

SIMULATION OF SURFACE HEATING FOR ARBITRARY SHAPE'S MOVING BODIES/SOURCES BY USING *R*-FUNCTIONS

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ABSTRACT. The purpose of this article is to propose an efficient algorithm for determining the place of an action of a heat source with a given motion law for a body of an arbitrary shape using methods of analytical geometry. The solution to this problem is an important part of a modeling of a laser, plasma, ion beam treatment. In addition, it can also be used for mass transfer problems, such as simulation of coating, sputtering, painting etc. The problem is solved by the method of *R*-functions to define the shape of the test body and the heat source and the analytical determination zone shadowing. As an example, we consider the problem of using the method of ion cleaning parameters optimization considering temperature limitations. Application of the *R*-functions can significantly reduce the amount of computation with usage of the ray tracing algorithm. The numerical realization of the proposed method requires an accurate creation of a numerical mesh. The best results in terms of accuracy of determination the scope of the source can be expected when applying adaptive tunable meshes. In case of integration of the *R*-functions into the CAD system, the use of the proposed method would be simple enough. The proposed method allows to determine the range of the source by the expression, which is constructed only once for the body and the source of arbitrary geometric shapes moving in any law. This distinguishes the proposed approach against all known algorithms for ray tracing. The proposed method can also be used for time-dependent multisource with arbitrary shapes, which move in different directions.

KEYWORDS: numerical methods; moving heat sources; ray tracing; *R*-functions method.

1. INTRODUCTION

Moving body/source heating analysis has an application in several manufacturing processes [1, 2]. In most well-known studies, in this formulation, the problem is considered for a circular heat source, which moves in a straight line [3, 4]. However, there are papers that outline the temperature distribution in a half-space, because of the complexity of the shape of the moving heat source [5], and because of the fact that a heat source moves according to a more complex laws [6].

The problem of heating bodies of finite dimensions by moving heat sources is considered in fewer studies. The objects of the study are likely to be the bodies of simple shapes (cylinder or parallelepipeds). For example, a number of studies were carried out by [7], to investigate the temperature distribution in a rotating cylinder heated with the laser heat source. This problem may be associated with the calculation of laser hardening regimes, laser-assisted machining, etc.

At the same time, it is necessary to calculate the temperature of an arbitrary shaped body caused by heating of a moving heat source. The law of motion and the shape of the heat source can be quite complex. Such problem is typical for cases, when body heat happens because of an energy flux action (radiation, heating, laser, ion or electron beam processing).

In this case, the definition of the heated area's borders is a complicated problem. In this paper, we propose an analytical method for the solution of this problem by using the *R*-functions. The geometric shapes of the body, the source and the law and their relative motion can be arbitrary. After definition of the action zone of the heat source, the further temperature calculation was determined numerically by a finite element method.

2. MATHEMATICAL FORMULATION

The problem with determining the action zone of the moving heat source is very similar to the problem with determining the shadow zones location that is typical to computer graphics.. Beginning with the studies [8, 9] such problems are solved by different algorithms of ray tracing. It required creating a lot of rays from points of the body surface in the direction of the radiation source.

These tasks require large amount of computations. At the same time, for complex shape bodies, the precise definition of the shaded area is associated with considerable difficulties in case of the moving sources, which change the intensity of the radiation.

We assume that the geometry of the source and the body is known. It can be independent of time,

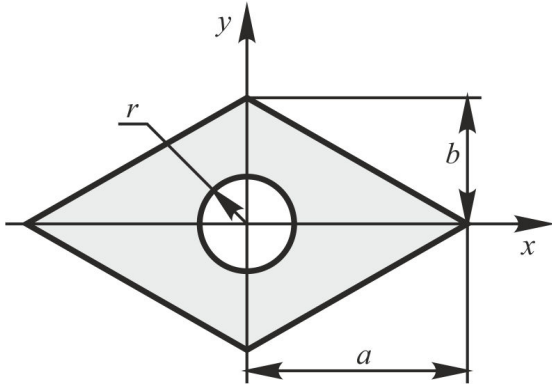


FIGURE 1. Description of geometric shapes with R -functions.

or change according to the known law. The source intensity is able to change arbitrary on time and on its cross section. The law of the source movement is also known.

Solution of the problem is reduced to the construction of a switch-function, which would be equal to 1 on the heated surface and to 0 on the rest of the surface of the part.

