JOURNAL OF ENGINEERING SCIENCES

Volume 10, Issue 1 (2023)

Antonyuk V. S., Bondarenko I. Iu., Vislouh S. P., Voloshko O. V., Bondarenko M. O. (2023). Heat exchange in a contact zone of nanoinstrumentation with elements of the microsystem technology. Journal of Engineering Sciences, Vol. 10(1), pp. F1-F6, doi: 10.21272/jes.2023.10(1).f1

Heat Exchange in a Contact Zone of Nanoinstrumentation with Elements of the Microsystem Technology

Antonyuk V. S.[1][0000-0003-0690-2411], Bondarenko I. Iu.[2][0000-0002-5179-8329], Vislouh S. P.[1][0000-0002-2204-2602], Voloshko O. V.[1][0000-0002-1067-2615], Bondarenko M. O.[3][0000-0002-5927-0326]

[1] National Technical University of Ukraine “Igor Sikorsky Kyiv Polytechnic Institute”, 37, Peremohy Ave., 03056 Kyiv, Ukraine;
[2] State Scientific Research Institute of Armament and Military Equipment Testing and Certification, 164, Chornovil St., 18028 Cherkasy, Ukraine;
[3] Cherkasy State Technological University, 460, T. Shevchenka Blvd, 18006 Cherkasy, Ukraine

Article info:
Submitted: February 24, 2023
Received in revised form: May 8, 2023
Accepted for publication: May 18, 2023
Available online: May 23, 2023

***Corresponding email:**
victor.antoniuk@gmail.com

Abstract. Theoretical studies of physical processes and phenomena in the zone of physical interaction of nanoinstruments with the surfaces of elements of microsystem technology are carried out in work. Based on the conducted research, mathematical models of energy heat exchange in the zone of physical contact of nanometric dimensions were compiled, and their analytical solution was obtained using the Fourier method of separation of variables and Goodman’s integral method. Simultaneously, the energy components of the processes in the nanocontact zone were considered. The numerical solution of the mathematical model of energy heat exchange in the zone of physical nanocontact was carried out using a software application based on the finite element method. The results were checked according to the equivalent thermal scheme to confirm the adequacy and accuracy of the obtained models. As a result, the mechanisms of energetic interaction of the nanoinstrument with the surfaces of the elements of microsystem technology devices were clarified. It is shown that the use of the proposed method of equivalent thermal circuits for the evaluation of mathematical models of the energy interaction of nanoinstruments with the surfaces of microsystem technology device elements, as well as the further study of the distribution of thermal fields in the nanocontact zone, differs from other numerical and analytical methods in terms of sufficient accuracy and speed of calculations. At the same time, it was established that the discrepancy between the results of mathematical modeling and the results obtained according to the equivalent thermal scheme does not exceed 5-8 %.

Keywords: energy heat exchange, mathematical modeling, physical contact, thermal energy, process innovation, equivalent thermal circuit.

1 Introduction

The intensive development of modern microelectronics and microsystem technology requires modern engineering sciences and technologies to comply with strict requirements for further miniaturization, increasing the functionality and manufacturability of elements of microdevices and systems based on them [1].

Compliance with such requirements is due, first of all, to the qualitative and quantitative growth of indicators of operational parameters of these devices, such as [2]: operating speeds, frequencies, and duration of operation, with a simultaneous increase in indicators of their reliability and accuracy. Simultaneous fulfillment of such mutually exclusive requirements is possible by observing the high stability of geometric shapes and sizes, as well as the physical and mechanical characteristics of microsystem technology devices in the process of their manufacture and operation [3, 4]. This, in turn, requires considering various physical processes that occur during the contact interaction between the elements of microsystem technology devices, both during their operation and during the manufacture and control of these elements with specialized nanoinstrumentation.

At the same time, physical processes (especially energy ones) that occur in the contact zone of nanometric instruments with the surface are little studied and are limited by known laws, which are based on the laws of classical physics for macro-objects [5, 6].

2 Literature Review

The issue of mathematical modeling of energy processes in micro- and nanosystems was considered by many scientists, such as Awrejcewicz J., Belmiloudi A., Hegde V., Laurencot Ph., Nik K., Ravikumar H.M., Senturia S.D., Walker Ch. and others [7-10].

However, in the scientific works of these scientists, the thermodynamic processes that occur during contact in the zone of interaction of a nanometer-sized tool with elements of microsystem technology have not been investigated.

