19,12

Modeling of thermal processes in a multilayer logic nanoelement consisting of NbN nanowires located in various functional layers and separated by a layer of Al_2O_3 dielectric

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A simulation of the temperature distribution in a three-layer functional nanoelement consisting of NbN nanowires separated by layers of Al_2O_3 has been performed. A nanowire with a built-in area of normal metal is located in the middle layer of the device. The simulation is performed for all three wires included in the device. A constant current of ≈ 0.9 from the I_c was passed through each of the wires. The time of transition of the upper nanowire to the normal state as a result of heating is estimated, taking into account its gradual warming up and the dependence of I_c on temperature.

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

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1. Introduction

Superconducting nanoscale NbN wires are widely used in cryoelectronics [1–3]. „Selective atom substitution“ (SAS) procedure developed by the Kurchatov Institute allows to change locally the composition and, consequently, properties of thin-film materials [4]. In particular, the use of this method makes it possible to create local modified areas in nanowires made from thin-film NbN, which exhibit resistive properties at temperatures below Tc of the wire itself. Also, the SAS procedure allows to produce multilayer functional nanostructures [5]. The SAS procedure offers the opportunity of creating both passive and active functional nanoscale elements. The switching mechanism in such elements is based on thermal effect of a control element („shutter“) on a controlled element (a superconducting channel of the adjacent nanowire) resulting in heating of the latter or its part to a critical temperature for its transition from superconducting to normal state. In [6], heating of a two-layer element was simulated and heating time was estimated for the whole nanowire heated up to T_c, however, the study did not consider current flow in the upper (switchable) nanowire, while current $\approx 0.9I_c$ flows in the switchable nanowires in real devices. Since switching in the element occurs due to heat exposure, to reduce the consumed power per single switching, it is reasonable to place a heating element between two superconducting wires. Such placement of the „shutter“ allows to switch two nanowires (located above and below the heater) simultaneously.

This study is devoted to simulation of heat release and propagation process in a multilayer logic nanogate consisting of NbN nanowires placed in various functional layers and separated by dielectric Al_2O_3 layers. The element consists of three NbN nanowires placed on a single-crystal sapphire substrate. A resistive region is created by the SAS method in the wire placed in the middle layer. The second and third superconducting NbN nanowires are placed on top and bottom through the separating dielectric layer (Al_2O_3, 10 nm). Each NbN wire is 4 nm in thickness. General view of the setup is shown in Figure 1. Near-critical DC current is applied via the middle nanowire. DC current $\approx 0.9I_c$ is also applied via the top and bottom nanowires.

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

2. Simulation

The simulation procedure is described in detail in [7], i.e. for heat distribution, the following thermal conductivity equation was used

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

Here, J is the current density, ρ is the resistivity of an area, κ is the thermal conductivity coefficient of NbN, α is the boundary thermal conductivity between NbN and sapphire, d is the wire thickness, c is the heat capacity per unit volume of NbN or unit volume of separating Al_2O_3

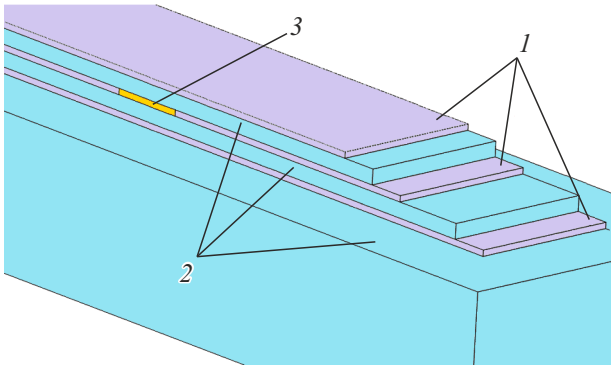

Figure 1. General view of the simulated device: 1) NbN nanowires, 2) substrate and Al_2O_3 separating dielectric layer, 3) normal metal section 50 nm in length built-in the nanowire by the SAS method.

