INTERNATIONAL JOURNAL OF CIRCUITS, SYSTEMS AND SIGNAL PROCESSING
DOI: 10.46300/9106.2023.17.21 Volume 17, 2023

Base Elements for Artificial Neural Network: Structure Modeling, Production, Properties

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Received: September 16, 2022. Revised: February 19, 2023. Accepted: March 7, 2023. Published: April 3, 2023.

***Abstract* — A radical reduction in power consumption is becoming an important task in the development of supercomputers. Artificial neural networks (ANNs) based on superconducting elements of spintronics seem to be the most promising solution. A superconducting ANN needs to develop two basic elements - a nonlinear (neuron) and a linear connecting element (synapse). The theoretical and experimental results of this complex and interdisciplinary problem are presented in this paper. The results of our theoretical and experimental study of the proximity effect in a stacked superconductor/ferromagnet (S/F) superlattice with Co-ferromagnetic layers of various thicknesses and coercive fields and Nb-superconducting layers of constant thickness equal to the coherence length of niobium and some studies using computer simulation of the formation of such multilayer nanostructures and their magnetic properties are presented in this article.**

Keywords*— *Artificial Neural Network , Base Elements, Modeling, Magnetic Properties, Structure

I. Introduction

One of the current trends in the development of supercomputers is the creation of an element base with low energy consumption and the development of optimal algorithms [1-3]. This problem has a multifaceted solution. One of them may be the development of artificial neural networks based on superconducting elements of spintronics. The competition between ferromagnetism and spin-singlet superconductivity leads to the appearance of new

phenomena, including the generation of an odd-frequency spin-triplet order parameter [4-6].

This exotic state has been widely studied both theoretically [7] and experimentally [8–10] in superconductor/ferromagnet (S/F) heterostructures and can be used to develop new superconducting devices in which the supercurrent is determined and controlled by the magnetic state of the heterostructure S/ F [11,12].

We experimentally study the in-plane transport properties of Nb/Co nanostructured multilayers (ML) with different number of layers and layer thickness.

The main goal of this part of the work is to demonstrate how conventional experimental methods can be used to estimate the magnetic states of S/F heterostructures and devices in situ.

Additionally, the article presents the results of mathematical modeling of the structure and magnetic properties of Nb/Co multilayers for designing artificial neuron nanostructures.

II. TRANSPORT CHARACTERIZATION OF MAGNETIC STATES IN SUPERCONDUCTOR/FERROMAGNET HETEROSTRUCTURES

We study two types of Nb/Co ML's with different number of layers and layer thicknesses. The simple S1: Nb(50 nm)/Co(1.5 nm)/Nb(8 nm)/Co(2.5 nm)/Nb(8 nm)/Si ML (bottom -to -top), has just two Co layers composing a single pseudo spin valve. A more complex sample S2: Nb(50 nm)/[Co(1.5 nm)/Nb(6 nm)/Co(2.5 nm)/Nb(6 nm)]$_3$Co(1.5 nm)/Nb(6 nm)/Si (block in square brackets is repeated 3 times) has five Co layers. ML's are deposited by magnetron sputtering in a single deposition run without breaking the vacuum.

Scanning electron microscope (SEM) image and contact configuration of one of the samples is shown in Fig.1.

Control of the magnetic state needs a possibility of variation of a relative magnetization orientation of the F-layers, which requires the different coercive fields. Resistance measured by the lock-in technique with different current amplitudes I_{ac}. Magnetic field is applied parallel to the film plane.

Multi-terminal geometry of the samples allows simultaneous four-probe measurements of different segments of the sample in longitudinal, R_{xx}, and Hall, R_{xy}, directions. When current is sent through the central vertical bridge, as sketched in Fig. 1b, measurements correspond to the easy-axis magnetization orientation. Alternatively, we can send current through horizontal bridges, that corresponds to the hard-axis magnetization orientation (perpendicular to the long side of the bridge).

Longitudinal magnetoresistance for a horizontal bridge S2, measured at different T are presented in Fig. 2.