Thus, an urgent issue is developing a mathematical model of energy heat exchange in the zone of physical contact of nanometric instruments with the surfaces of elements of microsystem technology.

The work aims to increase the accuracy and speed of determining the parameters of stable operation of nanometric instrumentation during its contact with the surfaces of elements of microsystem technology by developing a mathematical model of energy heat exchange in the zone of their physical contact.

Therefore, in the presented work, mathematical (analytical and numerical) modeling of the energy interaction of nanoinstruments with the surfaces of elements of microsystem technology is carried out, and the results are confirmed by the method of equivalent thermal circuits.

Thermal calculations are based on a complex of nonlinear, non-stationary equations that consider the nanotool's shape, dimensions, and thermophysical characteristics and the surfaces with which the interaction occurs [11].

Simultaneously, only heat exchange by heat transfer was considered (convective and radiant types of heat exchange were not considered due to their insignificance). It also does not take into account the energy impact on the nanotool and the surface in the contact zone from the action of external electric and electromagnetic fields when conductive diamagnets are in contact or, in the case of dielectric diamagnets, due to their insignificant effect due to the additional neutralization of surface charges during the interaction of the nanotool with the surface [12].

Conducting thermal calculations consists of compiling and analytically solving mathematical models of heating individual elements of microsystem technology devices when a nanoinstrument acts on them with the involvement of the inverse integral Fourier transform method [13].

Among the elements for which thermal calculations were carried out [14] is the surface of the object of interaction, the tip of the tool, and the cantilever, to which the nanotool is attached.

3 Research Methodology

3.1 General formulation of a problem

The electrically conductive (Au-999 gold coating) surfaces of the conductive collector's rings (3×3.0×0.1 mm) with an atomically smooth surface were chosen as model elements that were affected by the nanoinstrument. CSC38/No Al (Mikrotech) cantilever with a length of 12–18 μm and a conical tip made of single-crystal (n-Si(111) silicon), with a radius of 8 nm and a tip angle of 40° placed at its end was chosen as the tool model. Such a tool can be used as a measuring tool in scanning probe microscopy and for surface modification of surfaces in nanoprocessing technologies. The energy scheme in the zone of contact of nanometric dimensions is shown in Figure 1.

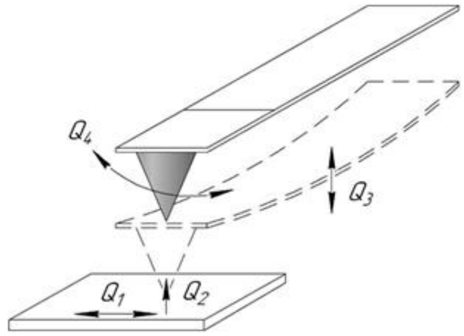

Figure 1 – Scheme of heat exchange in the zone of physical contact of nanometric dimensions (heat losses: Q_1 – during mechanical friction of the nanotool on the interaction surface; Q_2 – under the action of electromagnetic fields and electric charge; Q_3 – when bending the nanotool; Q_4 – when turning the nanotool)

3.2 Mathematical model of heating an interaction object

The thermal effect on the object of interaction (sample) is carried out by physical friction of the nanotool on its surface during the interaction of this sample in the contact mode. The total heat flow is uniformly distributed in the study area over the sample's surface (Figure 2).

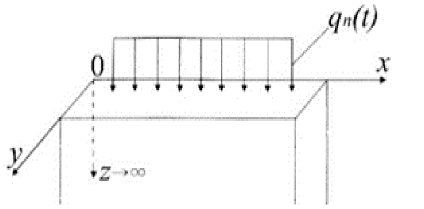

Figure 2 – Scheme of heating the working surface of the sample: $q_n(t)$ – the surface heat flux density, W/m^2

It is assumed that $\partial T/\partial x = \partial T/\partial y = 0$ (heat distribution occurs only in the depth of the plate) and $\delta = 2(a_0{}^2\tau)^{½} << H$ (thermal effects are superficial, and heat exchange on the bottom side of the plate is not considered).