layer (for the case of calculation in the NbN layer plane), T_{sub} is the substrate (or separating Al_2O_3 layer temperature); x describes the coordinate along the calculation line and is not associated with the coordinates shown in Figure 2. The right-hand side of the equation describes local energy density variations. In the left-hand side of the equation, the first term describes the Joule heating. This heating is a continuous process in the modified region and in the sections of the switchable nanowire whose temperature is $\geq T_c$. The second term describes the heat distribution along the calculation line. The third term describes the heat propagation into the sapphire substrate and separating dielectric layers. thermal conductivity data for Al_2O_3 substrate obtained in [8] were also used herein. Despite the fact that the substrate material is single-crystal Al_2O_3 and the separating layer material is Al_2O_3 produced by the atomic layer deposition method, dependences in the temperature range 4.2–20 K are probably very close to each other. Therefore, the same values were used for the separating layers and substrate. It should be noted that since the simulation of the total volume represented requires considerable computing power, the calculation was made only along lines A and B of the longitudinal section of the functional element (see Figure 2). The calculation along line A allows to estimate the temperature distribution in all layers of the functional element. For calculation along line A, which lies in the direction normal to the NbN layer plane, third-order boundary conditions were used ($\alpha(T_{sub}-T)$in our case): T_{sub} value was used for each of the interfaces in each design point of time. α value was constant (though it depends both on temperature and state) and was taken from [7]. The calculation along line B allows you to estimate the time required to heatup the heating element to a temperature above T_c and to estimate the temperature to which it is heated up. It should also be noted that there are two important differences from the case described in [7]. The first difference is that the modified area (heating element) in the simulated device is permanently integrated into the superconductor. The second important difference is that direct current is applied via each of the conductors. We also took into account the dependences of ρ and κ on the temperature and state (superconducting or normal) of the wire section. Resistivity ρ was assumed equal to zero if the temperature of the section was lower than T_c, and to $3 \cdot 10^{-6}\,\Omega \cdot$ m if the temperature of the section was above T_c. The modified wire section is always in normal state, its measured resistance per square was $6 \cdot 10^{-6}\,\Omega \cdot$ m. Thermal conductivity coefficient κ for NbN is determined by the Wiedemann–Franz law (when the conductor is in normal state). For the superconducting state, the same dependence as in [5] was used: $\kappa_s/\kappa_n = T/T_c$ (where κ_n is the thermal conductivity coefficient in the normal state, and κ_s — in superconducting state).

As opposed to [6], where heating of the whole switchable nanowire above T_c was calculated, current $\approx 0.9 I_c$ flowing via the switchable nanowires was taken into account herein. When a pat of the switchable wire is heated above T_c, current density is redistributed into the remaining part and the current density may exceed the critical value. In addition, during heating of the switchable wires up to T_c, I_c of its heated part will decrease. I_c values for superconducting wires (without built-in resistive region) were taken from the measured dependences of I_c on temperature (measurements are shown in Figure 3). The time of transition of the top wire can be defined as a point at which more than 10

Simulation was carried out for 2 temperatures 4.2 K and 5.5 K. As initial conditions in terms of temperature, the temperature for all components of the functional element was set to 4.2 K or 5.5 K. Since the geometry of the functional layers is significantly extended in real devices for electrical interface with measuring systems, a constant temperature of 4.2 K or 5.5 K was set as boundary conditions on the edges of the simulated element.

In the previous study of the authors [6], T_c of films was equal to 6.2 K, however, such low value was associated with non-optimum parameters of the film deposition parameters, because the films are deposited by the cathode sputtering method at low deposition temperatures (20–200°C). After

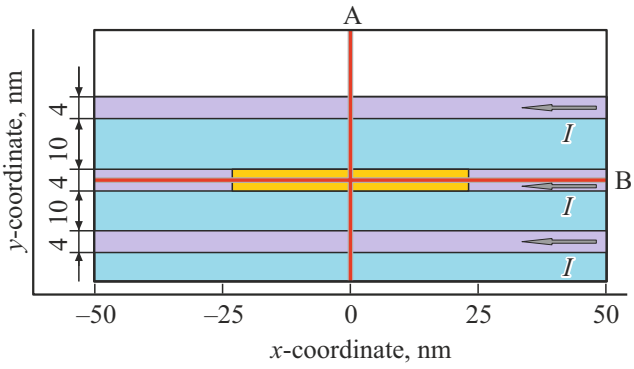

Figure 2. Longitudinal section of the simulated nano-element geometry. Red lines are the lines along which the calculation was made. The arrow indicates the current flow direction.