So, we have studied in-plane transport properties of micro-structured Nb/Co multilayers and demonstrated how conventional transport techniques can be used for the assessment of magnetic states of small S/F heterostructures and devices. For that we apply a number of experimental techniques, including magnetoresistance,

Hall effect, and first-order-reversal-curves analysis (FORC) and determined the range of parameters and the procedure for *in-situ* control of spintronic devices based on S/F heterostructures.

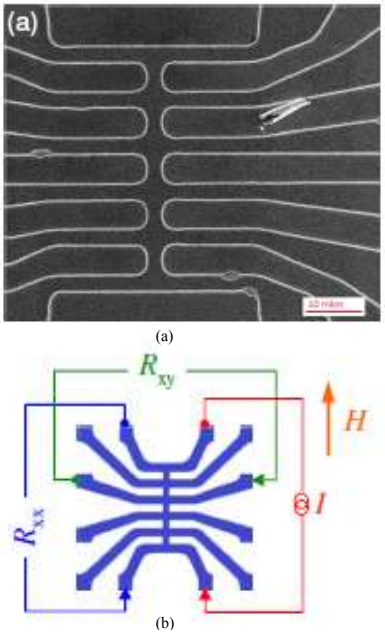

Fig. 1. a) (SEM) image of one of the studied samples; b) Contact configuration for measurement of longitudinal and Hall resistances

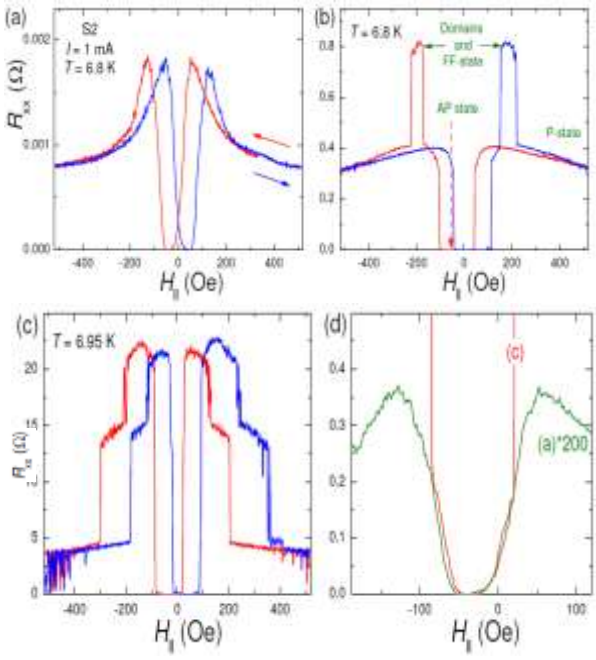

Fig. 2. Longitudinal magnetoresistances for a horizontal bridge S2, measured at different T. (a) the lowest T = 6.8 K, corresponds to the very onset of resistivity. (b) an additional maximum appears, which is attributed to the triggering of the flux-flow phenomenon by magnetic domain. (c) T = 6.95 K, corresponds to the middle point of the resistive transition. Steps are attributed to transitions of individual spacer layers. (d) Low-resistance parts of the curves from (a) and (c), which demonstrate a similar behavior in the AP-state.

III. MODELING OF ARTIFICIAL NEURON NANOSTRUCTRE FORMATION PROCESSES

This part of article presents the results of mathematical modeling of the artificial neuron nanostructure.

Design of artificial neuron is based on magnetic structures with controllable effective exchange energy for Josephson junctions and memory applications [13-14].

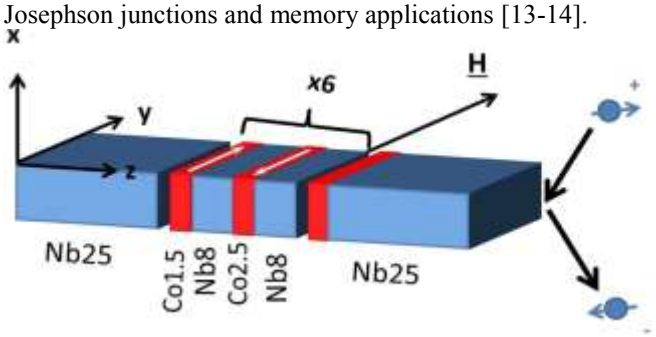

Fig. 3. The superlattice structure of ferromagnetic layers spaced by thin superconductors

Software package LAMMPS is applied to theoretical research. The statement of the simulation problem is shown in Fig. 4.

