V., SOLOVIEV, I. I. Proximity effect in multilayer structures with alternating ferromagnetic and normal layers. *În: JETP Letters*, 2015, vol. 102, p. 586–593. doi:10.1134/s0021364015210043.
19. OBI, Y., IKEBE, M., FUJISHIRO, H. Evidence for Zero–and  $\pi$ –Phase Order Parameters of Superconducting Nb/Co Tri–and Pentalayers from the Oscillatory Bahavoir of the Transition Temperature. *În: Physical Review Letters*, 2005, vol. 94, 057008. doi:10.1103/physrevlett.94.057008.
20. HUMPHREY, W., DALKE, A., SCHULTEN, K. VMD: visual molecular dynamics. *În: Journal of Molecular Graphics*, 1996, vol. 14, p. 33-38. doi:10.1016/0263-7855(96)008-5.
21. STUKAWSKI, A. Visualization and analysis of atomistic simulation data with OVITO–the Open Visualization Tool. *În: Modelling and Simulation in Materials Science and Engineering*, 2009, vol. 18, 015012. doi:10.1088/0965-0393/18/1/015012.

## LIST OF PUBLICATIONS ON THE TOPIC OF THE PhD THESIS

### Articles in journals from Web of Science and SCOPUS database with impact factor:

1. KARPAN, O., MORARI, R., GOLOD, T., BORODIANSKYI, E., **BOIAN, V.**, PREPELITSA, A., KLENOV, N., SIDORENKO, A., KRASNOV, V. In situ characterization of magnetic states in Nb/Co superconductor/ferromagnet heterostructures. În: *Beilstein Journal of Nanotechnology*. 2021, 12, 913–923. <https://doi.org/10.3762/bjnano.12.68>
2. SIDORENKO, A., MORARI, R., **BOIAN, V.**, PREPELITSA, A., ANTROPOV, E., SAVVA, Yu., FEDOTOV, A., SEVRYUKHINA, O., VAKHRUSHEV, A. Hybrid nanostructures superconductor-ferromagnet for superconducting spintronics. În: *Journal of Physics: Conference Series*, 2021, 1758, 012037. doi: [10.1088/1742-6596/1758/1/012037](https://doi.org/10.1088/1742-6596/1758/1/012037)
3. VAKHRUSHEV, A., FEDOTOV, A., **BOIAN, V.**, MORARI, R., SIDORENKO, A. Molecular dynamics modeling of the influence forming process parameters on the structure and morphology of a superconducting spin valve. În: *Beilstein Journal of Nanotechnology*, 2020, 11, 1776–1788. <https://doi.org/10.3762/bjnano.11.160>.
4. KLENOV, N., KHAYDUKOV, Y., BAKURSKIY, S., MORARI, R., SOLOVIEV, I., **BOIAN, V.**, KELLER, T., KUPRIYANOV, M., SIDORENKO, A., KEIMER, B. Periodic Co/Nb pseudo spin valve for cryogenic memory. În: *Beilstein Journal of Nanotechnology*, 2019, 10, 833–839. <https://doi.org/10.3762/bjnano.10.83>.
5. ALEXANDER, V., ALEKSEY, Yu F., OLESYA, S., ANASTASIA S., **VLADIMIR, B.**, ANATOLIE S. Numerical study of magnetic properties for Co-Fe-Nb nanofilms as promising materials for magnetoresistive memory. În: *Beilstein Archives*, 2024, 3, 28. <https://doi.org/10.3762/bxiv.2024.19.v1>

### Articles in conference proceedings and other scientific events

#### 2.1. in the works of scientific events included in the Web of Science and SCOPUS databases

6. **BOIAN VLADIMIR**, Modelarea proceselor de formare a valvei de spin supraconductoare bazate pe nanostructuri multistrat supraconductor-feromagnet. *Universitatea de stat Dimitrie Cantemir, Tendințe contemporane ale dezvoltării științei: viziuni ale tinerilor cercetători*, 2020, Ediția 9, Vol.1, 48–54. [https://ibn.idsi.md/ro/collection\\_view/700](https://ibn.idsi.md/ro/collection_view/700)
7. ANATOLIE, S., ROMAN, M., **VLADIMIR, B.**, EVGHENI, A., ANDREI, P., IURIE, S., NIKOLAI, K., IGOR, S., ALEXANDER, V. Nanostructures Superconductor/Ferromagnet for Superconducting Spintronics. "The 12th international conference on intrinsic Josephson effect and horizons of superconducting spintronics", Chișinău, Moldova, 2021, 22–25. [https://ibn.idsi.md/ro/collection\\_view/1566](https://ibn.idsi.md/ro/collection_view/1566)
8. **BOIAN, V.** Pregătirea și investigarea joncțiunii JOSEPHSON Nb/NiPt/Nb. *The 12th international conference on intrinsic Josephson effect and horizons of superconducting spintronics*. Chișinău, Moldova, 2021, 54–55. [https://ibn.idsi.md/ro/collection\\_view/1566](https://ibn.idsi.md/ro/collection_view/1566)
9. **BOIAN, V.** Determination of the critical thickness of Nb superconducting layers coupled proximiti with Co. *The 12th International Conference on Electronics, Communications and Computing*, 2022, 20–21, Chisinau, Republic of Moldova. [doi.org/10.52326/ic-ecco.2022/EL.08](https://doi.org/10.52326/ic-ecco.2022/EL.08)

