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PHYSICAL AND MATHEMATICAL MODELING OF UNSTEADY COUPLED HEAT AND MASS TRANSFER IN CVD-DIAMOND WINDOWS OF THE SIBERIAN CIRCULAR PHOTON SOURCE

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Abstract The results of physical and mathematical modelling in the ANSYS software package of three-dimensional unsteady coupled heat and mass transfer in the previously developed diamond vacuum window (DVW) of the workstation of the Siberian Circular Photon Source under construction are presented. Previous simulations have convincingly shown: the possibility of using a mini-channel cooling system to implement reliable and proper temperature management of this optical device, the advantage of a mini-channel cooling system over a one channel system in terms of fulfilling the optical requirements for DVW and its design. Here are detailed calculations of unsteady three-dimensional flow in the mini-channels of the cooling system, which will prevent possible dramatic destruction of the workstation due to local overheating of the CVD-diamond foil and its recrystallization.

Key words: cooling system, mini-channel, Siberian Circular Photon Source, Synchrotron.

AMS Mathematics Subject Classification: 76B47.

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1 Introduction

Calculation of non-stationary three-dimensional heat fluxes in coupled problems of heat and mass transfer becomes an integral part of the design of heat-stressed devices, in which there is a limitation both on the allowable temperature in local areas and on the magnitude of thermal deformations. An example of such devices that require reliable calculations of temperature fields and thermal deformations are the optical elements of workstations of synchrotron radiation sources (synchrotrons). Perhaps the main reason for the importance of such calculations is that they are unique and not previously used designs. Examples of both calculations and the uniqueness of devices are presented in [1-6]. And this is not surprising, since by the beginning of 2023 there were only twenty operating third-generation synchrotrons in the world and three fourth-generation synchrotrons: in Sweden, France, and Brazil. The designs of their workstations, which provide only relevant research, are unique, as they are located at the forefront of modern instrumental and technical capabilities. This paper presents the results of calculations and optimization of the most heat-loaded optical device of the Siberian Circular Photon Source (SKIF) workstations - a diamond vacuum window (DVW), separating a region with a high vacuum of 10^{-9} Pa.

SKIF is being built in the suburbs of Novosibirsk (Russia). At the first stage, six research workstations will be created to characterize the structure of objects in applied and fundamental science: materials science, new magnetic and superconducting materials, catalysts, current sources, nanoelectronics, geology, medicine, biology and archaeology. At several of the workstations, synchrotron radiation is produced by superconducting wigglers. In this case, the total radiation power approaches 49 kW, and the power density on the axis will be up to 92 kW/mrad^2. Thermal filters and DVWs are designed to absorb part of the radiation power on the order of hundreds of watts, up to a scale of 1 kW. The densities of thermal energy to be utilized are about 10 MW/m^2 [7-8]. All optical elements are subject to the most stringent requirements for reliability and, additionally, for maximum allowable strains. The requirements for admissible linear deformations caused by the emerging temperature gradients in the optical element body are sometimes less than 0.1 μm on length scales of the order of 100 mm, [5-6]. All of the above requires special approaches to the temperature management of workstation elements. This is what predetermines the need for physical and mathematical calculation of thermal and temperature fields.

Today, there are dozens of software systems that allow solving various problems of numerical simulation of physical processes. Two groups of complexes can be distinguished: CAD-systems (Computer-Aided Design) and CAE-systems (Computer-Aided Engineering). CAD-systems are software systems for preparing design drawings and 3D models. In turn, CAE-systems are designed for modeling and analysis of various physical processes. Such systems are based on physical and mathematical models, which are systems of partial differential equations, which are solved using the methods of finite differences, finite volumes and finite elements. One of the most complete computational software systems today is ANSYS, which combines both the features of a CAD-system that allows one to build various 3D-models, and a CAE-system that allows, among other things, numerical analysis of problems in continuum mechanics and provides wide opportunities for the preparation of geometric and grid models and subsequent processing of the calculation results, [9-10]. In addition, ANSYS is based on efficient parallelization algorithms.

To solve the problem, in this work, a special method for calculating unsteady coupled problems of heat and mass transfer was used, in which several modules of the ANSYS software package were used:

- the Design Modeler, which is used to create 2D/3D geometries, allowing one to import ready-made geometries from third-party CAD systems, as well as modify or simplify geometric models;

- the Meshing, which allows one to generate computational meshes taking into account a huge number of settings and parameters, including the use of various methods: 1) the Tetrahedrons method allows one to generate volumetric meshes with elements that have the shape of tetrahedra; 2) the Sweep method allows one to build a computational grid based on prismatic elements using the operation of pulling the elements of one layer along some axis; 3) The Hex Dominant method, which allows you to build computational grids based on hexahedra elements and can be used where the use of the Sweep method is impossible; 4) The Multi-

Zone method is based on block technology and provides automatic separation of geometry into two groups of geometric bodies [11];

- Fluent module designed to solve hydrodynamic problems and coupled heat transfer problems. It allows modeling a wide range of physical processes in liquids and gases, unsteady and turbulent processes in multiphase media.