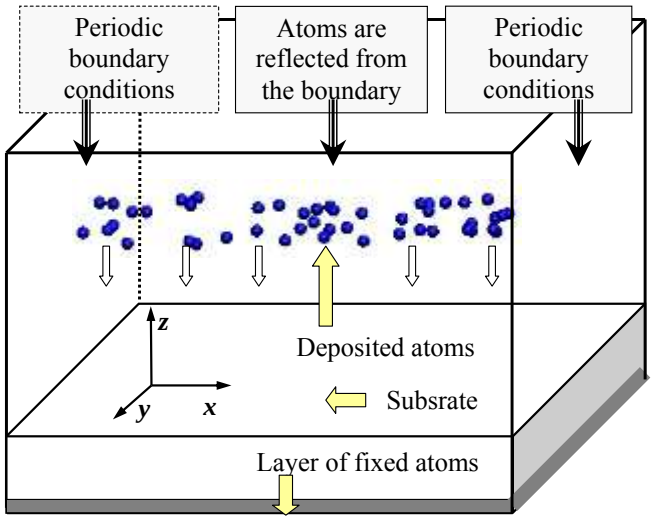

Fig. 4. Statement of the problem for the deposition of multilayers

The problem of precipitating nanofilms was solved by molecular dynamics method using theory of MEAM [15]. A more detailed mathematical model is considered in previously published works [16-18].

The main equations of this method are (1)-(7):

$$m_i \frac{d^2\bar{\mathbf{r}}}{dt^2} = -\frac{\partial E(\bar{\mathbf{r}})}{\partial \bar{\mathbf{r}}_i} + \bar{\mathbf{F}}_{ex}, \bar{\mathbf{r}}_i(t_0) = \bar{\mathbf{r}}_{i0}, \frac{d\bar{\mathbf{r}}_i(t_0)}{dt} = \bar{\mathbf{V}}_{i0}, \quad (1)$$

$$E = \sum_i E_i = \sum_i \left(F_i(\bar{\rho}_i) + \frac{1}{2}\sum_{j\neq i} \varphi_{ij}(r_{ij}) \right), \quad (2)$$

$$F_i(\bar{\rho}_i) = A_i E_i^0(\bar{\rho}_i) \ln(\bar{\rho}_i), \quad (3)$$

$$\bar{\rho}_i = \frac{\rho_i^{(0)}}{\bar{\rho}_i^0} G(\Gamma_i), \quad (4)$$

$$\Gamma_i = \sum_{k=1}^{3} t_i^{(k)} \left(\frac{\rho_i^{(k)}}{\rho_i^{(0)}} \right)^2, \Gamma_i^{\text{ref}} = \frac{1}{Z_{i0}^2} \sum_{k=1}^{3} t_i^{(k)} s_i^{(k)}, \quad (5)$$

$$E_{ii}^u(R_{ij}) = -E_{ij}\left(1 + a_{ij}^*(r_{ij})\right) e^{-a_{ij}^*(r_{ij})}, a_{ij}^* = \alpha_{ij}\left(\frac{r_{ij}}{r_{ij}^0} - 1\right), \quad (6)$$

$$\varphi_{ij}(r_{ij}) = \frac{1}{Z_{ij}}\left[2E_{ij}^u(r_{ij}) - F_i\left(\frac{Z_{ij}}{Z_i}\rho_i^{a(0)}(r_{ij})\right) - F_j\left(\frac{Z_{ij}}{Z_j}\rho_j^{a(0)}(r_{ij})\right)\right]. \quad (7)$$

As an example, to illustrate the modeling of a real material structure, we consider the structure of a multilayer Nb-Co spin valve nanosystem.

The result of numerical experiments on the deposition of alternating niobium-cobalt nanofilms is shown in Fig. 5. This figure illustrates the results of sputtering only the first three films, the other films are deposited in the same way. Fig. 5 shows that the nanofilms have different structures. In particular, the middle layer of niobium contains areas of crystallites with different spatial orientations. Cobalt nanofilms, due to their small thickness, have predominantly amorphous structure. This structure was also formed due to partial mixing of the contact areas between the cobalt and niobium layers. The mixing of the contact regions and the blurring of the nanofilm interfaces are undesirable technological effects. Such effects require additional investigation, including by means of mathematical modeling. The obtained results are in good agreement with the experimental data presented in [18].