For this purpose, it is enough to create a function that has the following properties:

$$\begin{cases} \omega(x, y, z, t) > 0 & \text{inside the heated surface part,} \\ \omega(x, y, z, t) = 0 & \text{on the border of the heated} \\ & \text{surface part,} \\ \omega(x, y, z, t) < 0 & \text{outside the heated surface part.} \end{cases} \quad (1)$$

Such relation can be described using the R -functions [10]. The R -function method was developed as an improvement of Ritz methods for solving boundary-value problems. It is known for its utilization of solving the heat conduction problems in [11]. However, in this paper it will be used only as a tool of analytical geometry.

The R -functions are functions of continuous real arguments. Their sign is determined by the sign of the argument. If, instead the sign of the “+” and “-”, we use the values 0 and 1, R -functions are equivalent to some Boolean logic functions. Boolean function equivalent to a particular R -function, called the companion function.

Almost in every CAD system, a geometric shape of a complex object is created by using Boolean operations with geometric primitives. These primitives can be defined by algebraic equations or inequalities. For example, inequality $\omega_1 = (R^2 - x^2 - y^2 \geq 0)$ in the plane XOY defines a circle of radius R centered at the origin.

It is proved by [12] that if the geometry of the complex object is created by using Boolean operations (\vee, \wedge, \neg) with geometric primitives which are described by the inequalities $\omega_i \geq 0$, the replacement of companion Boolean function with R -functions, al-

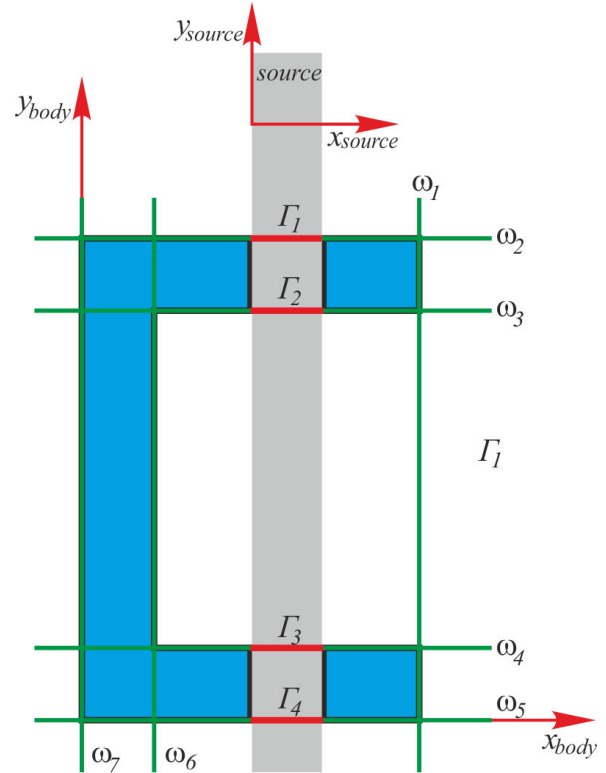


FIGURE 2. Definition of shadow zones.

lows to obtain the inequality $\omega = f(\omega_1, \dots, \omega_n) \geq 0$, with the properties (1).

The simplest complete system of these R -functions is the following one:

- $f \equiv -f$ (logical negation);
- $f_1 \wedge f_2 = f_1 + f_2 - \sqrt{f_1^2 + f_2^2}$ (logical conjunction);
- $f_1 \vee f_2 = f_1 + f_2 + \sqrt{f_1^2 + f_2^2}$ (logical disjunction).

Let it be required to create an expression $\omega(x, y) \geq 0$ for the area which is shown in Figure 1. As geometric primitives, the following items are selected: $\omega_1 = (1 - |x/a| - |y/b| \geq 0)$ – the part of the plane inside a diamond with vertices $(\pm a, 0), (0, \pm b)$; $\omega_2 = (x^2 + y^2 - r^2 \geq 0)$ – the part of the plane outside of the circle with radius r centered at the origin.

