Eurasian Journal of Physics and Functional Materials
2018, **2**(2), 159-164

Evaporation and thermal stresses in molybdenum irradiated by electrons

G.Z. Ganeev*, S.B. Kislitsin

[1] *Institute of Nuclear Physics, Almaty, Kazakhstan*
**e-mail: ganeev_07@mail.ru*

DOI: **10.29317/ejpfm.2018020208**
Received: 04.05.2018

Plasma disruption in the thermonuclear facility leads to a release of large energy flows to the chamber wall. The pulse duration is 10^{-6} -10^{-4} s, energy fluxes are of the order of 10^{8} -10^{11} Wm^{-2}. High temperature of the protective coating surface causes its evaporation and, probably, destruction under the action of thermal stresses. A promising material for the first wall protection is, in particular, molybdenum. In order to check suitability of molybdenum as a protective coating, an experiment on irradiation of a molybdenum sample with electrons (parallelepiped - 2 × 10 × 0.3 mm) was carried out. The energy flux was $J = 4 \times 10^{11}$ W m^{-2}; pulse duration t = 2 μs. The weight loss of the sample was 2.1 mg; cracking of the trained surface was observed. The purpose of this analysis is to calculate the temperature fields to estimate the mass of evaporated molybdenum and to determine critical thermal stresses.

Keywords: electron irradiation; molybdenum; evaporation; stress.

Introduction

The choice of materials for the divertor plates and the protection of the first wall of the thermonuclear reactor (TNR) is an important stage in the development of full-scale power synthesis reactors. Among the material problems of creating TNR, which include the problems of the first wall, systems for confining the plasma filament with superconducting magnets, etc., a very important role belongs to the problems of creating materials for the divertor device as one of the most energetic nodes of the TNR and protecting the first wall from energy flows.

The problems of creating and selecting structural materials for the TNS are an integral part of the problem of radiation resistance of materials for any nuclear installations, but at the same time they have their own peculiarities. For example, in the TNS materials are exposed not only to neutron irradiation and contact with the coolant, but also to the synergistic action of neutron and ion irradiation, which greatly enhances radiation effects, as well as the release of energy on the surface of the chamber when the plasma is disrupted.

One of the solutions implemented in the TNS with toroidal plasma confinement is coating of the chamber, i.e. the TNR first wall with special protection materials that take on the main thermal loads and protect the first wall from these impacts. The coating materials of the first wall are replaceable, and, as one of the most promising materials, graphite was previously considered, owing to its ability to retain its strength properties at high temperatures. Along with graphite, lithium, molybdenum and tungsten are used as coating materials. The experience

in the development of radiation materials science, in particular, material studies aimed at supporting the prototype of the ITER energy thermonuclear reactor, has shown that graphite is not an optimal material for protecting the TNR first wall. Therefore, it was decided to abandon graphite as a material for protecting the first wall of the ITER and concentrate efforts on choosing a more suitable material for protecting the TNR first wall.

One of the most promising materials is tungsten molybdenum. This is the reason for choosing the topic of research under the program "Scientific and technical support for creation and operation of the Kazakhstan thermonuclear material research reactor Tokamak", since KTM installation is primarily intended for testing structural materials of the TNR. Theoretical and experimental studies of the radiation resistance of molybdenum and tungsten, i.e. those materials that are used in KTM and close to the energy TNR "ITER" and "DEMO" will create a reserve for research and development of new structural materials for the TNR, which will replace the already used ones. Within the framework of this program, the present analysis has been carried out.

Plasma disruption in the thermonuclear facility leads to a release of large energy flows to the chamber wall. The pulse duration is $10^{-6} - 10^{-4}$ s, energy fluxes are of the order of $10^{8} - 10^{11}$ Wm^{-2}. High temperature of the protective coating surface causes its evaporation [1-3] and, probably, destruction under the action of thermal stresses.

In [1-3] and the bibliography presented in them, private problems are solved without giving details of calculations. Analysis of similar problems is based on well-known relationships. While the main difficulty lies in the correct representation of the parameters of the problem, which depend on temperature. The author does not set the task of analyzing works on this topic.

Determining equations

The dependence of temperature on time and on depth (z) of the sample was determined by the equation of thermal conductivity:

$$\rho C_p \frac{\delta T}{\delta t} = k\Delta T + \left(J + J_{ev} + \varepsilon\sigma_{SB}(T - T_{am})^4 \right), \qquad (1)$$

where ρ is the density of the matrix; C_p is the heat capacity; k is the coefficient of thermal conductivity; $T(r,z)$ is the temperature of the sample as a function of cylindrical coordinates; T_{am} is the ambient temperature; ε is the coefficient of thermal radiation; σ_{SB} is the Stefan-Boltzmann constant; J is the energy flux introduced by the eletrons; J_{ev} is the flux of energy carried away by evaporation.