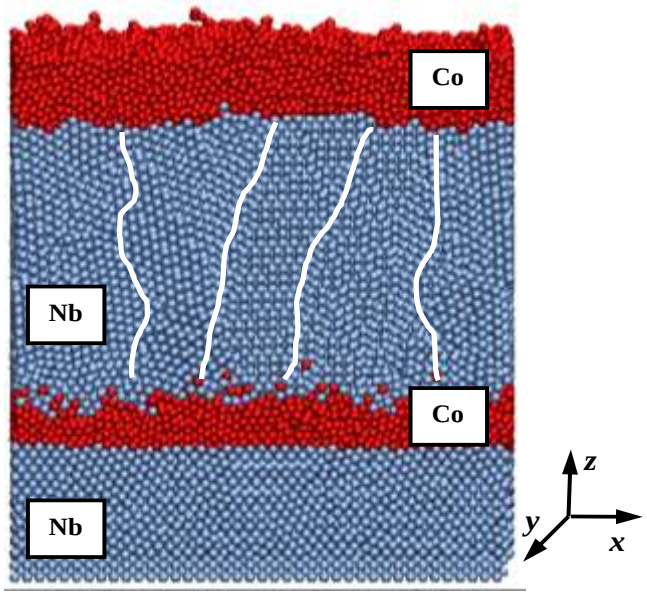

Fig. 5. Part of the Nb/Co multilayer structure included as part of the neuron (Josephson junction) or multilayered artificial synapse

IV. MODELING OF MAGNETIC PROPERTIES

The magnetic properties of nanosystems can be described using molecular dynamics methods in which, among other

things, a spin vector $\mathbf{s}_i$ is introduced for each i-th atom. In this case, the atoms and spins will move in accordance with the equations (8)-(10):

$$\frac{d\mathbf{r}_i}{dt} = \frac{\mathbf{p}_i}{m_i}, \tag{8}$$

$$\frac{d\mathbf{p}_i}{dt} = \sum_{i \neq j}^{N} \left[-\frac{dU\left(|\mathbf{r}_{ij}|\right)}{d|\mathbf{r}_{ij}|} + \frac{dJ\left(|\mathbf{r}_{ij}|\right)}{d|\mathbf{r}_{ij}|} \mathbf{s}_i \cdot \mathbf{s}_j \right] \mathbf{e}_{ij}, \tag{9}$$

$$\frac{d\mathbf{s}_i}{dt} = \mathbf{f}_i \times \mathbf{s}_i, \tag{10}$$

where $\mathbf{r}_i$ is the position vector of the atom i; along this vector a unit vector $\mathbf{e}_{ij}$ is directed; vectors $\mathbf{s}_i, \mathbf{s}_j$ characterizing the spins of the i-th and j-th atoms, respectively; the left part in (9) describes the change in the momentum vector; to each spin some vector $\mathbf{f}_i$ is applied; U describes potential energy.

The exchange interaction, Zeeman interaction, magnetic anisotropy, Dzialoshinsky-Moriya interaction, and dipole and magnetoelectric interactions will contribute to the total energy of the magnetic system (11):

$$H = H_{\text{ex}} + H_{\text{z}} + H_{\text{an}} + H_{\text{Neel}} + H_{\text{dm}} + H_{\text{di}} + H_{\text{me}}. \tag{11}$$

In modeling, the consideration of one or another type of interaction is determined primarily by the range of tasks that are considered in the study, as well as by the structure of the simulated systems. The values of the parameters included in the equations describing these or those kinds of interactions are determined from experiments and by means of auxiliary calculations. For the systems considered in this work, the pairwise anisotropy model of Neel was used.

