Hybrid nanostructures superconductor-ferromagnet for superconducting spintronics

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Abstract. The work is devoted to the study of the processes of formation of multilayer nanostructures, their vacuum deposition, and the manufacture of a novel functional element of spintronics - superconducting spin valve, which is a multilayer structure consisting of ferromagnetic cobalt nanolayers separated by superconductor niobium films. Multilayer nanostructures are fabricated by magnetron sputtering on (111) silicon substrates at a temperature of 300K. The prototypes of the superconducting spin valve are prepared from multilayer nanostructures by the method of sharp focus reactive ion etching (FIB). Modeling was carried out using molecular dynamics methods.

1. Introduction
Multilayer hybrid superconductor / ferromagnet nanostructures are the basic element of quantum electronics - spintronics, based on electron spin transport. Unlike conventional semiconductor electronics, superconducting spintronics consume a minimum of energy and has a high response rate. [1,2]. However, practice shows that the creation of multilayer superconductor-ferromagnet nanostructures with the required properties is an extraordinarily complex process, therefore, commonly, it is not possible to create an “ideal” nanosystem. The structure of real nanosystems is far from ideal one. In particular, it can be noted that the surface separating the various nanolayers of the system is not perfectly flat. The surface has noticeable irregularities that penetrating into the layers being in contact. Also, there is a mutual penetration of one contacting layer atoms into another due to the interdiffusion of the layer’s elements. Therefore, the layer interface has a certain, non-zero thickness. It should be noted that the atomic structure of each layer does not form an ideal single crystal, but a system of polycrystals is formed. In this regard, complex theoretical and experimental studies of such multilayer nanostructures are highly relevant.

The aim of the work was the experimental and simulation study of the influence on these nanosystems main technological parameters: temperature, concentration, and spatial distribution of deposited atoms over the nanosystem surface, and on the atomic structure and morphology of the fabricated nanosystem.
2. Experiments

Experimental studies are aimed at studying the formation of multilayer niobium / cobalt nanostructures manufactured by magnetron sputtering in a single deposition cycle in a modified vacuum system LEYBOLD-Z400. This vacuum system allows switching between several targets without depressurizing the chamber, with the target “rocking” during sputtering for the greater sprayed layer homogeneity.

Three targets were used in the experiments: niobium (99.95%) for the formation of thick S-layers (generators of Cooper pairs, 25 nm thick, much greater coherence length of niobium) and thin (6 nm) interlayer spacers between F-layers; a cobalt target (99.95%) for the deposition of F-layers, as well as a target of pure silicon (99.999%) for the buffer and protective layers deposition that prevent the prepared structures oxidation and the substrate influence.

Samples are grown on commercial (1 1 1) silicon wafers. Before deposition, all targets were preliminarily cleaned using Ar + plasma etching for 3 minutes before starting the deposition cycle and additionally for 1 minute after switching targets. The layers were deposited at an optimized temperature (Tp = 300 K) on a water-cooled substrate holder. Film thicknesses were determined using calibrated deposition rates: 3.5 nm / sec for niobium and 0.1 nm / sec for cobalt films.

For each layer set, three identical samples were prepared simultaneously, some of which were used to calibrate the ion rates etching of the films during further processing. Microbridges were formed from the prepared multilayer structures using optical photolithography, followed by reactive ion etching of a functional element - a spin valve.

In Figure 1a, a spin valve is shown housed in a holder for low temperature measurements. A scanning electron microscope (SEM) image of the prepared and investigated spin valve sample is shown in Figure 1b (a snapshot of a spin valve prepared by ion etching of a niobium-cobalt multilayer structure using a focused ion beam.

3. Simulations

As mentioned above, the creation of multilayer hybrid superconductor / ferromagnet nanostructures requires complex studies, including formation processes modeling and experiment series. Therefore, we used mathematical modeling to determine the optimal modes of formation and study the interface morphology of individual hybrid nanostructure layers.

The superconductor (niobium) - ferromagnet (cobalt) nanostructures simulation was carried out by the molecular dynamic’s method using the modified embedded atom many-particle potential method. Details of the mathematical problem formulation and the algorithms used for the calculations are given in the author’s works [3-7].

The schematic diagram of the simulated multi-layer hybrid superconductor / ferromagnet nanostructure is shown in Figure 2.
Figure 2. Sketch of a Nb / Co spin valve nanosystem. The numbers next to the elements in the layers represent the layer thickness in nanometers.

Figure 3 shows the general scheme of the modeling process. The nanosystem contains a material evaporation zone, atoms deposition area, a substrate with a fixed lower layer of atoms. During the first nanofilm formation, the deposition is carried out directly onto the substrate; for the subsequent ones, onto the substrate with previously formed nanofilms.

The temperature was controlled using a Nose - Hoover thermostat in the range of 300-800 K.

The image of a multilayer nanosystem formed as a result of mathematical modeling is presented in Figure 4.

The image in Figure 5 clearly demonstrates the niobium and cobalt layered nanosystem formation processes and the layers structure: the layers formed by niobium and cobalt atoms have a polycrystalline structure. In this case, groups of atoms are combined into domains with different spatial orientations. The blurring of the contact area between the layers and a less even surface profile compared to niobium are noticeable.

A quantitative characteristic of the material spatial structure can be obtained by calculating the coordination number. The coordination number in crystallography reflects the number of nearby equally distant atoms of the same type in the crystal lattice. The number of the nearest neighbors determines the material packing density. For different types of crystal lattices, the coordination number will be different. The cubic volume-centered lattice (characteristic of niobium) has a coordination number equal to 8, the hexagonal close-packed lattice (corresponds to cobalt) - 12. For the formed nanosystem, the
change in the average value of the coordination number in the layers was calculated (shown in Figure 5).

The change in the coordination number in Figure 5 correlates with the structure of the nanomaterial shown in Figure 4. The niobium substrate has a parameter value close to 8, which indicates its crystalline structure. Cobalt 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 close-packed lattice, indicating an amorphous-like structure of cobalt nanofilms. Variations in the coordination number within the intermediate niobium layer are more significant. When approaching the contact regions with cobalt, an increase in this parameter is observed.

![Figure 4. Multilayer nanosystem niobium and cobalt. The contact points of the nanofilms are indicated by letters (b) and (c). In the indicated contact points, the distribution of coordination numbers will be plotted below. Substrate temperature is fixed as 300 K.](image)

![Figure 5. Change in coordination (CN) number along the z-axis (shown in Fig. 5) in 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.](image)
Thus, it was shown that the structure of the nanomaterial depends not only on the current layer characteristics, but also on the structural features of the regions adjacent to it. In addition, temperature has a definite 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 the surface effects and boundary phenomena appearance in that region.

4. Conclusions
1. The optimal range of substrate temperatures during magnetron sputtering and deposition rates of materials, providing a sharp (high-quality) interface between layers, has been established.
2. The manufacturing technology parameters were estimated: the deposition intensity, the density of the deposition flux, and the temperature of the growth substrate.
3. As the studies result, the formed nanofilms structure and the distribution of atomic elements within the contact regions were obtained.
4. It is shown that the alternating layers of the formed nanocomposite have different atomic structures.
5. The atomic structure distribution in the horizontal sections of the nanosystem is demonstrated.
6. It is shown that a change in the deposition flux and the simulation cell size does not lead to a change in the composition of nanofilms and their contact regions.
7. An increase in the deposition rate above the critical value causes the coagulation of the deposited atoms in the evaporation region and affects the layers structure and composition, especially during prolonged deposition on the nanosystem upper layers.

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