Numerical model of high-power transient heating of tungsten with considering of various erosion effects

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Abstract. Surface melting of tungsten under exposure to a pulsed electron beam was simulated numerically, the evaporation process taken into account. The calculation is based on the experimental time dependence of the total beam power. The model of the tungsten heating process is based on solving the two-phase Stefan problem. The position of the phase boundary depends on discontinuous time- and space-nonlinear coefficients and boundary conditions. The aim of the study is to provide a detailed resolution of the heat flow deep into the material with a fine spatial grid step. As compared with the size of the tungsten plate, the heating depth is very small. The problem statement under consideration is multiscale. Further expansion of the model involves taking into account microcracks. Micro-cracks occur during the cooling process after exposure and affect the temperature of the tungsten surface during the subsequent heating process. The article presents a modeling of cracks of different geometries typical for this process. The results of the calculations correlate with the experimental data obtained on the experimental test facility BETA at BINP SB RAS.

1. Introduction
Results on the heating of a tungsten plate by a pulsed electron beam were obtained on the experimental setup BETA (Beam of Electrons for materials Test Applications) at BINP SB RAS [1]. The full-scale experiment goes in parallel with computational ones. The purpose of the work is to create and implement a model of melting and evaporation of refractory metals with formation of inhomogeneities, drops, and spills under pulsed heating with high amount of energy in small areas for short periods of time. The aim of the study is to obtain a detailed resolution of the heat flow deep into the material taking into account the inhomogeneities (microcracks). The cracks form in the surface layer of tungsten as a result of stresses that appear during pulsed heat load. It was found experimentally that after pulsed heating there arise cracks perpendicular to the surface, as well as cracks parallel to the surface. The latter may significantly affect the heat sink from the irradiated surface of the material. Calculations with a large number of cracks will require a detailed spatial grid, and calculations with involvement of more complex models of crack propagation will require even more computational resources.

There are some experimental works on pulsed heating of tungsten plates with numerical calculations of various characteristics of the process. However, no computational experiments similar to those in
this article have been conducted so far. The thermophysical properties of tungsten are studied in works by JIHT RAS [2]. Because of the specificity of the problem statement (temperature range and pressure and spatial scale), the known results cannot be used. In this work it is important that the problem statement should correspond to the experimental conditions. The results of the calculations correlate with experimental data obtained at the experimental setup BETA at BINP SB RAS.

2. Problem definition
Consider the following heat equation with surface heating:

\[
\begin{align*}
\left( c(T)\rho(T) \frac{\partial T}{\partial t} \right)_{T} &= \text{div}(\lambda(T)\text{grad}T), \\
(n,\text{V}T) &= \frac{W(t,r)}{\lambda(T)}, \\
(n,\text{V}T) &= 0 \text{ at other boundaries}, \\
T &= T_0 \text{ at } t = 0,
\end{align*}
\]

where \( T(\vec{x},t) \) is the temperature, \( c(T) \) is the specific heat, \( \rho(T) \) is the density, \( \lambda(T) \) is the thermal conductivity, \( W(t,r) \) is the power of the heat flux on the surface \( \gamma \), \( n \) is the normal to the surface, and \( T_0 \) is the initial temperature. In the experiments on the BETA facility, samples of rolled tungsten were exposed to an axisymmetric electron beam [3]. Electrons with an energy of 80–90 keV heat the material in a layer thin as compared with the characteristic depth of heating of the material. The power distribution over the surface \( \gamma \) is

\[
W(t,r) = W_{\max}(t) \cdot \exp(-A \cdot r^2), \quad A = 0.03088523.
\]

At each time step in the numerical simulation, the variable \( W_{\max}(t) \) is taken from the experimental data file, individual for each experiment. The distribution of the heating power density over the surface was measured using X-ray visualization [4]. The heat absorbed by the surface propagates into the material. A sample has dimensions of 25mm x 25mm and typical thickness of 4mm. Since in such a short time the sample is heated to a depth of several hundred microns, the simulation region was a transverse section of the sample, a region of 12 mm x 3 mm. As for the time, the numerical simulation continued until the moment at which the last measurement of the surface temperature was made.