In Ansys Meshing, elements can be tetrahedra, pyramids, hexahedra, prismatic elements [11]. Typical possibilities for building unsteady models in the Ansys Fluent shell are presented, for example, in [12, 13].

In the thermal management of optical devices using synchrotron radiation, one channel cooling techniques are most often used [5, 6]. This is due to the fact that one channel cooling techniques are quite simple and pragmatic, and also to the fact that the most heat-loaded devices have to be cooled, the total absorbed thermal power of which is 1-10 kW in order of magnitude. The characteristic transverse dimensions of the channels in these devices are significantly more than 1 mm, and the length is on a centimeter scale. However, one channel techniques are difficult to integrate into modern optical devices. The main reason for this is that the synchrotron radiation beam has dimensions that are smaller or much smaller than the channel size, and the dimensions of the object investigated area can even be several orders of magnitude smaller. Therefore, mini- and micro-channel cooling techniques are the most suitable in this case. Features of the calculation of flow regimes, heat transfer, hydraulic resistance of two-phase flow in mini- and micro- channel systems, as well as the size classification of channels can be found in [14-20].

When designing a DVW, it must be taken into account that the destruction of the CVD-diamond foil used in it leads to dramatic damage and destruction of not only the optical devices behind it and the sample under study due to a multiple increase in the radiation flux, but also the workstation elements located in front of it, due to the impact of the atmosphere penetrating into the zone, which was in a high vacuum. Synchrotron SKIF generation 4+ will operate at the limit of optical devices, as it is designed to provide workstations with the required quality optical beam of the maximum possible brightness. And high brightness leads to local release of high heat fluxes in the CVD-diamond foil. Local overheating from admissible values by only a few tens degrees will lead to localized recrystallization, a jump in the internal stress value in the foil and its destruction. That is why, the more accurately the physical and mathematical modeling of the cooling system is carried out, the more accurately the distribution of temperatures and stresses in the CVD diamond foil is predicted, the reliable the DVW will be designed.

Another important feature of heat transfer in the cooling system of the workstation optical devices, which is related to the fact that one is in a vacuum, is the presence of contact resistances between the optical element, the case, and the cooling system. This can significantly or even drastically impair heat transfer. However, the presence of contact resistances is a typical phenomenon for the operation of equipment in which there are high specific heat fluxes, for example, microelectronics. Methods for taking into account contact resistance at the designing of heat exchange devices are rapidly developing [21-23]. In practice, ones try to create metal or metal-like contacts that exclude the presence of the following types of gaps in the contact area: vacuum, gas, or non-metallic. For this, for example, welding, soldering or metal-containing thermal pastes are used. However, reliable methods for calculating such a phenomenon do not yet exist, and empirical corrections are introduced in the simulation.

There are very few examples of DVW physical and mathematical thermal modelling in the literature. The emphasis in them, most often, is on technical features and problems. We have previously carried out extensive modelling of three-dimensional unsteady coupled heat transfer in DVW for the SKIF workstation [5, 6, 24]. Examples of earlier DVW simulations for other synchrotrons are presented below shortly.

In study [25], the thermomechanical properties of DVW were optimized, which were planned to be applied at SPring-8, an accelerator complex with a third-generation synchrotron radiation source with the world's highest energy of 8 GeV, located in Hyogo Prefecture, Japan. Extensive calculations have been carried out for several beryllium and CVD-diamond foils. The glass thickness varied from 100 to 250 μm.

During the construction of the NSLS-II synchrotron at the Brookhaven National Laboratory, USA, numerical calculations were made of the absorption of the beam power part and heat removal from DVW, as well as from silicon carbide (SiC) foils, [26]. Calculations have shown that a DVW with a thickness of 1 mm CVD-diamond is able to absorb 850 W of energy, the maximum temperature in the DVW will be about 200°C. Approximately the same amount of energy can be absorbed by a 1 mm SiC filter, but the maximum temperature will be in this case 810°C.

Numerical simulation [2] by FEM of heat transfer in DVW was carried out when creating window samples capable of removing 600 W of thermal power released in diamond foil from a third-generation synchrotron radiation source ALBA (capacity storage ring 3 GeV, Spain). The diamond foil was placed between two Ø70 mm copper flanges and near one 5 mm water cooling channel. The synchrotron radiation beam had dimensions of 6.4×2.5 mm^2. The calculations showed that the maximum temperature on the diamond plate was 626°C, and the maximum thermal stress was 1.5 GPa.