The equations of the mathematical model of sample heating (thick plates) have the following form:

$$C_V(T)\frac{\partial T}{\partial t} = \frac{\partial}{\partial z}\left[\lambda(T)\frac{\partial T}{\partial z}\right],\ t>0,\ 0<z<+\infty. \quad (1)$$

$$-\lambda(T)\frac{\partial T}{\partial z}\Big|_{z=0} = q_n(t); \quad T|_{t=0} = T_0;$$
$$T \to T_0,\ \frac{\partial T}{\partial z} \to 0,\ z \to +\infty. \quad (2)$$

Taking into account $C_V(T)$ and $\lambda(T)$, as well as using the direct-inverse cosine Fourier transform along the z coordinate [15, 16], using the sequence of actions considered in [17], we find a general solution to the original problem:

$$T(z,t) = \left[T_0^{\nu+1} + \frac{(\nu+1)a_0 q_{n0}}{\sqrt{\pi}\lambda_0}\int_0^t \frac{e^{-\frac{z^2}{4a_0^2(t-\tau)}}}{\sqrt{t-\tau}}d\tau\right]^{\frac{1}{\nu+1}}. \quad (3)$$

3.3 Mathematical model of heating a cantilever

During the operation of the nanoinstrument, a uniformly distributed heat flow arrives on the free (unfixed) surface of its cantilever $q_n(t)$ (Figure 3):

$$q_n(t) \equiv q_{n0} = \frac{P_0}{B \cdot H}, \quad (4)$$

where P_0 – the power of the heat flow acting on the cantilever from the outside, W.

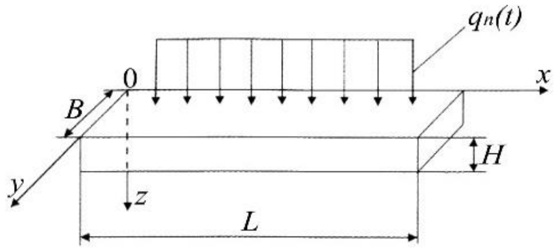

Figure 3 – Scheme of heating the free surface of the cantilever: B, H, L – width, thickness, and length of the cantilever, respectively, m; $q_n(t)$ – the surface heat flux density, W/m^2

As a model, a plate is considered, for which heat distribution occurs only deep into the plate: $\frac{\partial T}{\partial x} = \frac{\partial T}{\partial y} = 0$, as well as the depth of the zone of thermal influence $\delta = H$, i.e., heat exchange on the bottom side of the plate, is considered. When interacting with the plate, it is assumed that radiation heat exchange with the surrounding medium occurs on the plate's bottom side.

To find the values of $T(z, t)$, the following nonlinear equations of thermal conductivity are used [17]:

$$C_V(T)\frac{\partial T}{\partial t} = \frac{\partial}{\partial z}\left(\lambda(T)\frac{\partial T}{\partial z}\right),\ t>0,\ 0<z<H \quad (5)$$

with the initial condition

$$T|_{t=0} = T_0 \quad (6)$$

and boundary conditions

$$-\lambda(T)\frac{\partial T}{\partial z}\Big|_{z=0} = q_n(t);\ \lambda(T)\frac{\partial T}{\partial z}\Big|_{z=H} = \varepsilon\bar{\sigma}(T_0^4 - T_c^4)|_{z=H}, \quad (7)$$

where T_c is the ambient temperature, K; $\lambda(T)$, $C_V(T)$ are thermal conductivity coefficient, W/(m·K), and volumetric heat capacity, J/(m^3·K), of the plate material, respectively; ε is the blackness coefficient of the radiating surface; $\sigma = 5.67 \cdot 10^{-8}$ W/(m^2·K^4) is the Stefan–Boltzmann constant.

At the same time, empirical dependencies $C_V(T) = C_{V0}T\nu$, $\lambda(T) = \lambda_0 T_n$ [18] are taken into account in equations (5)-(7).

To solve the formulated nonlinear thermal problem (5)-(7), the method of substitution of variables, the Goodman integral method [19], and the previously mentioned method of Fourier transformation [20] were applied for the function $T(z, t)$ [17]:

$$T(z,t) = \left\{T_0^{\nu+1} + \frac{(\nu+1)q_{n0}}{\lambda_0}\left[\frac{a_0^2 t}{H} + \frac{3z^2 - H^2}{6H} + \frac{2H}{\pi^2} \times \right.\right.$$
$$\left.\left.\times \sum_{n=1}^{\infty}(-1)^{n+1}\frac{\cos\frac{\pi n z}{H}}{n^2}e^{-\left(\frac{\pi a_0 n}{H}\right)^2 t}\right]\right\}^{\frac{1}{\nu+1}}. \quad (8)$$

3.4 Mathematical model of heating a tip of the nanoinstrument

A solid hemispherical element of radius R in a range of 8-10 nm made of silicon is considered as the tip of the tool (Figure 4).

