Computer simulation of sublayer temperature mode during deposition of diamond coatings using gas-plasma method

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Abstract. The research presents a computer simulation of the temperature field on the sublayer surface, performed in a stationary mode during the deposition of diamond coatings using the gas-plasma method with different parameters of the cooling system. The optimization problem of mathematical programming with the search for the extremum of the performance function by varying the controlled parameters within the permissible range is considered.

1. Introduction

One of the main requirements for the deposition of diamond coatings is to maintain the temperature on the sublayer surface in a given interval, which is ensured by the balance of heat flux brought by the flow of deposited particles and removed by cooling system.

Diamond coatings are characterized by strength, hardness, high modulus of elasticity, low coefficient of linear thermal expansion, high thermal conductivity, good tribological properties, as well as erosion, thermal and chemical resistance. These properties can be used in various industries, in particular, for the improvement of the reliability and durability of machine parts and tools.

Among the existing plasma coating methods, one of the most high-performance is the method of gas-plasma deposition. It presents the subject of laboratory research since the late 80s of the last century [1–4]. The efficiency of diamond coating synthesis is determined by the parameters of the plasma flow, as well as the thermal mode of the sublayer on which the coating is deposited (Fig. 1). The optimum conditions are the surface temperature of the sublayer within 800, 900 °C, while the homogeneity of coating thickness depends on the uniformity of the temperature distribution on the sublayer surface. For a given thermal power of plasma flow, the optimum thermal mode of the sublayer can be achieved by selecting the parameters of cooling system.
2. Optimization of sublayer cooling system

Figure 2 shows a geometric model of an optimized cooling system [5].

The sublayer, a molybdenum disk with a diameter of 40 mm, is fixed on the end of the cooling manifold in the form of a quill cylinder with a diameter of 40 mm. The water-cooling unit has the shape of a cylinder with a diameter of 20 mm with a spherical top in the end. The heat carrier (water) is fed into the unit through a tube with dimensions of 6 × 0.5 mm; made of stainless steel. The background temperature is 20 °C; the integral thermal power of the plasma flow is 5000 Watts.

Figure 2. Geometric model of cooling unit of sublayer
1. Plasma flow;
2. A sublayer, a molybdenum disk with a diameter of 40 mm;
3. Cooling manifold;
4. Heat transfer tube made of stainless steel, 6x0.5 mm;
5. Heat carrier – water

The optimization task was formulated as a mathematical programming task — the search for an extremum of the performance function by varying controlled parameters within the permissible range.

$$\text{extrF}(X)$$

$$D_X = \left\{ X|_{\varphi(x) > 0, \psi(x) = 0} \right\}$$

where: F(X) – the performance function (temperature distribution over the surface of the molybdenum sublayer along the radius); X is the vector of controlled parameters (the thickness of the molybdenum sublayer is 1 mm and 0.1 mm; the material of the cooling collector is copper, zinc and steel; the flow rate of water in the cooling manifold is 1, 0.5, 0.08, 0.012 l/sec; the gap (from the top of the sphere of water-cooling unit to the sublayer) is 2 mm, 0.2 mm; \(\varphi(x)\) and \(\psi(x)\) - limiting functions (temperature range ~ 800 ... 900 °C); \(D_X\) - permissible range in the space of controlled parameters. The distribution of heat flux density over the sublayer surface is uniform, or according to Gauss.
The task was solved by direct search methods using the FlowSimulation module of the licensed package of SolidWorks.

There are methods of deposition of diamond coatings in streams of arc plasma torches of diamond coatings using a gas carrier from a mixture of argon and hydrogen and hydrocarbon reactant gases.

The disadvantages of these methods are a small deposition area, due to the small cross section of the stream of the arc plasma torch (the method of deposition of diamond coatings in plasma flow, utility patent № 204060010 mm), as well as the contamination of the deposition area with particles of electrode material.

The most appropriate technical solution to the proposed method is the deposition of diamond coatings in a stream of inductive thermal plasma containing a mixture of argon and hydrogen as a gas carrier and methane as a reactant gas.

Powerful plasma torches operate at relatively high flow rates of gas carrier (for example, a plasma torch with a capacity of 60 kW consumes 120 l/min at a pressure of 1 atm).

At the same time the gas path of high-power plants is open, i.e. the gas mixture is used once and then released into the atmosphere. The deposition process itself is long, with a characteristic time of about 1 hour or more. Gases are fed into the installation from cylinders; therefore, the existing methods are complicated by the procedure of periodic replacement of gas cylinders. The gas supply scheme is also complicated. It contains several cylinders with high-pressure reducers and gas paths that meet the safety requirements for work with explosive gases, which include hydrogen.