For the 2.4 GeV Swiss Light Source (SLS) synchrotron, the DVW design was optimized. The diamond vacuum window was installed at a distance of 5.5 m from the source; the thickness of the CVD diamond varied from 100 to 250 μm. It was necessary to absorb 160 W of beam energy and dissipate it in the form of heat. When modeling, it was achieved that the temperature in the center of the diamond plate with its thickness of 0.2 mm reached 330°C and decreased to 230°C near the flanges made of oxygen-free copper with high thermal conductivity and having a temperature of about 30°C [27]. Previously, a DVW prototype was made, consisting of only 1 channel [28].

This work presents new results of physical-mathematical modeling of three-dimensional unsteady coupled heat and mass transfer problem related to revealing the influence of the number and design of mini-channels on heat transfer and the ability to remove heat from the DVW. Previously, there were no similar studies in the literature in relation to diamond vacuum windows.

2 Design and physics and mathematics simulation of heat and mass transfer in DVW

One of the most difficult optical devices to temperature management is the DVW, which incorporates a single-crystal CVD-diamond plate obtained by chemical vapor deposition with a diameter of 25-90 mm and a thickness of 50-400 μm [29]. Thermal filters and DVW, Fig. 1, are located perpendicular to the synchrotron radiation axis and are designed to filter the radiation spectrum, as well as to extract the beam from the high vacuum region to the workstation optical systems. In the created workstation, the thermal power density perceived by the first thermal filters reaches 2.3 kW (2.0-2.5 kW/cm^2), and for DVW - up to 1.29 kW (1.5 kW/cm^2). Structurally, the DVW has the most complex design, since it is this device that separates the ultrahigh vacuum region from the surrounding space. The ability to remove heat from this element, which is released when part of the radiation of the working beam is absorbed without significant deformations and damage to the integrity of the diamond plate, largely determines the class of the synchrotron radiation source (4+), that is, the actual beam brightness available to the consumer.

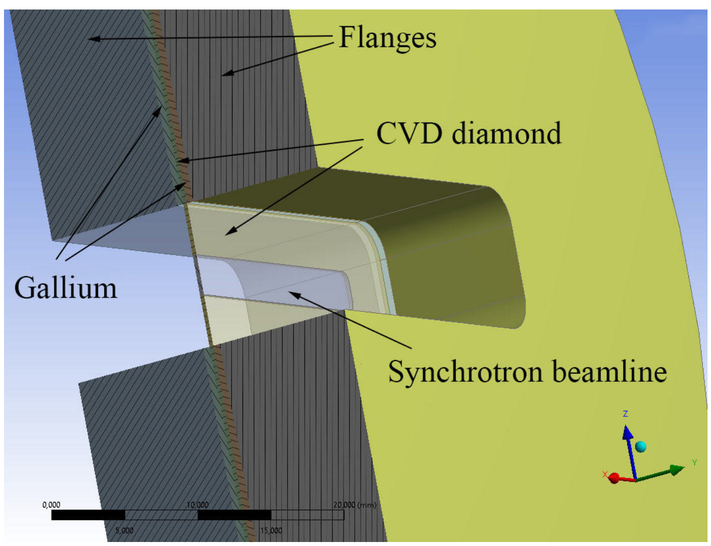

Figure 1: DVW scheme (cross section).

On Fig. 1 presents a DVW schematics by a cross section, the thermal simulation of which is carried out in this article. The main element of the DVW is a CVD-diamond foil through which a rectangular synchrotron beam passes. The foil is clamped between two round copper flanges with a through hole in the center (35×8 mm^2) for the passage of synchrotron beam. The heat absorbed by the foil enters the flanges and must be removed to dispose outside. A thin liquid metal film 0.5 mm thick, marked in Fig. 1 as Gallium, acts as a vacuum seal. It is this film that will significantly reduce the contact resistance between the diamond foil and the copper heat sink flange [5-6]. The coordinate center is located in the geometric center of the computational domain, the z-axis is directed upward, parallel to the gravity vector and opposite to the direction of the coolant flow, the y-axis is directed perpendicular to the flanges and the diamond plate.

