Numerical simulation of thermal diamond filter for working station 1-5 of synchrotron "SKIF"

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Abstract. Numerical 3D-simulations of thermal loads of thermal diamond filter for the working station 1-5 of synchrotron "SKIF" has been performed. An efficient version of a water-cooling system of a CVD diamond by means of mini-channels in copper flanges with a total heat release power of 1290 W is presented. The influence of various configurations of the cooling system, different boundary conditions (thermal insulation, radiation heat exchange), water supply pressure on the maximum temperature in diamond wafer has been investigated. The influence of the temperature dependence of the properties of diamond glass has been studied. The maximum temperature on the diamond wafer is found to be 317.6°C absorbing 1290 W of power correspond to the safe mode for some specific cooling system configuration. The corresponding flow rate of 7°C cooling water was 13.1 l/min.

1. Introduction
The synchrotron is a universal tool for solving problems in applied and fundamental researches, where particles move in a ring in a vacuum at almost the speed of light, and powerful electromagnets give them energy and set their trajectory. As a result, synchrotron radiation arises, which allows the study of the structure of any substance. One of the main challenges in the construction of a synchrotron is the development of a special design of cooled X-ray windows that can absorb the proper amount of power to prevent overheating. Diamond filters are X-ray windows that are made on the basis of CVD diamonds (diamond obtained by chemical vapor deposition, which has unique thermal and mechanical properties) [1,2]. CVD diamond has thermal conductivity of up to 85% of the thermal conductivity of monocrystalline diamond [3,4]. A high-quality diamond wafer has thermal conductivity of 2200 W/(m ·K) at a room temperature.

During the construction of 3GeV 3rd generation ALBA Light Source (Spain), numerical simulations were performed by means of the finite element method, experimental samples of filters with diamond X-ray windows were created to "remove" the required 600 W [1]. The diamond wafer with thickness of 300 μm was located between two copper flanges of Ø70 mm, each flange had one 5mm channel with cooling water. The dimensions of synchrotron beamline were 6.4 mm x 2.5 mm. The maximum temperature of diamond wafer was 626°C.

Optimized X-ray window design based on CVD diamond for the 2.4GeV Swiss Light Source (SLS) has been investigated in [2]. The X-ray window was placed at a distance of 5.5 m from the radiation source and had CVD diamonds with a thickness from 100 to 250 μm. The total power absorption was 160 W. The flanges were made of oxygen-free copper, i.e. from copper free of copper oxides (OFHC Cu). Edges of the copper flanges were kept at temperature of 30°C. Temperature at the center of the diamond wafer (0.2 mm) reached 330°C and decreased to 230°C near the copper flanges. As a result, a
prototype of a thermal filter based on 100 μm CVD diamond with a cooling system consisting of one channel was manufactured. The average surface roughness of the CVD diamond wafer measured by means of Zygo NewView 5010 interference microscope was 2.4 nm, and the maximum roughness was 16 nm. [2].

The third-generation synchrotron radiation facility SPring-8, situated in Japan, provides the most powerful synchrotron radiation currently available (8GeV). In [5], the coherent properties of X-ray sources were considered, experiments were carried out on SPring-8 for several beryllium and CVD diamond wafers. Glass thickness varied from 100 to 250 microns.

During the construction of the NSLS-II synchrotron at Brookhaven National Laboratory, USA, the booster was created in the INP SB RAS. Numerical simulations were carried out by means of the finite element method for the absorption of radiation by diamond filters, as well as filters on silicon carbide (SiC) [6]. Diamond filter with 1 mm glass thickness is capable of absorbing 850W of energy, while the maximum temperature is about 200°C. Roughly the same amount of energy can be absorbed by 1mm SiC filter, but the maximum temperature should be 810°C.

Construction of the Siberian Circular Photon Source (SKIF) is already underway in Novosibirsk. The power generated by the wiggler, which is a source of synchrotron radiation, will be up to 49 kW. The first heat-loaded element of the working station will be a collimator, which forms the geometrical dimensions of the X-ray beam for the subsequent elements and dissipates about 20.3 kW.

