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## The use of computational contact mechanics approaches to assess the performance of parts bearing stress concentrators

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#### ABSTRACT

**Purpose:** The purpose of this work is to build new computational schemes for assessing the strength parameters of parts with inhomogeneous properties of surface layers in the presence of stress concentrators.

**Design/methodology/approach:** Using the developed approaches of mathematical modeling and open software for calculating the structures of the FEM - FEniCS, the required thickness of the hardened zones of parts has been established, which ensures their minimum softening during operation, depending on the characteristics of the stress concentrator.

**Findings:** It is shown that for each size of the surface stress concentrator there is a critical value of the hardening thickness, the excess of which does not affect the operational strength of the parts, but increases the cost of technological operations.

**Research limitations/implications:** In this article proposes a method for calculating the influence of the dimensional characteristics of hardening zones on the contact strength of parts with stress concentrators under conditions of prevailing power loads.

**Practical implications:** The results obtained in this work were used to determine the technological modes of plasma hardening, which ensure an increase in the contact strength of parts with stress concentrators, depending on their dimensional characteristics.

**Originality/value:** Using the approaches of computational mechanics and mathematical and computer modeling, methods for controlling the contact strength of parts with inhomogeneous non-local properties in the presence of a surface stress concentrator are proposed for the first time.

Keywords: Power loads, Non-local mathematical model, Stress concentrators, Optimization

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ANALYSIS AND MODELLING

#### **1. Introduction**

Forecasting of operating parameters of parts working under intensive frictional loads is one of the most topical problems of mechanical engineering, the solution of which is based on the use of the apparatus of contact mechanics problems [1]. This class of problems constitutes an effective means of calculating the strength, durability and forecasting wear and tear of components and structural elements.

Depending on the target object and boundary conditions, methods for solving these problems are divided into analytical and numerical ones [2].

Analytical solutions of contact problems can be gained only for bodies of simple geometry and boundary conditions and they rather simplistically simulate working conditions of real constructions [3]. These contact problems were historically the first to be developed since there were no computational machines at the disposal of researchers in the first half of the 20th century. Since the second half of the 20th century, following the widespread introduction of computers, numerical contact problems that allow obtaining solutions for bodies with quite complex geometric parameters have been developing rapidly [3].

Subject to the type of boundary conditions, the simulation goal, and the study object, different algorithms are employed for solving this type of problems, a sufficiently wide overview of which is given in [3,4]. A fairly wide stand-alone class of contact problems is the problems that simulate the interaction of bodies occurring under friction, i.e. frictional interaction of bodies. In this case the formulation of boundary conditions is enhanced with friction parameters (relationship between the normal and tangential components of the load vector), thermal processes in the contact zone, laws of wear and tear describing timedependent changes in the surface geometry under the load applied in a variety of ways. The solution of such problems, even in the simplest formulation, requires the use of complex computational schemes, in which additional relations describing the behaviour of bodies under friction are introduced [5].

Modern tendencies in mechanical engineering are associated with the wide utilization of parts containing stress concentrators of structural, technological or operational origin [6]. Their existence requires the development of new approaches of computational mechanics, since classical analytical solutions can be received only for a limited class of problems [1,6].

It should be noted that determining of the stress field, deformations and strains in the considered structures, which most of the contact problems are reduced to, is only the first step in describing the behaviour of objects under given service conditions [7]. Depending on the study objective, it is often necessary to evaluate the strength parameters of a structure, its service potential, and possible remaining lifetime. Therefore, from the stress-strain state, one moves on to the evaluation of performance properties using various strength and durability criteria. The comparison of study results obtained for different bodies using these criteria makes it possible to establish the actual level of serviceability of structures and to optimise them [7,8].

An additional factor contributing to the necessity of designing new computational schemes for contact mechanics is the introduction of technological methods for part surface machining, which results in coordinate heterogeneity of properties [9,10]. In general, it can have a 3-dimensional form, which significantly complicates the calculations of applied and theoretical problems. As a result of technological processing, under load conditions the part stress-strain state changes as well as regions of increased or decreased performance originate, which significantly affect the behaviour of the entire structure during its operation [11].

The presence in the material of parts with pronounced spatial heterogeneity of properties causes the need to develop and use new mathematical models for solving contact problems, in particular, for locally inhomogeneous media. Their employment makes it possible to evaluate the effect of structural-energetic state distribution in a material (its spatial and local features) on the product functioning parameters in given operating conditions more efficiently [1,6,8].

It is worth mentioning that this problem is relevant to both general and transport mechanical engineering, since in this sector friction joints determine the operational safety of rolling stock to a considerable extent [12,13].

In this connection, we can conclude that the development of new approaches of computational contact mechanics for the evaluation of operational parameters of structural elements containing stress concentrators under frictional loads pertains to the topical issues of modern mechanical engineering [6,10,12].

### 2. Setting the problem for managing operational parameters of products from the standpoint of mechanics and mathematical modelling

One of the most effective approaches to the analysis of parameters of working structures is the use of mathematical modelling and computer systems [1,2,10]. Its implementation

makes it possible to determine the stress-strain state and strength properties of parts with sufficient accuracy for practice without carrying out costly field experiments.

At the same time, this approach raises a number of problems, one of which is an adequate formulation of the problem. They consist in recording mathematical ratios that most precisely correspond to the actual processes occurring in the study object, i.e. 1) a clear formulation of limiting conditions describing the physical pattern of part loading; and 2) the use of a mathematical model that takes into account the body's behaviour under external influences sufficiently well.