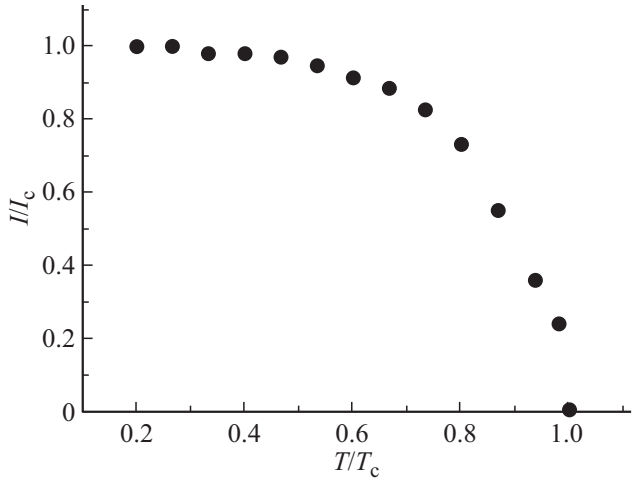

Figure 3. Measured decrease in the critical current at the temperature approaching T_c.

optimization of the deposition modes, measurements of $R(T)$ gave $T_c = 8.5$ K for NbN films of this thickness. This value was used for all superconducting nanowires.

3. Findings and discussion

The main objective of the study was to investigate the temperature distribution in a functional nano-element: it was necessary to determine the time spent to heat up 10% of the switchable NbN layer up to temperatures above T_c. Estimate of this time will help determine a possible operating frequency range of not conductively coupled logic gates which are produced by the SAS method and use thermal heating to switch the corresponding elements. Also, the maximum heating temperature of the heating element and also of the top/bottom nanowire should be determined.

The results of the heating simulation along line B line are given in Figure 4. The current applied through the nanowires was 20 μA, which corresponded to$\sim 0.9I_c$ of actually manufactured NbN nanowires with a pre-defined geometry. The diagram shows that the normal metal area warms up to 14 K, which considerable exceeds T_c of the original NbN.

The results of the heating simulation along line A for the top nanowire are shown in Figures 5 and 6. The diagrams illustrate the temperature distribution from the bottom to the top edge of the superconducting wire at different times. Figure 5 describes heating from the initial temperature of 4.2 K, and Figure 6 — from 5.5 K. We are interested in the point at 0.4 nm from the lower boundary of the wire (the points are shown in the illustrations)at which 8.5 K is reached (measured T_c of NbN films). The results of the heating simulation along line A for the bottom nanowire are shown in Figures 5 and 6. Generally, the results are the same subject to the caveat that the times required for heating up move upwards by 1–2 ps. This is likely caused by the effect of bulk Al_2O_3 substrate.

The simulation suggests that the time required for device actuation is $\sim 9-10$ ps for the initial temperature 4.2 K, and $\sim 6-7$ ps for 5.5 K. In [6] heating of the whole heated nanowire above T_c was calculated, and the result showed that the required time was ~ 150 ps. Consideration of the current flow and current density distribution over the superconducting switchable conductors has a significant effect on the assessment of the single switching time. Certainly, the total actuation time is also affected by the time required for the whole device to cool down and reset. This time can be considered, if the a description of the signal source, including the parameters of control signals, is added

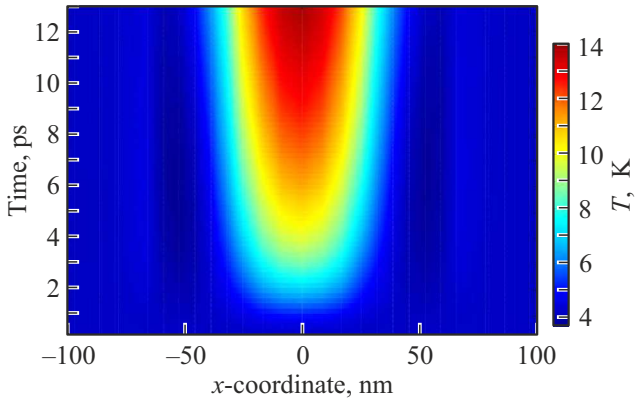

Figure 4. Simulation results along B line (heating of the heating element).