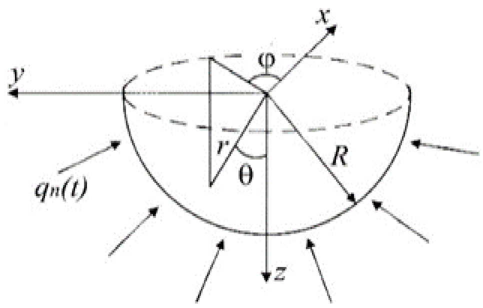

Figure 4 – Scheme of heating a hemispherical element: R – the radius of the element, m; $q_n(t)$ – the surface density of thermal influence, W/m^2; r, θ, φ – spherical coordinates

The depth of penetration of the heat wave into the tip $\delta = 2(a_0^2\tau)^{½} = 5.78 \cdot 10^{-9}$ m. Since the depth of penetration of the heat wave into the tip of the tool is less than its radius ($R > \delta$), it can be considered as a symmetric hemispherical element, the outer surface of which is heated by the heat flow arising as a result of the friction of this element on the surface of the sample. As a result, the total heat flow $\partial T/\partial\varphi = \partial T/\partial\theta = 0$, uniformly distributed over the surface, is formed. Convective and radiative heat losses are not considered.

Equations of the mathematical model of heat distribution in a hemispherical element have the form:

$$C_V(T)\frac{\partial T}{\partial t} = \frac{1}{r^2}\frac{\partial}{\partial r}\left[r^2 \cdot \lambda(T)\frac{\partial T}{\partial r}\right],\ t>0,\ 0<r<R; \quad (9)$$

$$T|_{t=0} = T_0;\ \lambda(T)\frac{\partial T}{\partial r}\Big|_{r=R} = q_n(t);$$
$$\frac{\partial T}{\partial r}\Big|_{r=0} = 0;\ T|_{r=0} \neq \infty. \quad (10)$$

Using the method of separation of variables (Fourier method [20]) and taking into account $q_n(t) \equiv q_{n0} = \text{const}$, as well as using the method of calculation according to formulas (1)-(3), the desired solution of the problem is obtained:

$$T(r,t) = T_0^{\nu+1} + \frac{(\nu+1)q_{n0}R}{\lambda_0}[\frac{3a_0^2 t}{10R^2} - \\ -\sum_{n=1}^{\infty}\frac{2R\sin\left(\mu_n \frac{r}{R}\right)}{\mu_n^3 \cos(\mu_n)R} \cdot e^{-\left(\frac{\mu_n a_0}{R}\right)^2 t}] \quad (11)$$

where μ_n – the root of the characteristic equation $J(\mu) = 0$.

4 Results

4.1 Numerical simulation results

For the numerical solution of the mathematical model of the process of heating nanoinstruments and elements of microsystem technology, the finite element method was used, which has proven itself well, for example, in researching new instrumental materials [22, 23].

The solution of the mathematical model of the energy effect in the zone of interaction of the nanoinstrument with the surface, as well as the study of the distribution of thermal fields, is implemented with the help of a software module [24]. The software module allows obtaining and investigating the thermal field distribution on the surface and in the volume of objects of nanometric dimensions with specified thermophysical properties.

Known values of geometric parameters and thermophysical characteristics of the materials from which both the elements of the nanometric tool and the objects with which this tool interacted and which are included in the expressions (3), (8), and (11) were used for the calculations. It was established that the most significant heat release occurs in the contact zone of the tool's tip with the surface (Figure 5).

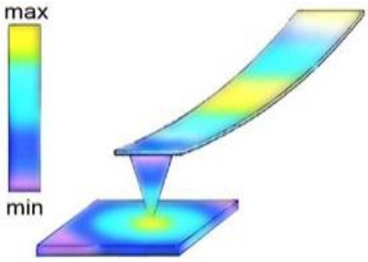

Figure 5 – Distribution of heat release in the zone of physical contact of nanometric dimensions (according to the results of analytical calculations)

4.2 Evaluation of the mathematical models

Mathematical heat exchange models were coordinated according to the heat balance scheme, in which the joint heat contribution was evenly distributed among all elements participating in heat exchange.