Synchrotron beamline (see Fig. 1) with a size of 30 mm horizontally and 3 mm vertically is directed to the center of the diamond plate. The histogram of the heat flux as a result of the absorption of its part, used in the calculations, is schematically shown in Fig. 2. The specific heat flux here varies from 1.35 to 1.50 kW/cm^2. The total generated thermal power is 1.29 kW. For the central region of the DVW, temperatures up to 500-540°C are acceptable, the cooled periphery can have temperatures up to 150°C [2]. Thermal deformation of diamond foil in the transverse direction should not exceed 3.0 μm. Heat removal should be carried out with distilled water pumped through mini channels. Flanges in which mini channels are formed are made of copper.

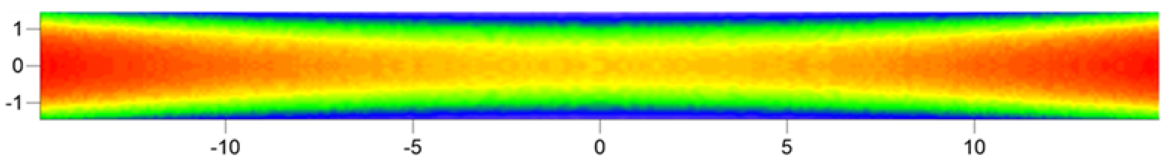

Figure 2: Heat flux distribution used in calculations (30×3 mm^2, 1290 W).

Previously, a new mini-channel cooling system for this DVW was developed, Fig.3, [5, 6, 24]. In this work, physical and mathematical modeling of heat and mass transfer between the Synchrotron beamline and a mini-channel cooling system, including copper flanges, was carried out. To do this, a three-dimensional problem of heat conduction and heat transfer was solved: inside the diamond foil, then by heat conduction through a thin liquid metal film into the copper flange and through it to the the mini-channel walls. The heat from the walls of the mini-channels by water, propagated through it by thermal conductivity and convection, and was carried away by the flow together with it. In addition, a small part of the heat was dissipated by radiation from the surface of diamond, copper, and the boundary of the liquid metal open into space due to the fact that they turn out to be hot in the surrounding space. As an example, gallium was taken as a liquid metal with thermophysical characteristics: density - 6095 kg/m^3, heat capacity 410 - J/(kg·K), thermal conductivity - 29.4 W/(m·K), melting point - 29.8°C.

Everywhere in the calculations, unsteady heat conduction equation (1) was used, as the boundary conditions at the surfaces of diamond-gallium, gallium-copper, copper-water contacts, the condition of temperatures equality $\delta T/\delta n = 0$ was used. Here t is time, T is temperature, α is the thermal diffusivity of the material, and n is the normal unit vector. The water flow was described by non-stationary Navier-Stokes equations (2-3), with the boundary condition for water velocity U=0. Here: $U(U_x, U_y, U_z)$ - velocity, ρ - water density, p - pressure, g - acceleration of gravity, ν - coefficient of kinematic viscosity. In the Fluent package calculations a unsteady k-omega turbulence model was used, the time step was 0.0001-0.02 s. All values of the used thermophysical properties of materials were taken for the current local temperature.

$$\frac{\delta T}{\delta t} = \alpha(\frac{\delta^2 T}{\delta x^2} + \frac{\delta^2 T}{\delta y^2} + \frac{\delta^2 T}{\delta z^2}) \tag{1}$$