The shape of the region is determined by $\omega = \omega_1 \wedge \omega_2$, or after replacing the Boolean operations with R -functions:

$$\omega = (1 - |x/a| - |y/b| + x^2 + y^2 - r^2 - \sqrt{(1 - |x/a| - |y/b|)^2 + (x^2 + y^2 - r^2)^2} \geq 0).$$

Further, for simplicity, the symbols \wedge_R, \vee_R will be used instead of the expanded form of R -function. Method of analytical determination of the coverage of the source considers the example of two-dimensional problem. We propose dependences that describe the geometric shape of the heat source $\omega_{\text{source}} \geq 0$ and body $\omega_{\text{body}} = R(\omega_i) \geq 0$, where $R(\omega_i)$ – system of R -functions; $\omega_i, i = 1, \dots, N$ – geometric primitives (Figure 2).

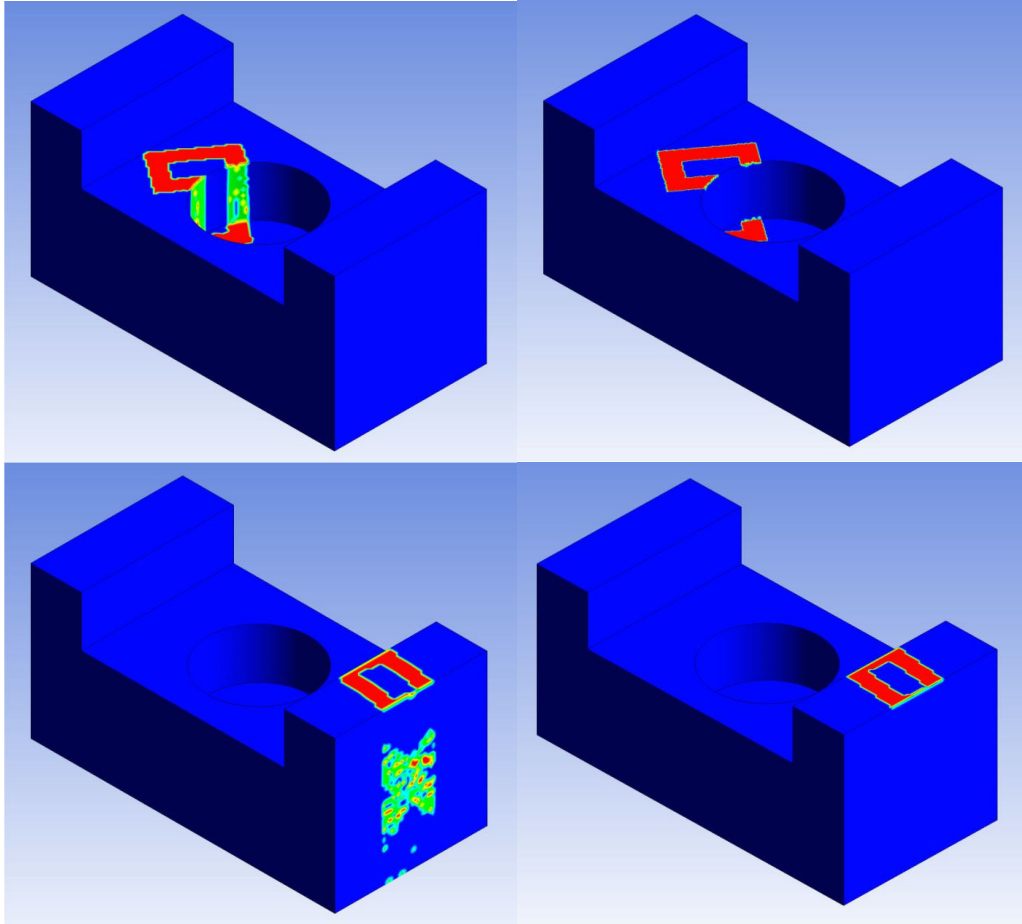


FIGURE 4. The results of numerical simulations using unstructured mesh without conditions (left) and mesh obtained by the forced association of mesh nodes from the body surface (right).

expressions:

$$\begin{cases} z_{\text{source}} = z_{\text{body}}, \\ x_{\text{source}} = (x_{\text{body}} + R \cos \varphi_1 t) \cos(-\varphi_2 t) \\ \quad + (y_{\text{body}} + R \sin \varphi_1 t) \sin(-\varphi_2 t), \\ y_{\text{source}} = -(x_{\text{body}} + R \cos \varphi_1 t) \sin(-\varphi_2 t) \\ \quad + (y_{\text{body}} + R \sin \varphi_1 t) \cos(-\varphi_2 t). \end{cases}$$

Blade surface geometry was defined by point cloud.

The heat flux is determined on the basis of the energy balance at the surface between input heat Q_{in} and heat loss Q_{out} .