10. LUPU, M., KLENOV, N., SOLOVIEV, I., BAKURSKIY, S., **BOIAN, V.**, MALCOCI, C., PREPELITSA, A., ANTROPOV, E., MORARI, R., SIDORENKO, A. Spintronic Functional Nanostructures for Artificial Neural Network. *International Conference on Electronics, Communications and Computing*, 2023, 20–21. [https://ibn.idsi.md/vizualizare\\_articol/177456](https://ibn.idsi.md/vizualizare_articol/177456).
11. **BOIAN, V.** Efectul de proximitate în microelectronica supraconductoare. *Conferința Tehnico-Științifică a Studenților, Masteranzilor și Doctoranzilor, Universitatea Tehnică a Moldovei*, 5-7 April, 2023, Vol. I, 270–273. ISBN 978-9975-45-957-0. [https://ibn.idsi.md/collection\\_view/2356](https://ibn.idsi.md/collection_view/2356).
12. SIDORENKO, A., KLENOV, N., SOLOVIEV, I., BAKURSKIY, S., **BOIAN, V.**, MORARI, R., SAVVA, Yu., LOMAKIN, A., SIDORENKO, L., SIDORENKO, S., SIDORENKO, I., SEVERYUKHINA, O., FEDOTOV, A., SALOMATINA, A., VAKHRUSHEV, A. Base Elements for Artificial Neural Network: Structure Modeling, Production, Properties. *International Journal of Circuits, Systems and Signal Processing*, 2023, Vol. 17, 177 – 18. DOI: [10.46300/9106.2023.17.21](https://doi.org/10.46300/9106.2023.17.21)
13. SIDORENKO, A., **BOIAN, V.**, ANTROPOV, E., SAVVA, Yu., LOMAKIN, A., VAKHRUSHEV, A. Functional superconductor–ferromagnet nanostructures for superconducting electronics. *Book of Abstracts JAPMED*, 2023, Vol. 12, 85–86. <https://japmed.bsu.edu.ge/index.php/japmed/issue/view/862/366>
14. **VLADIMIR, B.**, EUGEN, B. Using of the MEAM model for adjusting the technological parameters of magnetron deposition of Nb/Co nanolayers. *NANO-2024: “Quo Vadis – Ethics of the Scientific Research”*, 15 – 18. April 2024, Chișinău. <https://humboldt-kolleg.utm.md/>
15. VAKHRUSHEV, A., FEDOTOV, Yu., **BOIAN, V.**, SIDORENKO, A. Simulation of Multilayer Atom Nanostructures for Spinmechatronics. *Mechatronic Systems Design and Solid Materials*, 2021, pp. 187–203. ISBN 9781003045748.

## ADNOTARE

la teza cu titlul: “**Supraconductibilitatea tripletă ca bază a spintronicii supraconductoare**”, înaintată de candidatul Boian VLADIMIR pentru conferirea titlului științific de doctor în științe fizice la specialitatea 133.04 «**Fizica Stării Solide**».

**Structura tezei:** Teza înaintată spre susținere a fost realizată în cadrul Institutului de Inginerie Electronică și Nanotehnologii “D. Ghițu” al Universității Tehnice a Moldovei, Chișinău. Este scrisă în limba română și conține cinci capitole, concluzii generale, recomandări și bibliografie (161 de titluri) fiind expusă pe 112 pagini text de bază, conținând 56 de figuri, 6 tabele. Cercetările și studiile de bază în această teză au fost publicate în **15** lucrări științifice publicate în reviste la tema tezei; **5** articole în reviste din bazele de date SCOPUS și Web of Science; **7** publicații la conferințe naționale și internaționale; **4** articole cu un singur autor.

**Cuvinte cheie:** supraconductibilitatea tripletă, supapă de spin, elemente de memorie MRAM, depunere magnetron, modelare matematică.