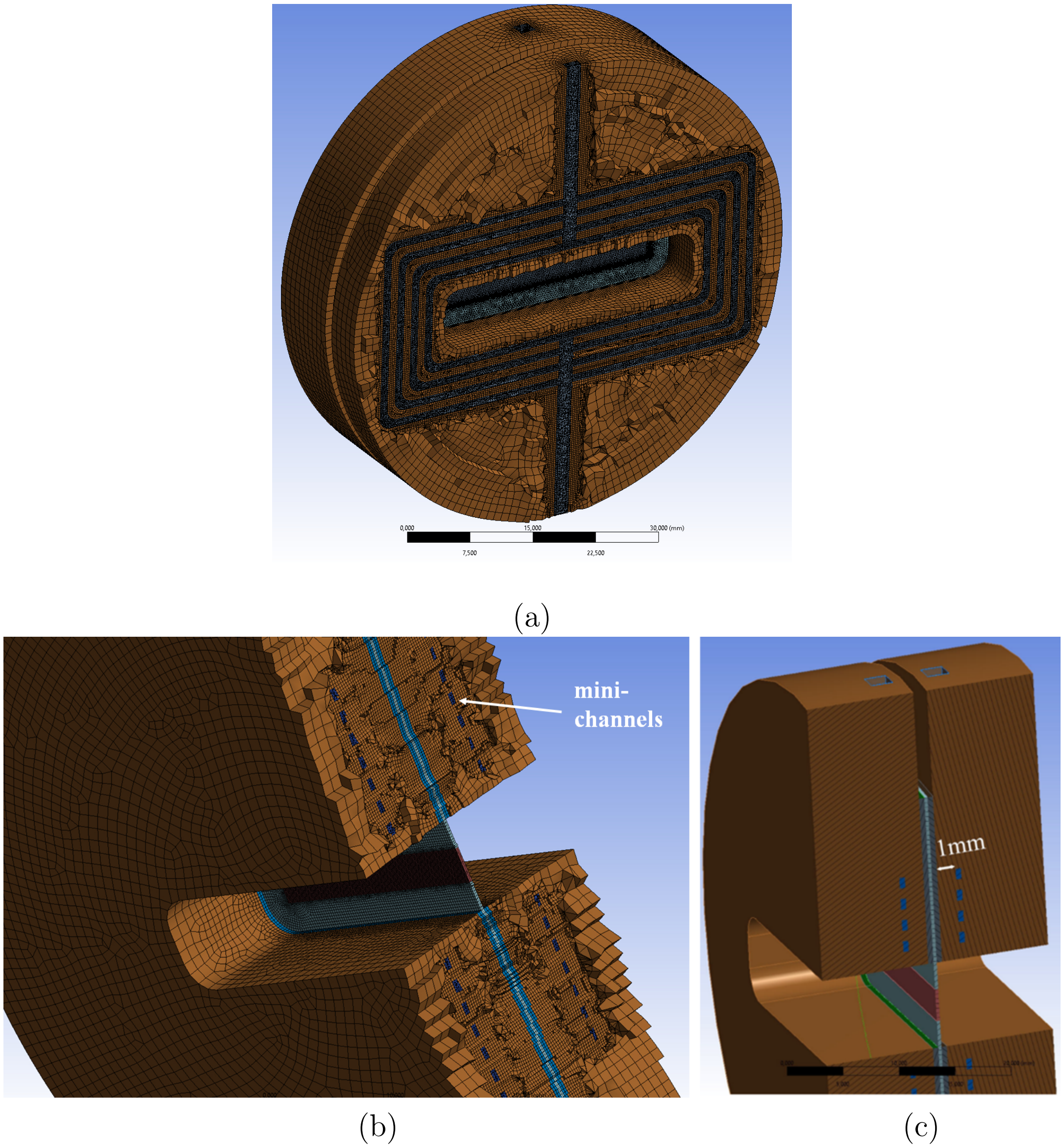

Figure 3: Calculation geometric schematics for DVW, the geometry of the mini-channels. Longitudinal section (a) and cross section (b, c).

$$\frac{\delta U}{\delta t} + (U \cdot \nabla)U = -\frac{1}{\rho}\nabla p + \nu \Delta U + g \tag{2}$$

$$\frac{\delta T}{\delta t} + U \cdot \nabla T = \alpha \Delta T; \nabla U = 0 \tag{3}$$

During the simulation, a non-uniform computational grid was built, consisting of about 5 million elements, with thickening (the Inflation parameter in Ansys Meshing) near the channels and in the region of heat release when part of the synchrotron radiation is absorbed, Fig.3. The size of the grid elements inside the mini-channels is 125 μm. The resolution of the grid elements inside the copper flanges is 1000 μm. The grid resolution in the region of heat flux from synchrotron radiation on diamond plate is 301×31 elements. In Ansys Meshing, the Hex Dominant method was mainly used, its choice was due to fast convergence, sufficient accuracy of the obtained solution, and the minimum number of computational grid elements, which affected the computation time.

According to the workstation design, the DVW is located in a vacuum, so there is no heat removal through the surrounding gas. However, radiative heat exchange with the surrounding space was taken into account by applying the real body radiation rules using the Stefan-Boltzmann law. To do this, in Ansys Fluent, the emissivity (material emissivity) $0 \leq \epsilon \leq 1$ and the ambient temperature [5, 6] were set as boundary conditions on copper flanges and the open part of the diamond foil. In this case, ϵ, depending on temperature, is equal to: for polished copper - 0.018 - 0.023, for diamond plate - 0.91 - 0.94, [30, 31]. Radiative heat transfer from the open surface of the liquid metal was neglected due to the obvious smallness of its area.