For plasma processes Q_{in} described by the expression [13]:

$$Q_{\text{in}} = J_{\text{rad,in}} + J_{\text{ch}} + J_{\text{n}} + J_{\text{ads}} + J_{\text{react,in}} + J_{\text{ext,in}}.$$

Here $J_{\text{rad,in}}$ is the heat radiation towards the surface; J_{ch} is the power transferred by charge carriers (electrons and ions); J_{n} is the contribution of neutral species of the background gas and the neutral particles; J_{ads} and $J_{\text{react,in}}$ are energies released by an absorption or a condensation and the reaction energy of exothermic processes including molecular surface recombination; $J_{\text{ext,in}}$ is an input heat flux by external sources that influences the thermal balance of the substrate.

Clearing by ion sputtering is carried out at low pressure with using a high-purity neutral gases, without additional heating and cooling. In this case, the expression for determining Q_{in} can be simplified [13]:

$$Q_{\text{in}} = J_{\text{rad,in}} + J_{\text{ch}} = \sigma(\varepsilon T_{\text{rad}}^4 - \varepsilon_s T_s^4) + j_i E_{\text{ion}} + \frac{4k_c M_i M_s}{(M_i + M_s)^2} \sin^2 \frac{\theta}{2} e_i V_{\text{bias}},$$

where ε is the spectral emittance of the radiation source at a temperature T_{rad} ; ε_s represents the spectral absorbance of the substrate surface at a temperature T_s ; σ denotes the Stefan–Boltzmann constant; j_i is the ion flux density of the surface; E_{ion} is the ionization potential of the incident ion; k_c is the energy transfer coefficient; M_i , M_s are masses ratio of the colliding particles (ion and surface atom); θ is the angle of incidence; e_i is the ion charge; V_{bias} is the sum of the plasma potential and the substrate potential.

The heat loss Q_{out} of the substrate during plasma processing consist of the following terms [13]:

$$Q_{\text{out}} = J_{\text{rad,out}} + J_{\text{particle}} + J_{\text{des}} + J_{\text{react,out}} + J_{\text{ext,out}}.$$

Here $J_{\text{rad,out}}$ is the energy radiated from the substrate at a temperature T_s ; J_{particle} is the energy transport

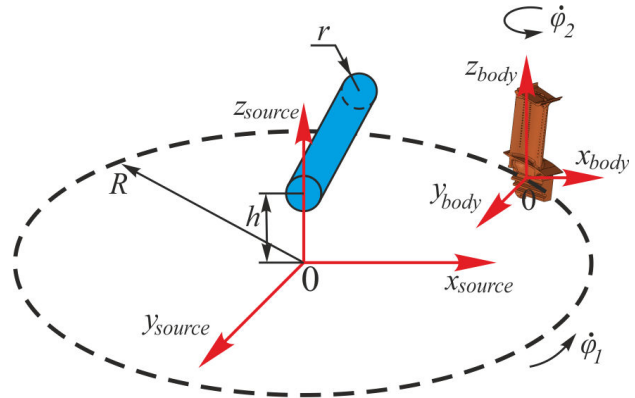
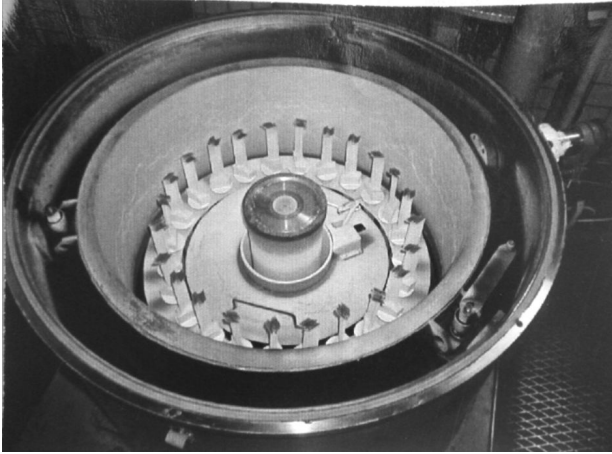


FIGURE 5. The equipment for sputtering and coating – turntable with blades and design scheme for the task of the blade heating under ion sputtering.

from the substrate due to sputtering of surface atoms and the secondary electron emission; J_{des} is the energy sink due to the desorption of particles into the gas phase and the diffusion into the solid bulk; $J_{react,out}$ is the reaction energy of exothermic processes, including molecular surface recombination; $J_{ext,out}$ is the heat loss caused by an external cooling.