Simultaneously, the thermophysical properties of the materials from which these elements were not considered. An equivalent thermal scheme (Figure 6) was drawn up and investigated to assess the adequacy of the considered heat exchange models based on thermal resistances connected to a thermal network.

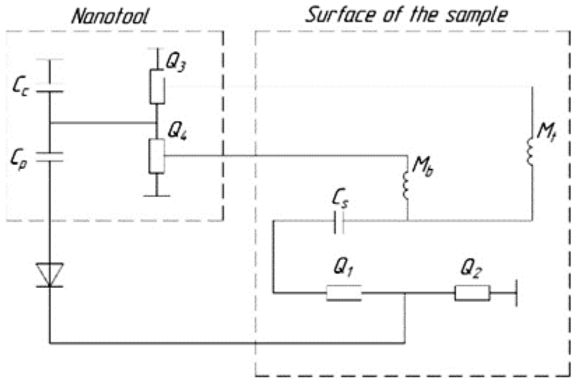

Figure 6 – Equivalent thermal scheme in the nanocontact zone (heat losses: Q_1 – during mechanical friction of the tip of the tool on the examined surface; Q_2 – under the action of electromagnetic fields and electric charge; Q_3 – when bending the cantilever; Q_4 – when the cantilever is twisted; C_c, C_p, C_s – specific heat capacities of the material of the cantilever, the tip of the tool, and the sample, respectively; M_b, M_t – energy dissipations resulting from the action of mechanical moments of bending and torsion of the cantilever)

Such a network simulates how heat flows are transferred into the nanocontact zone and provide an analogy of the heat flow with an electric current [25].

The diodes between the blocks on the equivalent thermal circuit are informative and determine the predominant direction of heat transfer between different functional blocks of the equivalent circuit.

After considering the features of the equivalent thermal scheme (Figure 6), the thermal models of heating in the nanocontact zone were compiled:

$$\begin{cases} C_s\left(\frac{dQ_1}{dt} + \frac{dQ_2}{dt}\right) = -\lambda_s(Q_1 + Q_2) + P_s; \\ \frac{C_s C_p C_c}{C_s C_p + C_s C_c + C_p C_c} \cdot \left(\frac{dQ_3}{dt} + \frac{dQ_4}{dt}\right) = -\lambda_c(Q_3 + Q_4) + P_c, \end{cases} \quad (12)$$

where C_p, C_s, C_c are coefficients of heat capacity of the materials of the tip of the tool, the sample, and the cantilever, respectively; λ_s, λ_c are thermal conductivity coefficients of sample and cantilever materials, respectively; P_s, P_c are heat losses on the sample and cantilever.

5 Discussion

System of differential equations (13) is the thermal model of heating individual elements in the contact zone of nanoinstrumentation with the surfaces of elements of microsystem technology.

The numerical solution of these systems of equations was carried out in the "ELCUT" software application and made it possible to conclude the primary heat consumption and energy impact in the zone of contact of the nanoinstrument with the surface.

It was established that the most significant heat release in the contact zone (about 70 %) occurs as a result of the friction of the nanotool on the surface, which is more than five times higher than the heat loss due to the bending of the cantilever, which fully confirms the results of the analytical calculation.

6 Conclusions

Thus, as a result of theoretical studies of thermophysical processes and phenomena that take place during the interaction of nanoinstruments with the surfaces of elements of microsystem technology, mathematical models of energy heat exchange in the zone of physical contact of nanometric dimensions were obtained, and their analytical solution was proposed.

A numerical calculation of the mathematical model of energy heat exchange in the zone of physical nanocontact was carried out. This calculation was carried out using the developed software application based on the finite element method.

The obtained analytical modeling results were checked using the equivalent thermal scheme, which allowed justifying the models' adequacy and accuracy. It is shown that the use of the proposed method of equivalent thermal circuits for the evaluation of mathematical models of the energy interaction of nanoinstruments with the surfaces of microsystem technology device elements, as well as the further study of the distribution of thermal fields in the nanocontact zone, differs from other numerical and analytical methods in terms of sufficient accuracy and speed of calculations.

It was established that the most significant heat release in the contact zone occurs due to the friction of the nanotool on the surface, which is more than five times higher than the second most significant heat loss, which occurs due to the bending of the cantilever. This fully confirms the analytical calculation results, and the discrepancy between the results of mathematical modeling and the results obtained by the equivalent thermal scheme is 5-8 %.

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