One of the important stages of the work is the numerical simulations of thermal filters containing CVD diamond wafers. Detailed numerical simulations of thermal filters and their cooling systems with further experimental verification will prevent overheating of CVD diamond wafers, as well as exclude limiting thermal stresses that can lead to temporary failure of the entire synchrotron.

It is assumed that the diamond filter of the workstation 1-5 of the SKIF synchrotron will consist of a CVD diamond wafer, clamped (through an interlayer of liquid metal) between two copper flanges with X-ray windows. Copper flanges must be provided with water cooling, the configuration and dimensions of which will be determined by numerical 3D-simulations. The dimensions of the synchrotron beamline on the 1st diamond wafer of the composite thermal diamond filter is 30 mm x 3 mm. The total absorption in 300 μm diamond wafer is 1290W (1.433 kW/cm²). The distribution of the absorbed power in 0.3 mm diamond wafer is uneven over the surface and is specified in the form of a matrix with a size of 301x31 elements. The values of the absorbed power are obtained from experimental measurements and carried out at the Institute of Nuclear Physics of the Siberian Branch of the Russian Academy of Sciences. The cooling system must remove heat in such a way that the temperature distribution in the diamond wafer does not exceed 500-600°C.

Despite the fact that there is a number of numerical and experimental studies of thermal filters, each synchrotron is a unique equipment (there are only 51 sources of synchrotron radiation in the world), for which it is necessary to carry out specialized calculations and experiments. In this work, 3D-numerical simulations of thermal loads, as well as various options for the cooling system, are studied using the Ansys Fluent. A cooling system with copper flanges is proposed, consisting not of a single channel, but of several mini-channels. Mini-channels are an effective means of cooling various electronic, optical and optoelectronic equipment with high heat dissipation [7-10]. In this study the usage of mini-channels ensures 1290 W total power absorption in the diamond wafer, while numerical 3D-simulations show that the maximum temperature will correspond to the safe mode.

2. Calculations and results
The geometry of the thermal diamond filter is shown in Figure 1. The center of coordinates is located in the geometric center of the domain, the z-axis is directed upward and 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 wafer. The Ø 70 mm CVD diamond wafer with a thickness of 300 μm is clamped (through a layer of liquid metal with a thickness of 0.5 mm) between two copper flanges with 35x8 mm X-ray windows. Liquid metal gallium is used to avoid hard contact of CVD diamond with copper flanges and prevent glass breakage when heated. The 30 x 3 mm synchrotron beamline is directed to the center of
the diamond wafer. In the first variant of the numerical simulation the specified heat flux had a constant value of 10.6 kW/cm². This value was chosen as the maximum of those considered at the stage of early 1-5 facility design. In the second variant, the heat flux was inhomogeneous and varied over the surface of the diamond wafer from 1.35 kW/cm² to 1.5 kW/cm². This heat flux distribution was determined during experiments at the Institute of Nuclear Physics SB RAS. In this case the total power released on the surface of the diamond wafer was 1290W.

Figure 1. – Geometry of the thermal diamond filter.

The thermal CVD diamond filter will be located in a vacuum, therefore the emissivity (emissivity of the material) 0 ≤ ε ≤ 1 and the ambient temperature 22°C are specified on the other external boundaries. According to the Stefan–Boltzmann Law emissivity ε defines the ratio of the thermal radiation energy of a "gray body" to radiation of an "absolutely black body" at the same temperature (emissivity of an absolutely black body ε = 1). For polished copper flanges, the value ε = 0.02 is specified; for diamond glass the value ε = 0.92 is specified [11].

In this work the temperature dependences of thermal conductivity and heat capacity C_P of the diamond wafer are taken into account. Tabular data are approximated by polynomials of the 5th degree.

Coefficient of thermal conductivity of CVD diamond λ > 2000 W/(m·K), but with increasing temperature the thermal conductivity decreases, and at 300°C λ is about 1000 W/(m·K). Other thermophysical properties of CVD diamond, liquid metal, and copper flanges are specified by constants (T=300°K), Table 1.