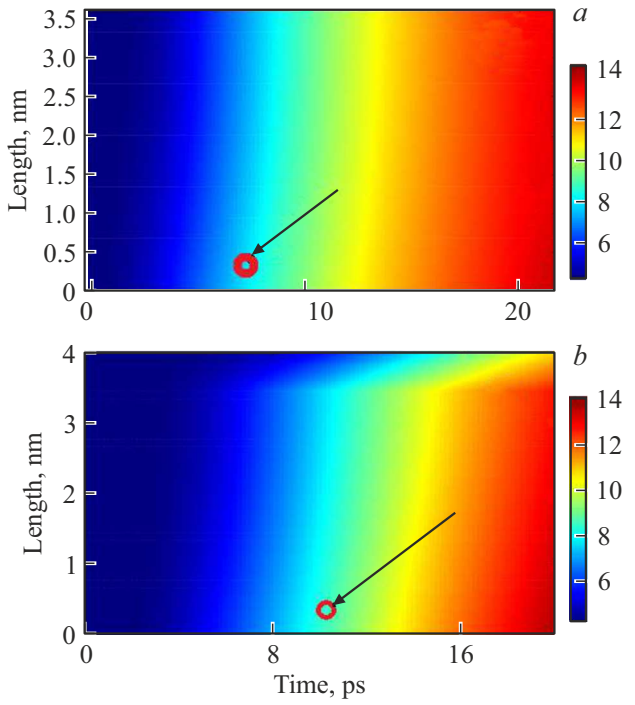

Figure 5. Simulation along line A for heating the top (a) and bottom (b) nanowire for the initial temperature of 4.2 K. The highlighted points are explained in the text.

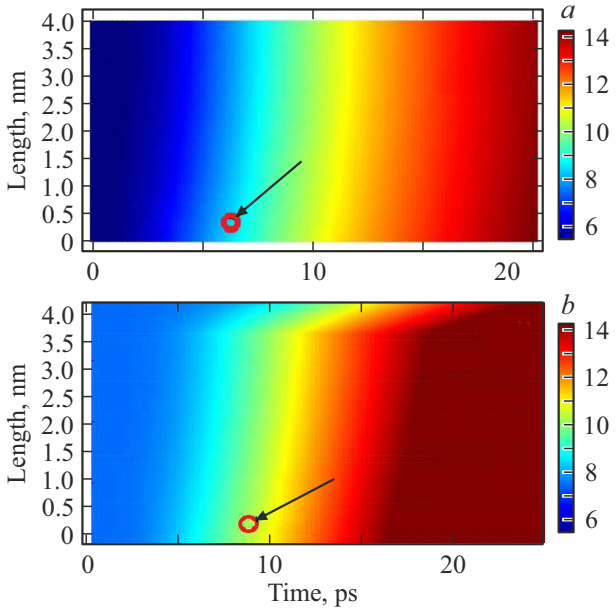

Figure 6. Simulation along line A for heating the top (*a*) and bottom (*b*) nanowire for the initial temperature of 5.5 K. The highlighted points are explained in the text.

to the model. current-limiting resistances incorporated in the real devices shall be also described. The work in this area will be continued.

4. Conclusions

The findings obtained herein regarding the temperature distribution along the transverse sections of the functional nano-element may be used to estimate the actuation time for the multilayer functional nano-elements described above.

Functional nano-elements manufactured using the SAS technology have different geometries. They may also have different positions relative to each other. The findings will help optimize the location and geometry of the nano-elements, as well as take into account possible mutual influence of the elements.

Conflict of interest

The authors declare that they have no conflict of interest.

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