Energy losses, in particular, by radiation (expression in parentheses) were taken into account only on the irradiated surface (z = 0.3 mm).

The obtained temperature fields determine thermal stresses. The equation of equilibrium for the displacement field $\vec{u}$ is determined by the equation

$$3(1-\nu)/(1+\nu)\nabla\nabla\vec{u} - 3(1-2\nu)/(2(1+\nu))\nabla\times\nabla\times\vec{u} = \alpha\nabla T, \qquad (2)$$

where α is the coefficient of volumetric expansion; ν is the Poisson's ratio.

The elastic bias field $\vec{u}$ determines the strain tensor u_{ik} and the stress tensor σ_{ik}:

$$\sigma_{ik} = E/(1+\nu)\,(u_{ik} + \nu/(1-2\nu)u_{ll}\delta_{ik}) - E/(3(1-2\nu))\alpha(T-T_0), \qquad (3)$$

where E is Young module; T_0 is the initial temperature of the irradiated sample; α is the coefficient of volumetric expansion.

The maximum values of invariants of the stress tensor or its components determine the regions of possible cracking of the matrix. In the ideal gas approximation, the flux of energy J_{ev} carried away by the sublimated atoms of the matrix is determined by the expression:

$$J_{ev} = P_{eq}\,[m_a/(2k_BT\pi)]^{1/2}\,H_{evap}, Wm^{-2}, \qquad (4)$$

where P_{eq} is the equilibrium pressure of the sublimated gas; m_a is the mass of the molybdenum atom; k_B is Boltzmann's constant; H_{evap} is the energy of evaporation of the liquid phase.

The defining equations with boundary conditions were solved by the finite element method, using the appropriate program packages. The task is complicated by the presence of three phases: solid, liquid and gas, the dependence of the parameters of the problem on the temperature of the analyzed region. Below Parameters of molybdenum at room temperature [4] are given below.

The atomic number is 42, the melting temperature is T_l =2895 K, the mass of the atom is m_A =95.94 a.m.u, the density is ρ =10.22 $\times 10^3$ kgm $^{-3}$,Young module is E =(300-330) GPa,the shift module is μ =120 GPa, the Poisson's ratio is ν =0.31, the yield stress is $\sigma_{0.2}$ =570 MPa, the ultimate strength is σ_B =670 MPa.

Dependence of parameters on temperature

In accordance with the tabular values [5], the heat capacity C_p at constant pressure, taking into account the phase transitions, is determined by the expression (here and below, the values are given in the SI system):

$$C_p = (202.85 + 0.15385T)_S + 10^4(T \le T_l)(T \ge T_c) + 420(T \succ T_c), Jkg^{-1}, \qquad (5)$$

where T_l =2895 K is the melting temperature; the temperature melting interval was 10 K-T $_c$; H_{SL} =10 ^{5} is the heat of transition from the solid to the liquid phase; C_L =420 Jkg $^{-1}$ is the heat capacity of the liquid phase; the signs of the ratio of the quantities are defined as Boolean variables.

The equilibrium pressure of the sublimated gas, used in the ratio (4), was determined by the expression for the gas [4]:

$$log(P_{eq}) = -32075T^{-1} + 11.567, Pa, \qquad (6)$$

The heat of formation of the gas phase H_{evap} (4) was given by equations:

$$\Delta H_{sub} = 6.6 \times 10^6 Jkg^{-1}; T = (1700K, T_{melt});$$

$$\Delta H_{evap} = 6.1 \times 10^6 Jkg^{-1} T \succ T_{melt}, \qquad (7)$$

The thermal conductivity, taking into account the phase transition of the solid phase to the liquid phase, was determined by the expression [6]:

$$k = (148.96 - 0.037683T)(T \leq T_1)_s + k_l(T \succ T_l), Wm^{-1}K^{-1}, \quad (8)$$

where k_l - the thermal conductivity of the liquid phase k_l is equal to k_s at the melting point.