The distinctive features of the proposed method are the use of air as a gas carrier and the injection of a hydrocarbon reactant gas into the area of interaction of air plasma stream with a sublayer onto which a diamond coating is deposited.

The use of air as a gas carrier makes it possible to simplify the method of deposition of diamond coatings and increase its cost-effectiveness, since it makes it possible to refuse from the use of expensive gases, the gas-cylinder economy accompanying them and ensure greater safety compared to the existing methods taking into account the absence of explosive hydrogen. In this case, the air for the implementation of the method is taken directly from the atmosphere and does not require any preparation except from dedusting.

According to the experiments the injection of a hydrocarbon gas-reactant into the area of interaction of air plasma stream with a sublayer leads to additional savings, since it reduces the energy consumption for the deposition process. In addition it becomes possible to vary the energy content of the stream in a wider range, and since the temperature of the sublayer in thermal plasma is determined by its energy content, the range of realizable temperatures of the sublayer expands. As a result it expands the scope of application of the method. In addition, the injection increases the concentration of the reactant gas in the deposition zone, which leads to its more economical use and contributes to the increase in the growth rate of the coatings.

3. Simulation results
During the course of the research of the effect of the collector material on the performance function, the calculations for stainless steel and copper were made. The Figures 3 and 4 show the temperature distribution over the sublayer surface for the case of a stainless steel cooling collector and two options for the distribution of the density of the thermal power of plasma stream: uniform and Gaussian.
**Figure 3.** Steel collector. Heat distribution is uniform. Water consumption is 1 l/s

**Figure 4.** Steel collector. Heat distribution is Gaussian. Water consumption is 1 l/s. Gap is 0.2 mm.

**Figure 5.** Copper collector. Heat distribution is Gaussian. Water consumption – 0.5 l/s. ΔT/T=1.5

**Figure 6.** Copper collector. Heat distribution is Gaussian. Water consumption – 0.08 l/s. ΔT/T=1.1.
In both cases, the temperature distribution over the sublayer is highly non-uniform, with \( \Delta T/T = 1.1 \) for the Gaussian flow, and the temperature maximum falls at the center of the sublayer, and for a uniform flow is \( \Delta T / T = 0.5 \) and the temperature reaches the highest value at the periphery. The same principle is observed in the case of a copper collector: the temperature distribution is more uniform for uniform plasma flow.

The effect of the coolant flow rate on the performance function is presented on Figure 5 and Figure 6. It can be seen that the reduction in the flow rate from 0.5 l/s to 0.08 l/s improves to some extent the uniformity of the temperature distribution over the sublayer surface, however the maximum temperature value deviates more strongly from the optimal range.

The removal of the water-cooling unit from the sublayer (the increase of gap) makes it possible to reduce the non-uniform distribution of temperature by reducing its maximum, however, both the maximum and minimum values remain far beyond the optimal range (Figure 5 and Figure 7).

The analysis of the results shows that the distribution of the thermal power density of plasma flow has the strongest influence on the performance function. With a uniform flow, it is possible to ensure that the temperature of all points on the surface of the substrate falls within the optimal range, however some non-uniform temperature distribution along the radius still remains (\( \Delta T/T = 0.06 \)), but it is significantly less than in all the investigated variants (fig. 8).

According to the above mentioned facts, in order to achieve the best uniformity of temperature distribution over the sublayer surface, the cooling system in the investigated geometric model should meet the following parameters: collector material is copper, 2 mm gap, molybdenum substrate thickness is 0.1 mm, and water consumption is 0.012 l/s. With a uniform distribution of the power density of plasma flow, the surface temperature is \((805 - 850) °C\).

A further reduction of the non-uniform temperature distribution on the molybdenum sublayer surface in the investigated geometric model of the cooling system can be achieved by additional heating of the outer part of the cooling collector to a temperature of \( \sim 800 °C \), or in the case of using a composite collector with varying thermal conductivity along the radius or the combination of these factors.
4. Conclusion
During the research a computer simulation of the sublayer cooling system was carried out using the installation for the deposition of diamond coatings by the gas-plasma method. The plasma flow enters the sublayer located at the end of the metal cylinder, in the unit of which the coolant (water) flows. The simulation showed that in the case of a uniform distribution of the power density of plasma flow, it is possible to ensure uniform temperature distribution over the sublayer surface in the range (805 - 850) °C. The variation of the parameters of the cooling system showed that the best temperature uniformity is achieved at a water flow rate of 0.012 l / s; in a water-cooled copper collector; with the thickness of the molybdenum sublayer of 0.1 mm. In this case, the non-uniformity of the temperature distribution along the radius is $\Delta T / T = 0.06$. The results obtained are of practical importance for the creation of highly efficient technologies for the synthesis of diamond coatings.

References
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