**Scopul lucrării:** realizarea unei supape de spin ca element de bază nedisipativ pentru calculatorul supraconductibil, și ajustarea parametrilor de depunere magnetron a nanostructurilor de Nb/Co, într – un singur ciclu de vid cu interfețele adiacente atomar netede.

**Obiectivele cercetării:** optimizarea parametrilor tehnologici de depunere a nanostructurilor supraconductor/feromagnetic, cu parametri dirijați și strict reproductibili într – un singur ciclu de vid, modelarea matematică a parametrilor tehnologici de depunere magnetron cu ajutorul pachetului LAMMPS, în scopul ajustării lor, studiul proprietăților supraconductoare a structurilor stratificate nanometrice, cu efecte valvă de spin și elemente de memorie.

**Noutatea și originalitatea științifică:** A fost optimizată tehnologia de depunere magnetron a nanostructurilor de supraconductor/feromagnetic cu interfețe atomar netede în care a fost înregistrată împerecherea tripletă – datorată nanostructurilor de feromagnetic cu magnetizări necolineare. Este propus un element de bază – valvă de spin în care rolul principal îl are supraconductibilitatea tripletă, alcătuit dintr – un metamaterial magnetic artificial.

**Problema științifică principală soluționată:** constă în optimizarea parametrilor de depunere magnetron a nanostructurilor cu interfețe atomar netede, și studiul caracteristicilor nanostructurilor pentru utilizarea lor în calitate de elemente de memorie și supape de spin.

**Semnificația teoretică și valoarea aplicativă a lucrării:** În baza măsurărilor caracteristicilor de transport a structurilor hibride de supraconductor/feromagnetic, Nb/Co, a fost realizat elementul cu comutare suficient de rapidă, cu orientările paralele (P) și antiparalele (AP) ale filmelor de feromagnetic. Elementul de bază valvă de spin –  $S/[F_1/s/F_2/s]n/F_1/S$ , în heterostructurile supraconductor/feromagnet este realizat dacă cel puțin două straturi feromagnetice  $F_1$ ,  $F_2$  au o aliniere necolinară a magnetizărilor lor – fapt ce generează componenta tripletă impară. În domeniul teoretic cu ajutorul dinamicii moleculare și a modelului atomului scufundat – MEAM, au ajustați parametrii de depunere magnetron în scopul îmbunătățirii calității interfețelor straturilor nanometrice, au fost depistați experimental parametrii de depunere magnetron a nanostructurilor ce contribuie semnificativ la îmbunătățirea interfețelor adiacente cu sporirea efectelor cuantice, cum ar fi temperatura substratului de siliciu (300 K).



## ABSTRACT

to the thesis with the title: "**Triplet superconductivity as the basis of superconducting spintronics**", submitted by Boian VLADIMIR for the obtaining of the scientific title of Doctor of Physical Sciences in specialty 133.04 "**Solid State Physics**".

**Structure of the thesis:** The thesis submitted was carried out within the Institute of Electronic Engineering and Nanotechnologies "D. Ghițu" of the Technical University of Moldova, Chisinau. It is written in Romanian and contains five chapters, general conclusions, recommendations and bibliography (161 titles) being presented on 112 pages of basic text, containing 56 figures, 6 tables. The basic research and applied studies are presented in **15** scientific papers published in journals on the topic of the thesis; **5** journal articles are included in the SCOPUS and Web of Science databases; **7** publications in proceedings of national and international conferences; **4** articles without co-authors.

**Keywords:** triplet superconductivity, spin valve, MRAM memory elements, magnetron deposition, mathematical modeling.

**The aim of the work:** the realization of a spin valve as a non-dissipative basic element for the superconducting computer, and the adjustment of the magnetron deposition parameters of Nb/Co nanostructures, in a single vacuum cycle with atomically smooth adjacent interfaces.

**The objectives of the research:** optimization of the technological parameters of the deposition of superconducting/ferromagnetic layers, with determined and strictly reproducible parameters in a single vacuum cycle, mathematical modeling of the technological parameters of magnetron deposition with the help of the LAMMPS package, in order to adjust them, the study of the superconducting properties of nanometric layered structures with spin valve effects and memory elements.

**Scientific novelty and originality:** The magnetron deposition technology of superconductor/ferromagnetic nanolayers with atomically smooth interfaces was optimized and the triplet pairing was detected – due to presence of ferromagnetic nanolayers with non-collinear magnetizations. A basic element is proposed - spin valve with artificial magnetic metamaterial in which triplet superconductivity plays the main role.

**The main scientific problem solved:** optimizing the magnetron deposition parameters of nanostructures with atomically smooth interfaces, and studying the characteristics of the nanostructures for their use as memory elements and spin valves.