The structure of the material in question, in particular its crystal lattice, has a direct influence on the type of magnetic anisotropy to be observed in the system. The magnetic properties of ferromagnetic are influenced by the direction of the magnetization vector with respect to the structural axes of the crystals that form these ferromagnetic. This dependence is described by magnetic anisotropy. In ferromagnetic materials, the orientation of the magnetization vector also affects the change in internal energy. The appearance of magnetic anisotropy can be caused by the following factors: mechanical deformation, temperature effects, sample characteristics, and dipole-dipole interaction. The symmetry of a ferromagnetic material crystal depends on the internal energy if there are no external influences in the system.

For magnetically ordered substances, magnetic crystallographic anisotropy is often a consequence of spin-orbit interaction.

The dipole-dipole interaction is small, so it has little effect on the anisotropy energy.

The dipole-dipole interaction is worth considering for some rare-earth metals, because the lattice constants in these kinds of materials are small and the magnetic moments of the particles are large.

Approaches to modeling the magnetic properties of materials with spin-orbit coupling at the atomic level are described in [19 - 21]. Magnetic anisotropy between pairs of magnetic spins can be described using the previously mentioned Neel pair anisotropy model. This model considers more complex forms of magnetocrystalline anisotropy, which is characteristic of most crystals of magnetic materials. The Neel model can be described using equation (12):

$$\begin{aligned} H_{\text{Neel}} = &- \sum_{i,j=1, i \neq j}^{N} g_1\left(r_{ij}\right)\left(\left(\mathbf{e}_{ij} \cdot \mathbf{s}_i\right)\left(\mathbf{e}_{ij} \cdot \mathbf{s}_j\right) - \frac{\mathbf{s}_i \cdot \mathbf{s}_j}{3} \right) + \\ &+ q_1\left(r_{ij}\right)\left(\left(\mathbf{e}_{ij} \cdot \mathbf{s}_i\right)^2 - \frac{\mathbf{s}_i \cdot \mathbf{s}_j}{3} \right)\left(\left(\mathbf{e}_{ij} \cdot \mathbf{s}_j\right)^2 - \frac{\mathbf{s}_i \cdot \mathbf{s}_j}{3} \right) + \\ &+ q_2\left(r_{ij}\right)\left(\left(\mathbf{e}_{ij} \cdot \mathbf{s}_i\right)\left(\mathbf{e}_{ij} \cdot \mathbf{s}_j\right)^3 + \left(\mathbf{e}_{ij} \cdot \mathbf{s}_j\right)\left(\mathbf{e}_{ij} \cdot \mathbf{s}_i\right)^3 \right), \end{aligned} \tag{12}$$

where g_1, q_1, q_2 functions defining the intensity of dipole and quadrupole contributions determined according to (13)-(15):

$$g_1\left(r_{ij}\right) = g\left(r_{ij}\right) + \frac{12}{35} q\left(r_{ij}\right), \tag{13}$$

$$q_1\left(r_{ij}\right) = \frac{9}{5} q\left(r_{ij}\right), \tag{14}$$

$$q_2\left(r_{ij}\right) = -\frac{2}{5} q\left(r_{ij}\right). \tag{15}$$

The functions $q\left(r_{ij}\right)$ and $g\left(r_{ij}\right)$ are determined with the Bethe – Slater curve:

$$f\left(r_{ij}\right) = 4\alpha\left(\frac{r_{ij}}{\delta}\right)^2\left(1 - \gamma\left(\frac{r_{ij}}{\delta}\right)^2\right) e^{-\left(\frac{r_{ij}}{\delta}\right)^2} \Theta\left(R_c - r_{ij}\right), \tag{16}$$

where α (in eV), δ (in Å), γ (dimensionless value) are the three constant coefficients; the last factor in the right-hand side of equation (16) is the Heaviside function $\Theta\left(R_c - r_{ij}\right)$. The coefficients α, δ, γ must be chosen so that the above function corresponds to the values of the magnetoelastic constant of the materials under consideration.

The spin temperature is determined from (17):

$$T_S = \frac{h}{2k_B} \frac{\sum_{i=1}^{N} \left|\mathbf{s}_i \times \boldsymbol{\omega}_i\right|^2}{\sum_{i=1}^{N} \mathbf{s}_i \cdot \boldsymbol{\omega}_i}, \tag{17}$$

where $\mathbf{s}_i$ is spin vector of the magnetic particle, $\boldsymbol{\omega}_i$ describes magnetic moment, h stands for Planck constant. This method of determining the spin temperature is described in detail in [22].