Figure 2. – Thermal conductivity of CVD diamond vs temperature.
Table 1. Thermophysical properties of materials used in calculations.

|                 | CVD-diamond | Gallium | Copper flanges |
|-----------------|-------------|---------|----------------|
| ρ, kg/m³        | 3.520       | 6.095   | 8.978          |
| Cₚₜ, J/(kg·K)  | Polynomial  | 410     | 381            |
| λ, W/(m·K)     | Polynomial  | 29.4    | 387.6          |

Inside the copper flanges water cooling is provided consisting of several mini-channels 0.5x1.0 mm² located around the X-ray window, one input and one output of 2.6x2.6 mm² channels (connected to thermostat in a real technology). The computational mesh, consisting of about 5 million elements, with inflation near the channels is shown in Figure 3. The dimension of mesh elements inside the mini-channels is 125 µm. Non-stationary k-omega turbulence model is used.

At the inlets, the water temperature and pressure are specified. It should be noted that in this work several test calculations were performed, i.e. the dimensions of the cooling water channels and collectors have not yet been optimized.

First, numerical simulations were performed for a constant specified heat flux 10.6 kW/cm². The maximum temperature in the CVD diamond was about 950°C, it means such a heat flux is not applicable in a real SKIF synchrotron manufacturing technology, since the temperature distribution in a diamond wafer should not exceed 500-600°C.

In case of 10.6 kW/cm² heat fluxes, it is necessary to consider other, more efficient methods of cooling of thermal diamond filter or another filter design. The influence of the initial temperature of the cooling water from the thermostat on the temperature in the system is given in Table 2.

Table 2. The influence of the initial temperature of the cooling water from the thermostat on the temperature in the system.

|                 | Max. temperature in CVD diamond, °C | Max. temperature in gallium (at y=0.4 mm section), °C | Max. temp. in mini-channels (at the y=5.65 mm section), °C |
|-----------------|--------------------------------------|--------------------------------------------------------|----------------------------------------------------------|
| Water: 17°C, pressure: 5 atm | 954.2                                | 584.4                                                  | 115.7                                                    |
| Water: 7°C, pressure: 5 atm | 951.9                                | 579.4                                                  | 105.5                                                    |
| Water: 7°C, pressure: 10 atm | 948.1                                | 565.8                                                  | 90.0                                                     |

With specified 10.6 kW/cm² heat flux, a decrease in the water supply temperature by 10 degrees leads to a decrease in the maximum temperature in the diamond wafer by 2.3 °C, in the liquid metal this temperature decreases by 5°C, and in the area of mini-channels it decreases by 10.2°C (Table 2). In this calculation, water should be considered as a model liquid, i.e. high-temperature heat carrier, which has some properties like water. When the temperature of the cooling water from thermostat was 17°C and

Figure 3. – Computational mesh in copper flange and around mini-channels at the center of mini-channel level (at the y=5.65 mm section).
the pressure was 5 atm, the corresponding water flow rate was 9 l/min. The leaving water temperature was 31.8°C.

The influence of boundary conditions on the temperature distribution is also investigated. The maximum temperature inside CVD diamond, liquid metal and copper flanges at different boundary conditions is given in Table 3: ε = 0.02 (copper), ε = 0.92 (CVD diamond), ambient temperature is 22°C. The water supply temperature is 17°C, Table 3.

\begin{table}[h]
\centering
\begin{tabular}{|c|c|c|c|}
\hline
Boundary condition & Max. temperature in CVD diamond, T°C & Max. temperature in gallium (at y=0.4 mm section), T°C & Max. temp. in mini-canals (at the y=5.65 mm section), T°C \\
\hline
Thermal insulation & 960.2 & 586.6 & 115.7 \\
Radiation heat transfer & 954.2 & 584.4 & 114.5 \\
\hline
\end{tabular}
\caption{The influence of boundary conditions on temperature.}
\end{table}

As compared to thermal insulation, when specifying radiation heat transfer at the boundaries, the maximum temperature in CVD diamond dropped down by 6°C, in liquid metal the temperature dropped down by 2.2°C, and in the area near mini-channels the temperature dropped down by 1.2°C (Table 3).