The volume expansion coefficient α and Young's modulus E were determined by expressions [1]:

$$\alpha = 6.6381 \times 10^{-13}T^2 + 1.1335 \times 10^{-9}T + 4.8856 \times 10^{-6}, \quad (9)$$

$$E = (2.9617 \times 10^{11} - 3.7372 \times 10^4 T^2 + 2.2334 \times 10^7 T)(T \leq T_l), Pa, \quad (10)$$

The last relation assumes that E =0 for the liquid phase, that is, for T $\succ T_l$.

The coefficient of thermal radiation ε, in accordance with tabulated values [3], was determined by the expression

$$\varepsilon = 1.0457 \cdot 10^{-1} + 1.8962log(T/1100), T \geq 800, K, \quad (11)$$

Calculation of temperature fields, evaporation

The analysis was carried out in a cylindrical coordinate system, in the approximation of the axial symmetry of the analyzed matrix. The determining equations (1) were solved by the finite element method (software package "Femlab"), triangulation of the region was taken with condensation to the irradiated surface.

The energy flux is J =4 $\times 10^{11}$ (t $\leq 2 \times 10^{-6}$ s), Wm $^{-2}$; pulse duration is t=2 $\times 10^{-6}$ s; the evaporated mass was determined in accordance with formula (4).

As expected, the temperature of the irradiated surface reaches a stationary value rather quickly. This is seen from Figure 1. After switching off the irradiation, the surface temperature decreases rapidly due to the radiation and evaporation of the matrix. This circumstance is due to the power and exponential dependences of energy loss by these mechanisms. Further, the main contribution to the lowering of the surface temperature is due to the diffusion mechanism of energy absorption by the layers of the next layer in depth.

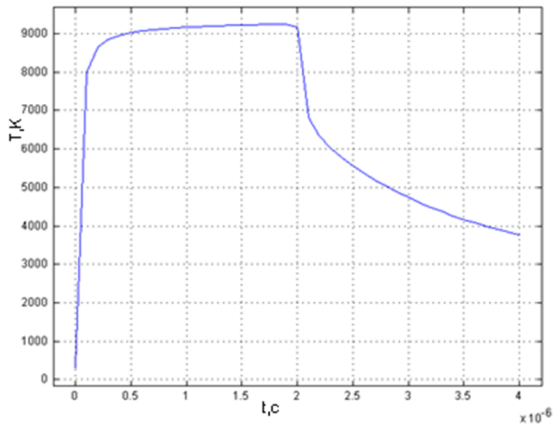

Figure 1. Dependence of the temperature T (K) on the time t(s) on the surface of the sample.

It follows from Figure 2 that the thickness of the molten layer is of the order of 3 μm. Figure 3 shows the dependence of mass loss on time, caused by the evaporation of molybdenum As can be seen from the figure, the mass loss ceases with the end of the pulse. The total weight loss was $Dm_{tot} = 1.9733 \times 10^{-6}$ kg; experimentally the value of $Dm_{exp} = 2.1 \times 10^{-6}$ [6], i.e, the thickness of the evaporated layer is of the order of 0.01 mm. This comparison is the argument of the relative correctness of these calculations.

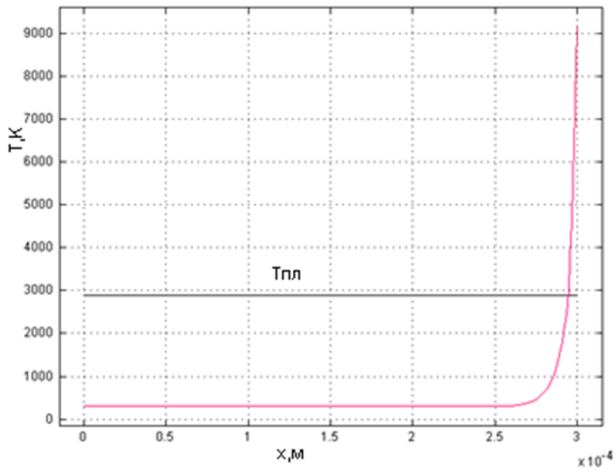

Figure 2. Dependence of the temperature T (K) on the depth of the sample z, t = 2 μs .