Mathematical models for describing the spin behavior of nanomaterials include phenomenological models, quantum mechanics, statistical methods, and direct simulation by particle dynamics. The latter approach [23] has a number of advantages over alternative methods, since it allows us to describe sufficiently large systems and is not

computationally expensive. Direct particle dynamics simulation methods are based on a combination of the classical method of molecular dynamics and atomic spin dynamics. The calculation of the spins distribution, coordinates, and velocities of atoms is performed sequentially, step by step, but, of course, requires a number of empirical constants responsible for interparticle and magnetic interactions.

In the following, the classical and spin mechanics of cobalt atoms for two variants of nanosystems will be considered. In the first case, the cobalt atoms were located near the equilibrium state, which corresponds to the nodes of the hexagonal close-packed crystal lattice. In the second case, the structure of cobalt had structural defects and was distorted to some extent, since it was formed by simulation methods during the deposition of cobalt nanofilms, which are shown in Fig. 3 and 5 and described earlier in Section 3. The size of the nanosystems was chosen to be small, approximately 0.5 nm x 0.9 nm x 0.8 nm, due to the small thicknesses of the cobalt nanofilms used. The boundary conditions in all directions were periodic.

Despite the fact that the final nanocomposite includes an alternating combination of cobalt and niobium films (Fig. 3), consideration of niobium at this stage on the effect of spin distribution was excluded, since niobium belongs to the group of superconductors, in which the phenomenon of displacement of the magnetic field from the internal volume of the material is observed due to the Meissner effect [24]. The operating modes of the proposed composite based on cobalt and niobium assume the use of superconductivity mode, so the spin behavior of cobalt atoms was modeled at a system temperature of 5 K, which is below the superconducting transition temperature for niobium (9.25 K).

The results of modeling the magnetic behavior of two nanosystems with ideal and real (obtained by molecular dynamics simulation) structures as a spin temperature distribution are shown in Fig. 6. An external magnetic field with induction along the x-axis direction was applied to the nanosystems.

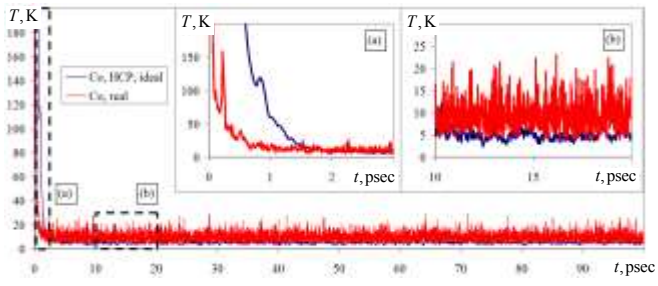

Fig. 6. Dynamics of spin temperature for ideal and real cobalt structures in an external magnetic field with an induction of 1.0 T. The data were obtained by mathematical modeling

The spin temperature at the initial moments of time (Fig. 6(a)) is characterized by significant changes and jumps, which is associated with the initial nonequilibrium state of both systems.

The set reorientation of spins of the cobalt atoms leads to a significant decrease in the instantaneous values of the spin temperature, which indicates some stabilization of the magnetic state of both versions of the systems. Nevertheless, for the real cobalt structure, large values are observed in the spin temperature variations (Fig. 6(b)), which may be due to the presence of structural defects and the deviation, for this reason, from the most stable magnetic state.

Another macro characteristic of a nanostructured material is its magnetization. Magnetization characterizes the total distribution and behavior of atomic spins and allows us to determine which group of materials (dielectric, magnetic) the studied sample belongs to. For the two versions of the cobalt structure considered in this work, the aggregate magnetization is shown in Fig. 7.