**Theoretical significance and applied value of the work:** Based on the measurements of the transport characteristics of the superconductor/ferromagnetic hybrid structures, Nb/Co, the sufficiently fast switching element, the spin valve, was realized with the parallel (P) and antiparallel (AP) orientations of the ferromagnetic films magnetizations. The basic spin valve element –  $S/[F1/s/F2/s]n/F1/S$ , in superconductor/ferromagnet heterostructures is realized if at least two ferromagnetic layers F1, F2 have a non-collinear alignment of their magnetizations – a fact which generates the superconducting odd triplet component. In the theoretical part, with the help of molecular dynamics and the immersed atom model (MEAM), it were adjusted the magnetron deposition parameters in order to improve the quality of the interfaces of nanometric layers. Than the optimised parameters of magnetron deposition of nanolayers were experimentally checked (for example, the temperature of the silicon substrate, 300 K), which significantly improved the interfaces quality with the enhancement of quantum effects.

## АННОТАЦИЯ

на диссертацию на тему: «Триплетная сверхпроводимость как основа сверхпроводниковой спинтроники», представленную кандидатом Бояном ВЛАДИМИРОМ на соискание ученого звания доктора физических наук по специальности 133.04 «Физика твердого тела».

**Структура диссертации:** Представленная на защиту диссертация выполнена в Институте электронной инженерии и нанотехнологий «Д. Гицу» Технического университета Молдовы, Кишинев. Диссертация написана на румынском языке и содержит пять глав, общие выводы, рекомендации и библиографию (161 наименование), представлена на 112 страницах основного текста, содержащих 56 рисунков, 6 таблиц. Фундаментальные и прикладные исследования данной диссертации представлены в **15** научных статьях, опубликованных в журналах по теме диссертации; **5** журнальных статей из баз данных SCOPUS и Web of Science; **7** публикаций на национальных и международных конференциях; **4** статьи с без соавторов.

**Ключевые слова:** триплетная сверхпроводимость, спиновой клапан, элементы памяти MRAM, магнетронное осаждение, математическое моделирование.

**Цель работы:** реализация спинового клапана как бездиссипативного базового элемента сверхпроводящего компьютера и настройка параметров магнетронного осаждения наноструктур Nb/Co в одном вакуумном цикле с атомарно-гладкими соседними интерфейсами.

**Задачи исследования:** оптимизация технологических параметров нанесения сверхпроводящих/ферромагнитных слоев с заданными и строго воспроизводимыми параметрами в одном вакуумном цикле, математическое моделирование технологических параметров магнетронного напыления с помощью пакета LAMMPS, и с целью их корректировки - исследование сверхпроводящих свойств нанометровых слоистых структур с эффектами спиновых клапанов и элементами памяти.

**Научная новизна и оригинальность:** Оптимизирована технология магнетронного осаждения нанослоев сверхпроводник/ферромагнетик с атомарно-гладкими границами раздела, в которых зафиксировано триплетное спаривание – за счет наличия ферромагнитных нанослоев с неколлинеарными намагниченностями. Предлагается базовый элемент - спиновый клапан, в котором главную роль играет слабая связь сверхпроводимость, состоящая из искусственного магнитного метаматериала Nb/Co.

**Основная решаемая научная задача:** заключается в оптимизации параметров магнетронного осаждения наноструктур с атомно-гладкими границами раздела и изучении характеристик наноструктур для их использования в качестве элементов памяти и спиновых клапанов.

**Теоретическая значимость и прикладная ценность работы:** На основе измерений транспортных характеристик гибридных структур сверхпроводник/ферромагнетик Nb/Co реализован достаточно быстро переключающийся элемент с параллельной (P) и антипараллельной (AP) ориентациями намагниченности пленки ферромагнетика. Базовый элемент спинового клапана –  $S/[F1/s/F2/s]n/F1/S$ , в гетероструктурах сверхпроводник/ферромагнетик реализуется, если два ферромагнитных слоя F1, F2 имеют неколлинеарное направление намагниченностей. В теоретическом разделе с помощью молекулярной динамики и модели погруженного атома (MEAM) оптимизированы параметры магнетронного осаждения с целью улучшения качества границ раздела нанослоев Nb/Co, экспериментально установлены оптимальные параметры магнетронного осаждения нанослоев (например, температура кремниевой подложки 300 K), что существенно улучшает соседние интерфейсы наноструктуры с усилением квантовых эффектов.

**BOIAN VLADIMIR**

**TRIPLET SUPERCONDUCTIVITY AS THE BASIS OF  
SUPERCONDUCTING SPINTRONICS.**

**133.04 – Solid state physics**

**Abstract of the PhD thesis**

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