The correctness of numerical calculations was controlled in two ways. The first one is to check the balance of the heat flux through the heated and cold boundaries of the region. In the model used: the hottest boundary of the computational domain is located where the heat flux with a total power of 1290 W is released when part of the synchrotron radiation is absorbed, and heat is utilized: 1) by water cooling the system through the inlet/outlet openings going to the thermostat, 2) through the radiation heat transfer from surfaces open to the surrounding space (copper flanges, parts of CVD diamond and edges of the liquid metal layer). For example, the integral over all surfaces showed that the thermal imbalance in the system is

Strength calculations, optimization of cooling water flow, pressure and initial temperature of water, geometric dimensions of the flange design, thickness of CVD diamond foil were performed. In the developed DVW, the maximum temperature of 300 mum diamond plate was 542.6°C, thermal deformations at thermal stresses of 842.7 MPa (with a tensile strength of 1200 MPa) with a 30% margin do not exceed the limiting values at the maximum temperature. With this option, the cooling system is capable of removing up to 1.7 kW of heat (about 2.0 kW/cm^2 at the centre of diamond foil). However, it was found that a twofold margin of safety in the case of thermal stresses occurring in CVD-diamond foil of DVW can only be achieved by reducing the heat power of release to the level of 1.29 kW. Taking into account this requirement, the DVW geometric dimensions were finalized. The simulation of the mini-channel cooling system convincingly showed that the proposed version fully satisfies the requirements for the workstation of the first stage of the SKIF.

Below are the results of physics and mathematics modeling performed during the development of the DVW cooling system and to refine the design of mini-channels.

3 3-D calculations of mini-channel cooling parameters under unsteady coupled heat and mass transfer. refined design of mini-channels

Detailed calculations of the unsteady coupled problem of heat and mass transfer in a diamond vacuum window have been performed, which, in particular, have resulted in the flow velocity and overpressure profiles of cooling water in the minichannels of the DVW cooling system. These parameters are important in identifying possible problems in the functioning of mini-channel cooling systems, in particular, due to the possibility of critical flow regimes or heat exchange between the channel wall and cooling water. An example of the calculated profiles of the flow velocity and overpressure of cooling water in the mini-channels of the DVW cooling system is shown in Fig. 4 for the case of the final [24] DVW cooling system (CVD-diamond thickness - 0.3 mm, its diameter - 40 mm, copper flanges - Ø60 mm, four mini-channels 0.5×1.0 mm^2, one inlet and one outlet channels with a size of 2.0×2.0 mm^2, the initial water temperature is 7°C, its pressure at the inlet to the mini-channels is 10 atm). An enlarged image of the corresponding profiles and their magnitudes on the section plane are shown on the right. The study of the physical information obtained from Fig. 4 showed that one should not expect crises in the water flow or the appearance of features in the heat transfer from the channel wall to the water. However, at the initial stage of DVW design, such information made it possible to avoid errors in the cooling system development; in addition, it was possible to ensure heat exchange between the mini-channel walls and water without boiling one.

Possible designs of mini-channels were studied: their number (from 8 to 1), the number of input and output channels (one or two each) and the location of the output channel. In this case, all physical information obtained as a result of model calculations was studied. In Fig.5 and in Table 1, as an example of such information, for the final cooling system (Fig.5, left) and its version with a single channel 1.42×1.42 mm^2 (Fig.5, right), the temperature profiles are presented: the surfaces of the copper flange in contact with liquid metal (above); surfaces of the mini-channel system (in the middle part); CVD-diamond foil (bottom). The study of the obtained physical information showed that when using only one channel, the value of the maximum temperature in the CVD-diamond foil increases by 5.8°C, see bold in the third column of Table 1. And this becomes critical due to a significant increase in thermal stresses in the foil. In this case, it was taken into account that the margin of safety of the DVW elements should be twofold. At the same time, if the number of channels is more than four, the value of the maximum temperature in the foil does not decrease by more than 0.4°C. In this case, there is no reason to change the parameters of the mini-channel system, thus complicating it. Thus, the choice of the final DVW design was justified.

It can be seen from Table 1 that the maximum temperature in the liquid metal, when using a non-optimal mini-channel scheme, increases above 126°C, that is, by almost 15°C higher. This significant temperature change can shorten the life of both the flanges and the single crystal CVD-diamond. It is known that liquid metal alloys of gallium and indium, having a melting point below room temperature, dissolve well in copper and other materials. Even the application of refractory metal protective coatings does not prevent gallium and indium from dissolving in them, reducing the number of flange heating and cooling cycles. The liquid metal interaction at elevated temperature with single-crystal diamond foil also reduces its lifetime. Therefore, the choice of the final mini-channel scheme is also optimal from this point of view.