It is more convenient to proceed in non-dimensional variables, for example, as follows:

\[
\begin{align*}
r^* &= \frac{r}{r_0}, \quad \lambda^* = \frac{\lambda}{\lambda_0}, \quad \rho^* = \frac{\rho}{\rho_0}, \quad c^* = \frac{c}{c_0}, \\
\tau^* &= \frac{\lambda_0 \gamma}{\rho_0 c_0 r_0^2}, \quad T^* = \frac{T}{T_0}, \quad W^* = \frac{\lambda_0 T_0 W}{r_0},
\end{align*}
\]

The numerical values of the parameters are given in Table 1.

**Table 1.** Dimensional parameters of nondimensionalization.

| Parameter | Typical value | Units |
|-----------|---------------|-------|
| \( r_0 \) | \( 10^{-1} \) | mm    |
| \( t_0 \) | \( 10^2 \)    | \( \mu s \) |
| \( \lambda_0 \) | \( 10^{-1} \) | W/mm⋅K |
| \( \rho_0 \) | \( 10^{-5} \) | kg/mm² |
| \( c_0 \) | \( 10^6 \)    | W⋅μs/kg⋅K |
| \( T_0 \) | \( 10^3 \)    | K     |
| \( W_0 \) | \( 10^3 \)    | W/mm² |
The phase transitions inherent of the problem under consideration are included in the coefficients of Eq. (1). The density (Fig. 1), thermal conductivity (Fig. 2), and specific heat (Fig. 3) are given as dependencies on the temperature of the material in the range of $300K \leq T \leq 8000K$. These functions have discontinuities or lose smoothness at the melting point $T_m = 3695K$.

![Figure 1](image1.png) Figure 1. Graph of temperature dependences of density for evaporation that were used in numerical simulation.

![Figure 2](image2.png) Figure 2. Graph of temperature dependences of thermal conductivity for evaporation that were used in numerical simulation.

![Figure 3](image3.png) Figure 3. Graph of temperature dependences of specific heat for evaporation that were used in numerical simulation.

![Figure 4](image4.png) Figure 4. Graph of temperature dependences of power loss for evaporation that were used in numerical simulation.

Measuring the thermophysical characteristics of refractory metals is a difficult task. Many reference books and articles give an approximate or theoretically predicted dependence with an accuracy estimate of 10% and worse. The thermal conductivity and heat capacity of solid tungsten are taken from [5]. The estimates for the thermal conductivity of liquid tungsten are taken from [6, 7].

3. **Numerical simulation**

For the melting process to be taken into account, the enthalpy of the phase transition $L_m$ was introduced into Eq. (1) [8].

$$\left(\varepsilon(T)\rho(T) + L_m\delta(T, \Delta)\right) \frac{\partial T}{\partial t} = div(\lambda(T)gradT),$$

where the melting point is $T_m = 3695K$.

$$\delta(T, \varepsilon) = \begin{cases} 
\frac{1}{2\varepsilon}, & |T - T_m| \leq \varepsilon, \\
0, & |T - T_m| > \varepsilon.
\end{cases}$$
with the smoothing interval \([\varepsilon, \varepsilon]\), \(\varepsilon = 5K\), and the heat of fusion \(L_w = 51.1 \cdot 10^3 \frac{W \mu S}{mm^3}\).

The process of evaporation at the boundary is taken into account via setting the resultant energy flux \(W(t, r) = W(t, r) - N(T)|_{r}\), where \(W(t, r)\) is the power of the heat flux (see (2)), \(N(T)|_{r} = L_e \cdot \frac{1}{S} \frac{dm}{dt}\) is the power loss (Fig. 4), \(T|_{r}\) is the boundary temperature, \(P(T)\) is the saturated vapor pressure, and \(\frac{1}{S} \frac{dm}{dt}\) is the mass evaporation rate. The power loss is calculated with the following parameter values:

\[
L_e = 4.482 \cdot 10^{12} \frac{W \mu S}{kg}, \quad \frac{1}{S} \frac{dm}{dt} = P(T) = \sqrt{\frac{M}{2\pi RT}} = \exp \left[ 26.19104 \cdot \frac{83971.3}{T} \right] \sqrt{\frac{0.184K}{2\pi 8.314T}} \cdot 10^{-12} \frac{kg}{mm^2 \cdot \mu S}.
\]