Subject to the terms of the ion cleaning, the expression for determining Q_{out} can be written as:

$$Q_{out} = J_{rad,out} + J_{particle} \approx J_{rad,out} + J_{sputtering} = \sigma(\varepsilon_s T_s^4 - \varepsilon_{env} T_{env}^4) + k_{sput} j_i E_{coh},$$

where ε_{env} is the emissivity of the environment; T_{env} is the environmental temperature (reactor walls, etc.); k_{sput} is the sputtering coefficient dependent on the ion energy and angle of incidence; E_{coh} is the cohesive energy of sputtered material's atoms.

The temperature field in the clearing blade was calculated during the simulation. For this, the transient heat conduction equation was solved. The heat flux through surface of the blade was specified by the expression:

$$W = \sigma(\varepsilon_s T_s^4 - \varepsilon_{env} T_{env}^4) + \Phi \left(\sigma(\varepsilon_{rad} T_{rad}^4 - \varepsilon_s T_s^4) + j_i E_{ion} + \frac{4k_c M_i M_s}{(M_i + M_s)^2} \sin^2 \frac{\theta}{2} e_i V_{bias} - k_{sput} j_i E_{coh} \right),$$

where Φ is a switch-function, which is determined by the expression (2).

Dependence of the heat flux value on the angle between the direction of ions flux and the blade surface is a feature of the process. This feature required calculating the directional cos of the normal to the surface. Using R -functions makes it simple to solve this problem. If the equation $\omega_i \geq 0$ for geometric primitives is known, and for a complex domain the equation $\omega(\omega_i) \geq 0$ is constructed by using R -functions, than

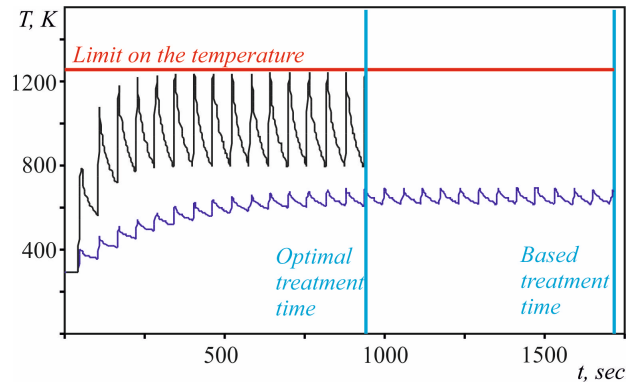


FIGURE 6. Maximum blade surface temperature versus the sputtering time.

for the function $\omega_i^* \geq 0$, where

$$\omega_i^* = \frac{\omega_i}{\sqrt{\omega_i^2 + (\text{grad } \omega_i)^2}},$$

the expressions $\partial\omega(\omega_i^*)/\partial x$, $\partial\omega(\omega_i^*)/\partial y$, $\partial\omega(\omega_i^*)/\partial z$ will determine the direction cosines of the interior normal to the corresponding coordinate axes [12].

Parameters of sputtering (such as value of the ions energy, rotation speed of the turntable and the blade) have been determined with respect to the temperature limit, so the maximum surface temperature should not exceed the temperature of the material phase transition. Additionally, the condition, in which the minimum value of the sputtered material layer should not be less than a predetermined value throughout surface of the blade, was applied.

The graphs of the maximum temperature change in a checkpoint of the blade at a various ion beam energy is shown in Figure 6. Based on the simulation results, recommendations on the choice parameters of the sputtering of the blades have been made. Criterion of choice was the minimum time of the sputtering while respecting the temperature limitations.

4. CONCLUSIONS

The use of R -functions can significantly reduce the amount of tracing computations. The above-mentioned effect is due to the analytical determination of points falling within the scope of the source. The point clouds produced by the 3D scanners can be used for this purpose.

The numerical realization of the proposed method requires an accurate build numerical mesh. The best results in terms of accuracy of determination the scope of the source can be expected, when applying adaptive tunable meshes.

The proposed approach can be applied to cases with an arbitrary number of heat sources considering that the law of body motion is known. It can also be used in mass transfer problems, such as simulation coating, painting or clearing bodies with complex geometric shapes. In case of integration of the R -functions in CAD system, the use of the proposed method would be simple enough.

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