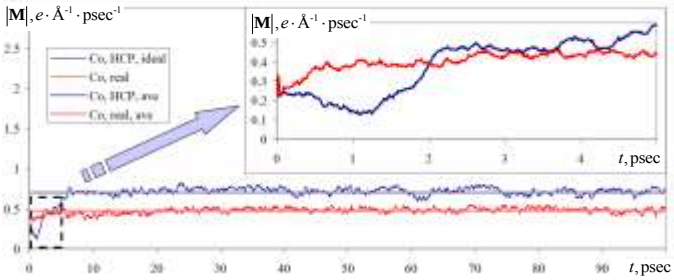

Fig. 7. Dynamics of the magnetization value of the material for the ideal and real cobalt structure in an external magnetic field with an induction of 1.0 T. The data were obtained by mathematical modeling

The behavior of the magnetization vector module generally correlates with the behavior of the material's spin temperature. At the initial moments of time, oscillations and significant changes in the magnetization magnitude are noticeable (enlarged region in Fig. 7), which occurs due to spin rearrangement and mutual reorientation under the action of the external magnetic field. Further behavior of the magnetization modulus can be characterized as slightly changing. There are some fluctuations in this magnitude, but they occur near the mean values. From the graphs in Fig. 7 shows that the average value for the real structure of cobalt is $0.47\, e/(\text{Å}\cdot\text{psec})$. The ideal hexagonal crystal structure of cobalt has an average magnetization modulus of $0.7\, e/(\text{Å}\cdot\text{psec})$. In these expressions, e represents the value of the electron charge.Analysis of the magnetization modulus values obtained indicates that this characteristic depends on the structure of the nanomaterial. The presence of defects and deviation from the ideal structure leads to a decrease in the total magnetization by up to 40%. This effect can be explained by a disturbance in the cumulative ordering of the magnetic moments of the atoms in the material with a distorted structure. In spite of this, the ferromagnetic behavior of cobalt is preserved for both variants of the nanosystems under consideration.

V. Conclusion

Analysis of the field state in the design and fabrication of modern electronic devices demonstrates the need to create new nanomaterials that would be devoid of the drawbacks of existing ones and would solve a number of problems, such as those related to excessive heat dissipation. These promising materials can be found using the effects of spintronics. One such material is a multilayer nanocomposite based on cobalt and niobium.The results of theoretical studies processes of formation of the multilayer nanostructures are used for the

development of vacuum technology of functional S/F nanostructures fabrication for application in spintronics

The proposed mathematical model of particle dynamics, supplemented with the spin dynamics of atoms, allows the magnetic behavior of nanomaterials to be described and investigated considering their atomistic structure. The model is able to reproduce both the spin behavior of individual atoms and obtain integral material characteristics, such as spin temperature and magnetization value. In the absence of magnetic fields, the model is a classical molecular dynamics method, which is a convenient tool for working out technological processes and searching for optimal modes of nanomaterial fabrication.

Simulating the deposition of multilayer nanofilm coatings in the cobalt-niobium nanocomposite showed the presence of regions of different structure in the material. The sputtering processes depended on the supported substrate temperature, and the nanofilm interface region was not always compact. In the case of niobium deposition on cobalt, the interfaces were more blurred. Mathematical modeling in this case makes it possible to select the most optimal variants of film deposition processes in order to qualitatively improve the structure and interfaces of the nanocomposite layers.

Numerical experiments on the investigation of the magnetic properties of cobalt nanofilms showed that the spin temperature and magnetization value depend on its atomic structure. Distortion of the ideal structure and the presence of possible defects leads to a less stable behavior of integral characteristics and causes partial disorientation of atomic spins. The magnetization vector modulus decreased by 40% due to defects in the cobalt nanofilm structure. The ferromagnetic behavior of cobalt was preserved.

ACKNOWLEDGMENT

The work was supported by the Russian Science Foundation Grant Nr. 20-62-47009 “Physical and engineering basis of computers non-von Neumann architecture based on superconducting spintronics” (modelling and calculations), and partially by the Moldova State Program Project «Functional nanostructures and nanomaterials for industry and agriculture» Nr. 20.80009.5007.11.(formation of nanostructures)

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Contribution of individual authors to the creation of a scientific article (ghostwriting policy)
We confirm that all Authors equally contributed in the present research, at all stages from the formulation of the problem to the final findings and solution.

Sources of funding for research presented in a scientific article or scientific article itself
No funding was received for conducting this study.

Conflict of Interest
The authors have no conflict of interest to declare that is relevant to the content of this article.