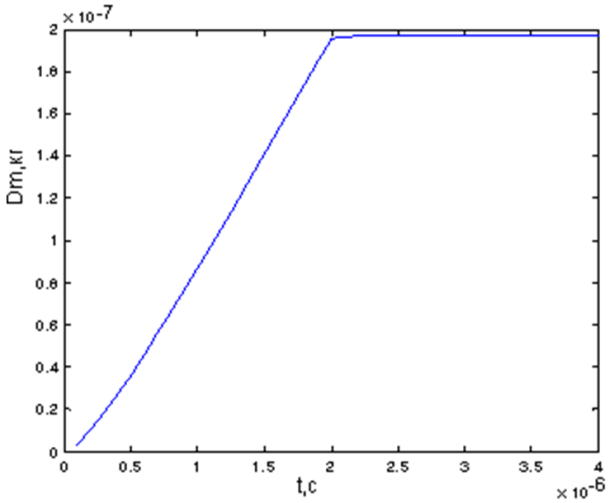

Figure 3. Dependence of the mass loss Dm, kg, on time t, s; total mass loss $Dm_{tot} = 1.9733 \times 10^{-6}$ kg, ($Dm_{exp} = 2.1 \times 10^{-6}$ kg).

Thermal stress

For a given temperature field, stress fields are determined in accordance with formulas (2-3). These equations were solved by the finite element method with the corresponding software packages (software package "Femlab").

The strength limit of metals σ_B, quite rapidly decreases with temperature, $\sigma_B \approx 200$ MPa ($\approx 10^3$ K), [3]. It follows from Figure 4 that it is possible that the near-surface layer of molybdenum is destroyed. The compression area changes to stretching in the direction towards the irradiation surface; the maximum stress values significantly exceed the strength limit of molybdenum.

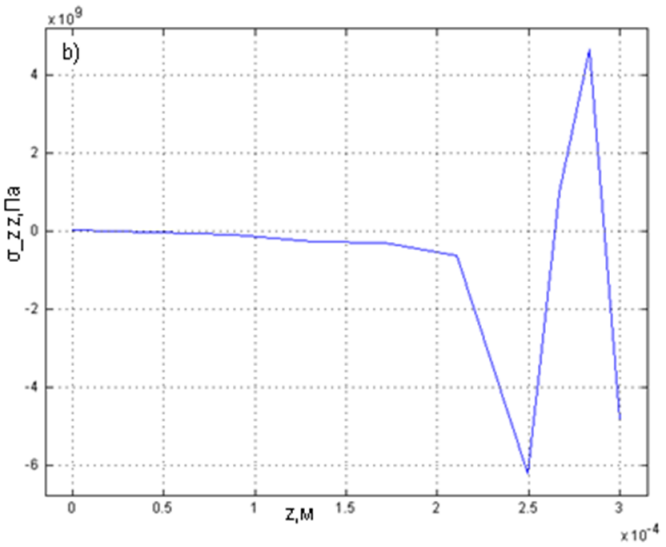

Figure 4. Dependence of the stress component σ_{zz} for t=10 $^{-7}$ s along the cylinder axis.

Conclusion

In the framework of existing concepts, the mass loss of the molybdenum sample was estimated for pulsed exposure to an electron beam. The obtained result is consistent with the results of the experiment. The values of tensile thermal stresses were estimated. The obtained results do not exclude cracking of the irradiated molybdenum surface under the given irradiation parameters.

A special scheme is proposed for calculating the temperature fields and related to them thermal stresses caused bythe thermal shock produced by a short-time electron pulse. The coincidence of the calculated mass loss with the results of the experiment confirms the correctness of the proposed model. The obtained results on thermal stresses correspond to the observed cracking of the irradiated surface of the sample.

It is possible to develop the proposed approach by taking into account the actual composition of the acting plasma, and a more complex composition of the coating, in particular, of stainless steel 304.

Note, as follows from a preliminary estimate, more significant contribution to the stress is made by He ions introduced into the protective coating. This is due to the intrinsic volume of the introduced interstitial atoms. Within the framework of the proposed scheme, consideration of this circumstance is possible.

References

[1] A.M. Hassane et al., J.Nucl. Mater. **103&104** (1981) 321.
[2] I.S.Grigor'eva, E.Z. Melihova, Fizicheskie velichiny. Spravochnik (Moskva: Energoizdat,1991) 1232 p. (in Russian)
[3] O.M. Wirtz, PhD dissertation, The Rhine-Westphalian Technical University of Aachen (2012) 144 p.
[4] G. Li and B.G. Thomas, Proceedings of the 16 th IEEE/NPSS Symposium on Fusion Engineering, part 1. Champaign, IL, USA (1995) 406.
[5] P.D. Desai, J.Phys.Chem.Ref.Data **16**(1) (1987) 91.
[6] K.W.R.Johnson, J.F. Kerrisk, Eleventh international conference on thermal conductivity, Los Alamos (1971) 3.