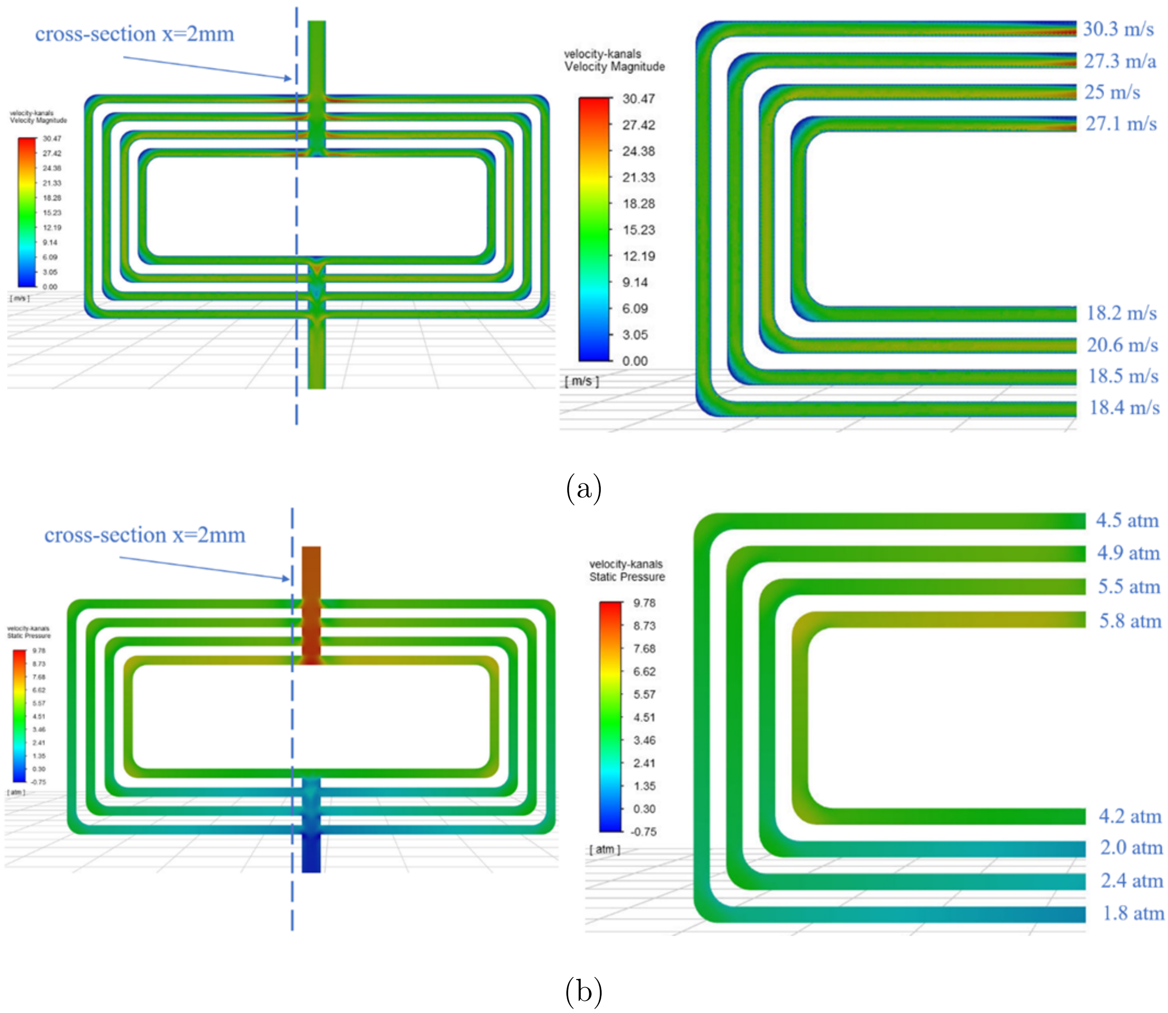

Figure 4: Calculated profiles of the flow velocity (a) and overpressure (b) of cooling water in the mini-channels of the DVW cooling system. An enlarged image of the corresponding profiles and their magnitudes on the section plane are shown on the right.