Eq. (1) has a divergent form. We use a uniform rectangular grid on spatial variables \((r, z)\). The numerical implementation is based on the Douglas-Rachford scheme [9]. Homogeneous Neumann boundary conditions and boundary conditions describing the heating and evaporation of the material are used. As compared with the size of the tungsten plate, the heating depth is very small. The aim of the study is to provide a detailed resolution of the heat flow deep into the material with a fine spatial grid step. This statement of the problem is multiscale. Further expansion of the model will involve gas dynamics equations to simulate the dynamics of the liquid and gaseous phases of the metal. The equations for the density and momentum will be implemented by explicit schemes. The calculation of the temperature equation by the run method will greatly slow down the program. For simplification of further parallelization of the algorithm, the Konovalov-Popov method is used instead of the run method. The explicitly solvable finite-difference Konovalov-Popov discretization model [10] is expected to result in conjugate-consistent approximation [11]. Obviously, this method exceeds the run method in the acceleration and efficiency. Thus, the temperature is found using a discrete model that inherits the properties of the continuous problem. Implementation of this method has an important feature of selection of agreed boundary conditions at a semi-integral time step. For the problem under consideration, homogenous Neumann boundary conditions are used at all boundaries except the heated surface. The boundary conditions describing the heating and evolution of the material are similar to those of the run method.

The solution of Eq. (1) with constant coefficients is tested on the analytical solution in [12]:

\[
T - T_0 = \frac{1}{c \rho_0} \int_{t'} \int_{t'} e^{-\frac{1}{\lambda(t-t')}} e^{-\frac{v}{\lambda(t-t')}} dt'.
\]

The solution of Eq. (1) with variable coefficients is tested on experimental data. It is known that heating with a power density of \(10^3 \text{ watt/mm}^2\) for 1000 \(\mu s\) increases the surface temperature by about 2000 degrees.

4. Crack geometry setting

Micro-cracks occur during the cooling process after the exposure and affect the temperature of the tungsten surface during the heating by subsequent pulses. The presence of cracks violates the symmetry of the solution of the problem only at large times (more than 500 \(\mu s\)). The crack geometry is defined at the initial moment and is considered to be unchanged throughout the calculation. This is due to the peculiarities of the formulation of the practical problem. Cracks are defined similarly to the boundaries of the region, with a boundary condition \((\hat{n}, VT)|_{r} = 0\). If necessary, one can add heating from the vertical cracks near the surface of the plate, which is associated with increase in absorption of
electron beam in cracks. We assume that the heat does not pass through the cracks since at the characteristic times of the calculations this process be neglected. Let us consider the most common cases. Let \((i, k)\) be the number of the node on which a crack passes.

The simplest case is a symmetric crack. The Y axis is parallel to the line of symmetry of the crack and is directed into the plate. The X axis is directed along the surface (Fig. 5). Calculations are carried out only in a quarter of the space. The conditions on such a crack are set as follows:

\[
T_{i,k}^n = T_{i,k-1}^n, \quad T_{i,k+1}^n = T_{i,k+2}^n, \quad 1 \leq i \leq l_c.
\]

If the lengths of horizontal cracks on the opposite sides of the vertical are not equal (Fig. 6), the following boundary conditions are set at a crack:

\[
\begin{align*}
T_{i,k}^n &= T_{i,k-1}^n, & & 1 \leq i \leq i_c, \\
T_{i,k+1}^n &= T_{i,k+2}^n, & & 1 \leq i \leq i_c, \\
T_{k+1, i}^n &= T_{k+2, i}^n, & & 1 \leq k \leq k_c.
\end{align*}
\]

An inclined crack (Fig. 7) is set in a more complex way. We need to construct an approximation on a rectangular grid. Because of the need to take into account the boundary conditions on the upper heated surface of the plate on the OX axis, the crack is vertical in the first three nodes. The first and second nodes participate in the boundary condition on the surface, and the second and third ones in the condition for the crack. In the corner nodes there are just two conditions, both for vertical and horizontal cracks.

