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Simulation of temperature distribution in a functional NbN nanoelement with an embedded normal metal region

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A simulation of the temperature distribution in a functional NbN nanoelement with a built-in normal metal region has been carried out. The functional element consists of two NbN nanowires with a thickness of 4 nm, located on a substrate of monocrystalline Al_2O_3 . The wires are separated by a 10 nm thick dielectric layer. A region of normal metal is embedded in the lower nanowire using the ZA technology. An approximate estimate of the performance of functional nanostructures, for the creation of which such a hike is used, is given.

Keywords: Thin superconducting NbN films, functional superconducting nanoelements from NbN, modeling of thermal processes.

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1. Introduction

The application of the developed by the Kurchatov Institute „selective substitution of atoms“ (SSA) allows to change locally the composition and, consequently, properties of thin-film materials [1]. The use of this method makes it possible to create modified areas in nanoconductors made of thin-film NbN, which exhibit resistive properties at low temperatures. Also, SSA technology allows manufacturing not only single-layer, but also multi-layered structures. Thus, it is possible to create passive [2] (resistance), and active (logic elements „NOT“, „AND“, „OR“) functional nanoscale elements. If you alternate nanoconductors with and without built-in modified areas in a certain way, you can achieve the effect of adjacent nanoconductors on each other. The switching mechanism in such elements is based on the thermal action of the control element („shutter“) on the controllable element (the superconducting channel of the adjacent nanowire) which causes the latter or part of it to heat to a critical temperature for its transition from superconducting state to normal. In work [3] it has been shown that embedding the normal metal regions into the superconducting wire leads to a decrease in the critical current value, which is likely to be associated with heat generation in the normal metal area. In work [4] a single-layer functional multistage nanoscale element was described, which was created using SSA technology and performed the logical „NOT“ function. However, the arrangement of the heated nanowire and shutter in the same plane [4] is not optimal in terms of minimizing unit element switching energy. As shown in work [4], the minimum switching power is characteristic of two-layer vertical structures, as the shutter and the heated

nanowire are under each other and separated by a thin dielectric layer. The purpose of this work is to describe the heating process in such a vertical geometry, which is the closest to the forward-looking arrangement of the elements in terms of minimizing the power required to switch the superconducting conductor to the normal state.

This paper is devoted to modelling the process of heat separation and propagation in a functional nano-element of NbN with a built-in normal metal region. The element is embodied in the form of a NbN nanowire located on a monocrystalline sapphire substrate, in which a resistive area is created by the SSA method. Above it through a separating dielectric layer (Al_2O_3 10 nm thick) is a second superconducting NbN nanowire 4 nm thick. General view of the setup is shown in Fig. 1. Near-critical DC current is passed through the lower nanowire. Since exclusively thermal calculation is carried out in the work, no current is passed through the top nano-conductor. In the process of operation of the real device, a current close to the critical is also flowing along the upper nano-conductor, but there is no heat dissipation, because the upper nano-conductor is in a superconducting state.

The results can then be used to design topologies for both single-layer and multi-layer structures.

2. Simulation

The simulation was done using the technique described in detail in [5], that is, the heat conductivity equation was used to distribute the heat along the calculation line

$$J^2\rho + \kappa \frac{\partial^2 T}{\partial x^2} + \frac{\alpha}{d} (T - T_{sub}) = \frac{\partial cT}{\partial t}.$$

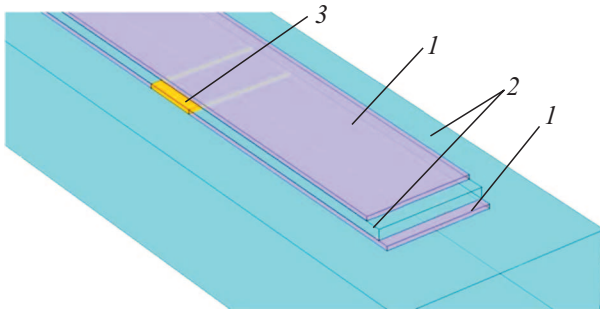


Figure 1. The general appearance of the simulated device is 1) NbN, nanowires, NbN, 2) substrate and separative dielectric layer Al_2O_3 , 3) area of the nanowire with the length of 50 nm built-in by the SSA method into the normal metal.