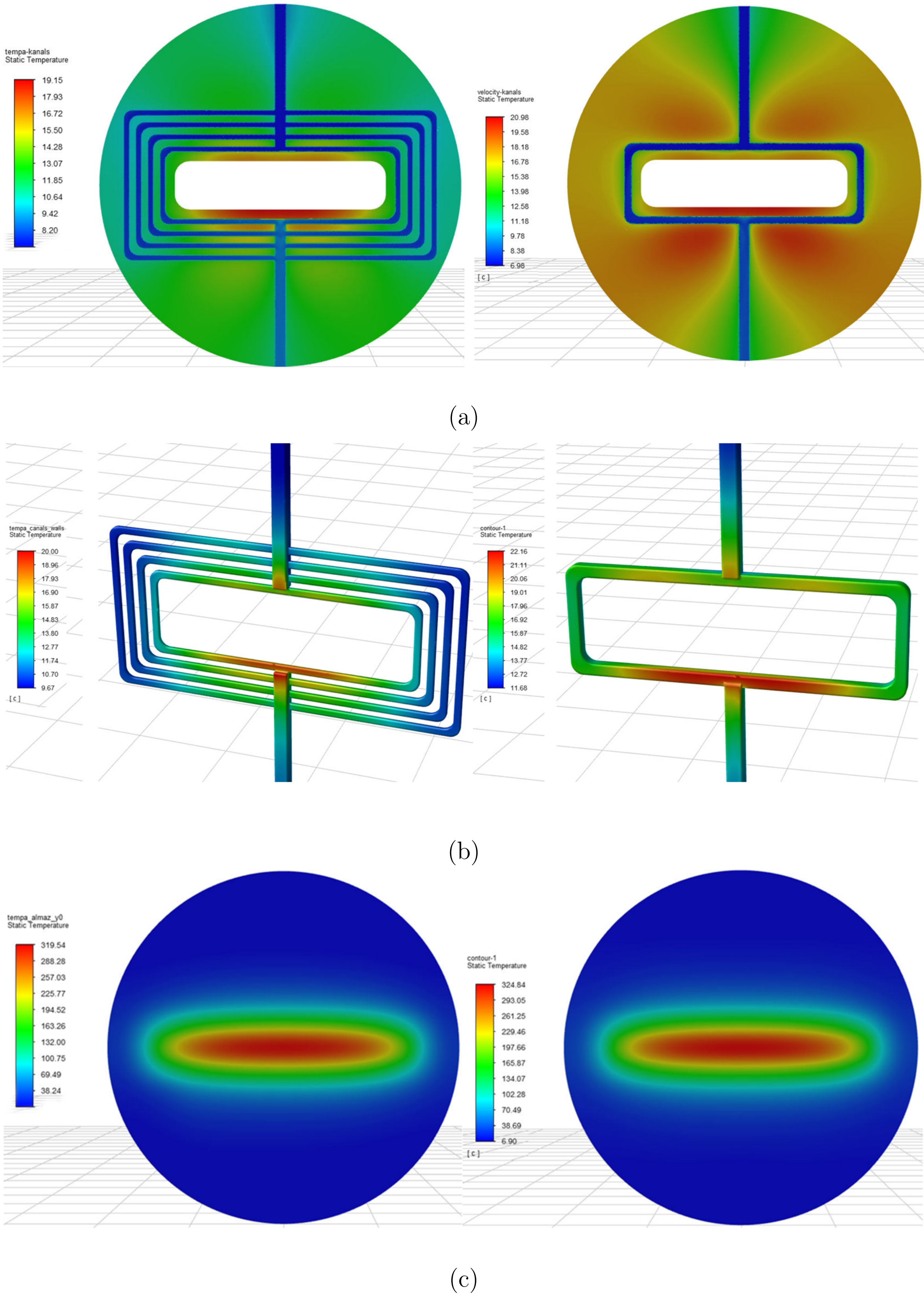

Figure 5: Temperature profiles in the final cooling system [24] (left) and its version with one channel 1.42×1.42 mm^2 (right) for: copper flange surface (a), mini-channel system surface (b), CVD-diamond foil (c).

Table 1: Maximum temperatures in the cooling system depending on the parameters of the minichannels.

cooling system	foil maximum temperature, °C	mini-channel maximum temperature, °C	liquid metal maximum temperature, °C
final: four mini-channels 0.5×1.0 mm^2, one input and one output channels with a size of 2.0×2.0 mm^2 (Fig.5, left)	319.0	20.0	112.6
one mini-channel 1.42×1.42 mm^2, one input and one output channel with a size of size 2.0×2.0 mm^2 (Fig.5, right)	324.8 (+5.8)	22.2	123.8
one long mini-channel 1.42×1.42 mm^2, input and output channel with size 2.0×2.0 mm^2 are side by side	325.8 (+6.8)	24.9	126.2
eight mini-channels 0.5×1.0 mm^2, two input and output channels each 2.0×2.0 mm^2	318.6 (-0.4)	19.5	112.5

4 Conclusion

Detailed calculations of the three-dimensional unsteady coupled problem of heat and mass transfer in a diamond vacuum window have been carried out, which resulted in a reasonable choice of a mini-channel cooling system, namely: the number and size of the inlet and outlet channels of the system, the number of mini-channels directly for cooling. As a result of physico-mathematical modeling, an effective option for cooling CVD-diamond devices using mini-channels has been developed, in which a level of specific heat release power up to 1.5 kW/cm^2 can be achieved, the total heat power will be 1.29 kW. Calculations convincingly show that the proposed version of DVW cooling by mini-channels satisfies the requirements for workstations of the first and second stages of SKIF.

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