The next series of numerical simulations was performed for a variable heat flux, which varied from 1.35 kW/cm² to 1.5 kW/cm², Figure 4. The total radiation power dissipated by the thermal filter was 1290 W.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure4.png}
\caption{Radiation beam dimension: 30 x 3 mm, heat flux: 1.35 kW/cm² – 1.5 kW/cm², total power: 1290 W. Radiation beam applies to the center of the CVD diamond wafer.}
\end{figure}

The effect of the temperature dependence of the thermal conductivity and heat capacity of CVD diamond was investigated. First, numerical 3D-simulation was performed for constant values of the thermal conductivity of CVD diamond (λ = 2000 W/(m·K)); this corresponds to the thermal conductivity at room temperature. Water supply temperature was 17°C, water supply pressure was 5 atm. The maximum temperature in the CVD diamond wafer was 235.6°C. In the second calculation, the thermal conductivity coefficients λ and C_p were specified as polynomials of the 5th degree (Figure 2). The maximum temperature in CVD diamond increased by 107°C (i.e. 45%) from 235.6°C to 342.6°C. These numerical simulations show that it is important to take into account the dependence of material properties on temperature.

The temperature distribution inside the CVD diamond wafer in the section y = 0 and the temperature profile T (0,0,z) along the height of CVD diamond are presented in Figure 5 and 6. Water supply temperature is 7°C, water supply pressure is 10 atm. The corresponding cooling water flow rate is 13.1 l/min. The temperature inside liquid metal (Figure 1) in the section y=0.4 mm does not exceed 77°C. The maximum temperature in the CVD diamond wafer is 317.6°C (at a water temperature of 17°C and pressure 5 atm, the maximum temperature of a CVD diamond was 342.6°C). As it is shown above the configuration of water cooling using mini-channels with a total heat release power of 1290 W (1.433 kW/cm²) allows us to avoid an excess of the maximum temperature in the CVD diamond wafer of 500-600°C (specified by the SKIF synchrotron designers). The maximum temperature in gallium was 119.7°C (at the contact plane between the liquid metal and the diamond wafer), the maximum temperature of the channel walls was 20.3°C.

The effective way to check the correctness of the numerical simulation is to check the balance of the heat flux through the heated and cold boundaries of the region. In this work, the heated boundary of the
computational domain is a given heat flux with a total power of 1290 W, and heat is removed through the inlet / outlet openings going to the thermostat, as well as through radiation heat exchange from other surfaces (copper flanges, parts of CVD diamond and liquid metal).

Figure 5. – Profile of the temperature $T(0,0,z)$ in diamond wafer $\varnothing 70 \text{ mm} \times 300 \mu\text{m}$.

![Figure 5](image)

$T_{\text{MAX}} = 317.6^\circ \text{C}$

Figure 6. - Temperature distribution $T (x,0,z)$ in $^\circ \text{C}$ in diamond wafer resulting from heat load of 1290 W applied in the center of the window (beam footprint: 30 x 3 mm, window thickness: 300 μm).

Water temperature at the outlets is 9.1°C. The integral over all surfaces indicates that the thermal imbalance in the system is 0.06630713 W or 0.005%. The second way to check the correctness of the numerical simulation is to control the mass flow rate of cooling water passing through the inlets and outlets. The water flow rate through the inlet was 13.1 l/min, the mass imbalance was $3.56 \cdot 10^{-6}$ l/min or less than 0.00003%.

3. Conclusion
Numerical 3D-simulations of the thermal diamond filter of the working station 1-5 of synchrotron "SKIF" have been performed. An efficient version of water-cooling of CVD diamond using mini-channels in copper flanges with a total heat release power of 1290 W is presented, when the maximum temperature of the diamond wafer (317.6°C) does not exceed the safe temperature range 500-600°C. The corresponding flow rate of 7°C cooling water was 13.1 l/min. The influence of the temperature and pressure of the cooling water, as well as the influence of boundary conditions (thermal insulation, radiation heat transfer) on the 3-dimensional temperature distribution in CVD diamond, liquid metal layers and mini-channels has been studied. Temperature-dependent properties of CVD diamond are critical for the result. The thermal imbalance in the system during the calculations did not exceed 0.005%.

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