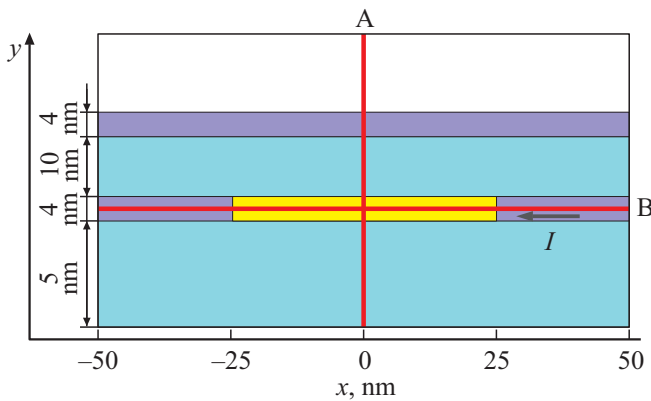


Figure 2. Longitudinal section of the simulated nano-element geometry. The red lines are the lines along which the calculation was made. The arrow indicates the current flow direction.

Here is the ρ — specific phase resistance, J — current density, κ — NbN thermal conductivity ratio, α — boundary thermal conductivity between NbN and sapphire, d — wire thickness, c — heat capacity of a unit with the capacity of NbN, T_{sub} — temperature of substrate (or separative layer Al_2O_3). The right side of the equation describes changes in local energy density. In the left side of the equation, the first term describes the Joule heating. This heating is constantly occurring in the modified area. The second component describes the heat distribution along the calculation line. The third component describes the propagation of heat into the sapphire substrate and dielectric separative layer (since the substrate and separation layer material are the same). It should be noted that since the simulation of the total volume represented requires considerable computing power, the calculation was made only along the lines A and B of the longitudinal section of the functional element (see Fig. 2). The calculation along the A line allows to estimate the temperature distribution in all layers of the functional element. The calculation along the B line allows you to estimate the time required to warm the heating element to a temperature above T_c . In addition, it is possible to estimate the size of the area adjacent to the heating element of the lower nanowire,

which goes into normal condition and begins to take part in heating itself. It should also be noted that there are two important differences from the case described in work [5]. The first difference is that in the simulated device the modified area (heating element) is permanently integrated into the superconductor. The second important difference is that we pass direct current through the conductor. We also took into account the dependence of ρ and κ on the temperature and condition (superconducting or normal) of the wire section. Electrical resistivity ρ is defined as zero if the temperature of the site is lower than T_c , and is $3 \cdot 10^{-6} \Omega \cdot \text{m}$ if the temperature of the site is above T_c . The coefficient of thermal conductivity κ for NbN is determined by the Wiedemann–Franz law (when the conductor is in normal condition). For superconducting states we have used the same dependency as in [5]: $\kappa_s/\kappa_n = T/T_c$ (where κ_n — conductivity ratio is in normal condition, and κ_s — in superconductive condition). In the simulated device the current is passed only on the lower nanowire. In this work we calculate only with respect to the thermal heating of the upper nanowire or its part up to T_c . In real devices, the current close to I_c will pass through the top nanowire. Heating the wire part above T_c should lead to an increase in the current density in it. Increasing current density will lead to the destruction of superconductivity. The destruction of superconductivity in the top nanowire of the simulated device is its actuation, so we do not take into account the current flow in the top nanowire.

The temperature of all components of the functional element was set at 4.2 K as initial conditions. Since the geometry of the functional layers is significantly extended in real devices for electrical interfacing with measuring devices, a constant temperature of 4.2 K was set as boundary conditions on the edges of the simulated element. The T_c value for all NbN wires was 6.2 K, which was taken from $R(T)$ measurements for NbN films of a given thickness [6].

3. Results and discussion

The main task of the paper was to study the temperature distribution in a functional nano-element: it was necessary

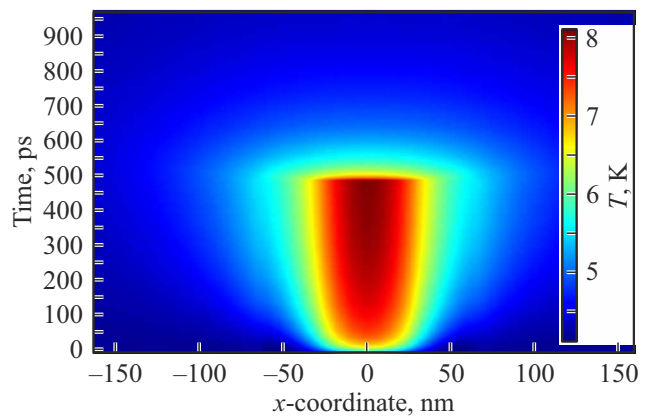


Figure 3. Simulation results along B line (heating and cooling of the heating element).