![Figure 5. Crack scheme: symmetric.](image)

![Figure 6. Crack scheme: asymmetric.](image)

![Figure 7. Crack scheme: inclined.](image)

The program developed enables calculation of heat distribution in the tungsten plate in consideration of heterogeneity of different geometries (Figs. 8-10). The graphs show the temperature distributions in a cross section of tungsten plate heated with a constant power of the heat flux \( W = 5 \times 10^3 \text{ W/mm}^2 \) for 200 µs for the case of a symmetric crack, for 300 µs for the case of an asymmetric crack, and for 70 µs for the case of an inclined crack. The presence of microcracks increases the surface temperature (Figs. 11-13), including temperatures above the melting point. Further developed, the model may be able to predict location of cracks inside the material using known temperature data for the heated surface.

![Figure 8. Temperature graph around symmetric crack.](image)
5. Simulation results
On the BETA facility, several photographs of the sample surface were taken during pulsed heating and cooling after exposure. The melt regions are experimentally registered, which can be used for estimation of the accuracy of calculations. It is shown that the evaporation model accurately describes the movement of the free boundary of the molten metal during cooling. Development of a discrete model allows calculations for experiments with large delay times between measurements and large exposure times. The radius of the melt regions was experimentally registered at four time moments, which can be used for estimation of the calculation accuracy, as done in [13]. It is shown that the evaporation model accurately describes the movement of the free boundary of the molten metal during cooling.

Figure 5a presents the time dependence of the maximum of power density of heating by the electron beam. Figure 5b presents surface temperature graph this heating pulse. The moment for which the calculation result is output corresponds to the time of measurement. For example, calibration frames was made in the interval of 145 to 155 µs with an exposure time of 10 µs (black rectangle in Fig. 14). The surface temperature graphs were made for a non-stationary beam power at 150 µs (Fig. 15); the graphs are used in analysis of the measurements. The straight line in the graph shows the level of the melting point \( T_m = 3695 \, K \) and separates the melt area. In this exposure the heating duration was 119 µs. Due to the heating, the sample temperature is as high as 7000 K. At 150 µs the tungsten cools...
down; the surface temperature decreases to 4700K; the depth of heat propagation into the bulk of the sample is less than a quarter of a millimeter.

![Figure 14](image1.png)  
**Figure 14.** Time dependence of power density in the center of exposure area and moment of measurement.

![Figure 15](image2.png)  
**Figure 15.** Surface temperature graphs: preliminary experimental data (black line), results of calculations (red line).

The kind of the thermal conductivity function has a great influence on the nature of the solution. The function $\lambda(T)$ is the argument of the operator $\text{div}$ in Eq. (1). The discontinuous nonlinear function of thermal conductivity $\lambda(T)$ affects the smoothness of the derivative of the solution with respect to the radius $\partial T/\partial r$. Moreover, the boundary condition on the heated surface involves division by $\lambda(T)$. This leads to the appearance of non-smoothness of the solution. It is necessary to choose the function $\lambda(T)$ at large temperature values such that there is no division by zero. The results of the calculation of the radial temperature distribution over the sample surface are consistent with experimental data and analytical estimates.

6. Conclusion

The paper describes a numerical simulation of melting of material exposed to an electron beam on the BETA facility during experiments on simulation of pulsed thermal loads on tungsten in a fusion reactor. Further expansion of the model involves taking into account microcracks. Micro-cracks occur during the cooling process after exposure and affect the temperature of the tungsten surface during the heating by subsequent pulses. The article presents a modeling of cracks of different geometries typical for this process. The results of the calculation of the radial temperature distribution over the sample surface are consistent with experimental data and analytical estimates. This work was supported by the Russian Science Foundation (project №17-79-20203).

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