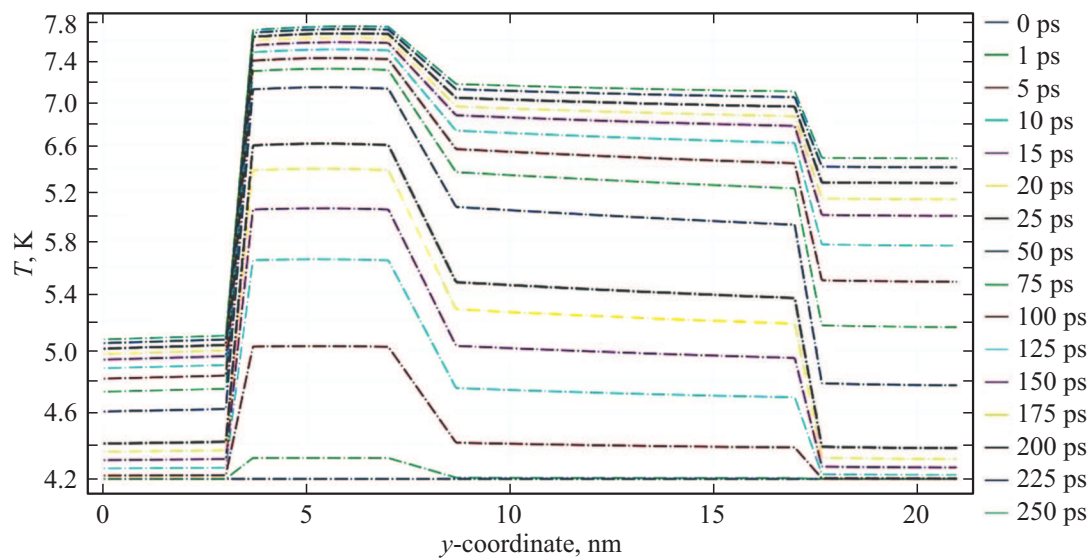


Figure 4. Simulation results along A line for heating the entire system.

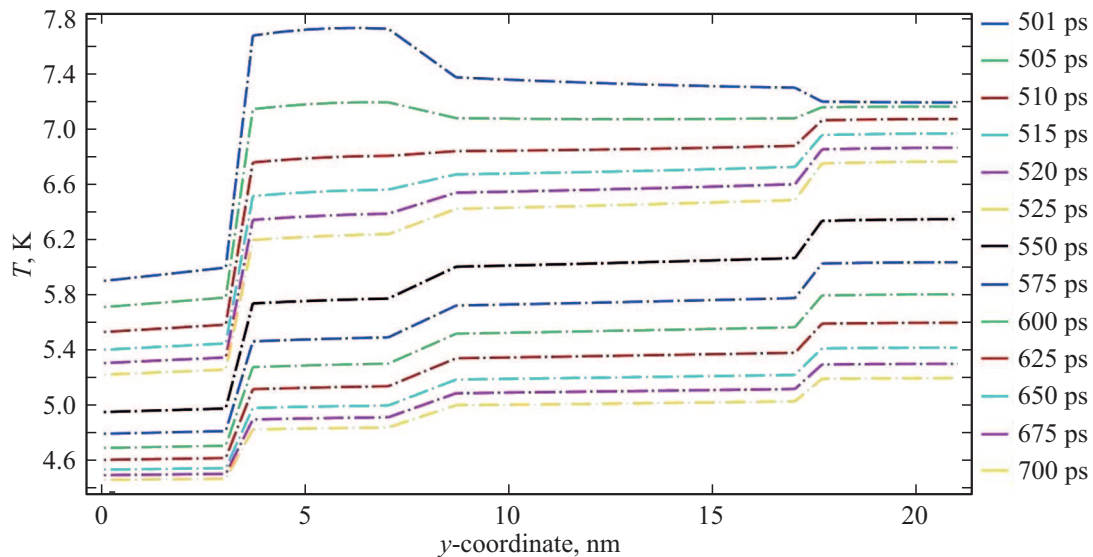


Figure 5. Simulation results along the line A for heating the entire system.

to find out whether the upper NbN layer (or at least part of it) was warming up to temperatures above T_c . It was also necessary to find out the characteristic heating and cooling times of both the directly heating element and the upper nanowire to a temperature of T_c to determine the possible frequency range of operation of logic devices without galvanic communication, which are produced by the SSA method and use thermal heating to switch the corresponding elements.

The results of heating simulation along the **B** line are given in Fig. 3. The current passed through the nanowire was $20 \mu\text{A}$, which corresponds to $\sim 0.9I_c$ of actually manufactured nanowires of NbN with a given geometry. The current passed the first 500 ps, after which the transmission of current ceased. The graph shows that the normal metal area warms up to a temperature of 8 K, which exceeds T_c

of the original NbN. Areas adjacent to the heating element become normal, and they themselves begin to participate in the Joule heating.

The results of heating simulation along the line **A** are given in Figs. 4 and 5. Graphs illustrate the temperature distribution from the substrate to the top of the whole geometry at different times. Fig. 4 describes heating and Fig. 5 — cooling. Four different areas are clearly visible. From left to right: substrate Al_2O_3 , heating element (normal metal area), separator dielectric Al_2O_3 , and finally top layer of NbN. From the graphs it is seen that the influence of the heater on the upper layer of NbN begins after ~ 50 ps. The temperature of the upper layer approaches that of T_c after 150 ps value. After the current is removed, the cooling process begins (Fig. 5), and the temperature in the area of the upper nanowire drops below T_c for about 75 ps.

Simulation results suggest that the full heating-cooling cycle for the upper NbN layer (in the functional element it is a heat-switched element) takes $\sim 150\text{--}200$ ps. In real devices, the operating temperature of the entire device may be higher than 4.2 K and be 0.8–0.9 from T_c , so it is possible to reduce, the heating–cooling cycle time. In addition, it is possible to reduce the thickness of the interlayer dielectric to 3–5 nm, which should also reduce the heating time of the upper layer.

4. Conclusion

The results obtained on temperature distribution along the transverse section of the functional nano-element can be used to calculate the critical current density in the upper nano-conductor. This will allow to realize its transition to a normal state taking into account the amount of current flowing through it. This calculation will give more realistic values of the time of switching the upper nanowire to the normal state and back.

The real devices will operate at temperatures above 4.2 K ($\sim 0.8T_c$). In each of the nanowires included in the device, as the temperature rises, the critical current density will drop, and therefore the critical current will also decrease. To account for this effect, it is necessary to experimentally measure the temperature dependence of the critical current density for each of the nanowires. Based on the results of this work and experimental data, the model will need to take into account the current flow on the upper nanowire.

Functional nano-elements manufactured with SSA technology have different geometries. They may also have different positions relative to each other. The obtained results will optimize their location and geometry, as well as take into account the possibility of mutual influence.

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Conflict of interest

The authors declare that they have no conflict of interest.

References

- [1] B.A. Gurovich, K.E. Prihod'ko, M.A. Tarkhov, A.G. Domantovsky, D.A. Komarov, B.V. Goncharov, E.A. Kuleshova. *Micro Nanosystems* **7**, 172 (2015).
- [2] B.A. Gurovich, B.V. Goncharov, M.M. Dementyeva, K.E. Prihodko, L.V. Kutuzov, D.A. Komarov, A.G. Domantovsky. *IOP Conf. Ser.: Mater. Sci. Eng.* **699**, 012016 (2019).
- [3] B.A. Gurovich, K.E. Prihodko, B.V. Goncharov, M.M. Dementyeva, L.V. Kutuzov, D.A. Komarov, A.G. Domantovsky, V.L. Stolyarov, E.D. Olshansky. *ZhTF* **90**, *11*, 1860 (2020) (in Russian).
- [4] B.A. Gurovich, K.E. Prihodko, L.V. Kutuzov, B.V. Goncharov. *FTT* **62**, 9, 1420 (2020) (in Russian).
- [5] J.K.W. Yang, A.J. Kerman, E.A. Dauler, V. Anant, K.M. Rosfjord, K.K. Berggren. *IEEE Trans. Appl. Supercond.* **17**, 2, 581 (2007).
- [6] B.V. Goncharov, B.A. Gurovich, K.E. Prihodko, M.M. Dementyeva, V.L. Stolyarov, E.D. Olshansky, A.G. Domantovsky, L.V. Kutuzov, E.M. Malieva, A.A. Cherepanov. *IOP Conf. Ser.: Mater. Sci. Eng.* **1005**, 012023 (2020).