In this connection, we consider a generalised mathematical formulation for the analysis of processes that occur during operation in structural elements with stress concentrators:

- 1. Let the study object (part) occupies the region of space X, let us identify the body surface as  $\partial X$ .
- 2. Let us set regions  $Y_1, \ldots, Y_n$  in the body, which are the sources of stress concentrations  $(Y_i \subset Y, i = 1..n)$ .
- Let us present the body surface as an assemblage of non-overlapping sets ∂X = ∂X<sub>1</sub> ∪ ∂X<sub>2</sub> ∪ ∂X<sub>3</sub>, where ∂X<sub>1</sub> is the body region undergoing physical loads, ∂X<sub>2</sub> is body region with predetermined displacement limitations, ∂X<sub>3</sub> is an unloaded surface. Regions ∂X<sub>1</sub>, ∂X<sub>2</sub>, ∂X<sub>3</sub>, in turn, <sup>i=1</sup>/<sub>k</sub> can include simple sub-regions: ∂X<sub>j</sub> = ∪ ∂X<sub>j</sub><sup>i</sup>, j =

1,2,3.

- 4. In each elementary sub-region ∂X<sub>1</sub><sup>i</sup> a force vector F<sub>1</sub><sup>i</sup> is set, and on ∂X<sub>2</sub><sup>i</sup> the displacement vector u
  <sup>j</sup><sub>2</sub> is set, both of which in ∂X demonstrate the following distribution F<sub>1</sub><sup>i</sup> = F<sub>1</sub><sup>i</sup>(x), u
  <sup>j</sup><sub>2</sub> = u
  <sup>j</sup><sub>2</sub>(x), x ∈ ∂X.
- When considering the behaviour of parts under contact loads, we use a non-local mathematical model of the distributed elastic continuum damageability given in [14]:

$$\vec{\nabla} \cdot \left(\frac{K(x)}{1 - \sqrt{Z(x)}} \left(\vec{\nabla} \cdot \vec{u}\right) \hat{I} + \frac{2G(x)}{1 - \sqrt{Z(x)}} \left(\vec{\nabla} \otimes \vec{u} - \frac{1}{3} \left(\vec{\nabla} \cdot \vec{u}\right) \hat{I}\right) \right) = 0, \quad (1)$$

where  $Z(x) = \alpha_1(\omega(x))^2 + \alpha_2(|\vec{\nabla}\omega(x)|)^2 + \alpha_3(\frac{1}{V_0}\int_V \omega dV)^2$ generalized damageability functional,  $\alpha_1$ ,  $\alpha_2$ ,  $\alpha_3$ numerical constants,  $\omega(x) -$  damageability rate,  $\vec{u} -$  a displacement vector,  $\hat{I} -$  an ordinary tensor,  $\vec{\nabla} -$  the Hamiltonian differential operator, K(x) - a compression bulk modulus, G(x) - modulus of shear,  $\otimes -$  a tensor product,  $\cdot -$  a dot product,  $V_0 -$  a typical size of the material zone at the mesolevel is equal to three grain diameters.

- 6. As a result of physical loads, a stress state is formed in the part, which is described at each point by a tensor  $\hat{\sigma} = \hat{\sigma}(x), x \in X$ .
- 7. Since rated stresses do not clearly specify the operational parameters of structures [8], for the analysis of contact strength we use the following expression:

$$k(x) = 1 - \frac{\sigma_m(x)}{\sigma^*(x)},\tag{2}$$

where k(x) is the contact strength safety factor,  $\sigma_m(x)$  is the equivalent representation of a stress tensor according to von Mises,  $\sigma^*(x)$  are strength properties of the material at a point.

- The value k(x) changes within the interval -∞; 1, at k(x) = 1 no softening occurs, at k(x) ≤ 0 softening has occurred.
- 9. The task of enhancing the contact strength of a body X bearing the given set of stress concentrators {Y<sub>1</sub>,...,Y<sub>n</sub>} is to find such a distribution of body material properties that offers the stability of structural softening state:

$$L = \dim_{x \in V} (k(x) \le 0) \to const, \tag{3}$$

where dim(...) is the size of a region that meets the specified condition.

Condition (3) is a modified condition of "structure strength balance", which is the most effective optimization criterion from the point of view of structure functioning [8,11]. This way, the structure material fulfils its functions evenly, and furthermore, this condition ensures a minimum product weight.

We use the FEniCS finite element analysis package and its implementation in Python to calculate the stress-strain state and optimise the strength parameters of the structure [15]. This framework has been chosen through its wide range of features regarding the analysis of various mathematical models of the material continuum, including those built by the authors themselves, the available scalability, suitability for distributed calculations, as well as the absence of any restrictions on its use for commercial, educational or scientific purposes. Post-processing of finite element analysis results has been carried out using free MatPlotLib software for the Python language [16].

Flowchart of the proposed algorithm (steps 1-9) is shown in the Figure 1. As it is rather difficult to optimise a structure without clear specification of parameters of stress concentrators, given set of mechanical properties and boundary conditions, in the Figure 1 is shown a generalised block-scheme describing the problem of solution according to the above algorithm.



Fig. 1. Flowchart of the solution of the problem of finding the optimal mechanical parameters of the surface layers of parts: 1 - define initial parameters block, 2 - optimizationprocess initialization block, 3 - stresses and softening setting block, 4 - surface layer optimal parameters solving block, 5 - results output block

The proposed flowchart of the algorithm consists of:

- block of initialization of the computational model, in which the investigated body (region zone), the stress concentrators, the boundary conditions, as well as the relations of the mathematical model are defined (according to steps 1-5 of the algorithm);
- block of initialization of the optimization process, in which the initial value of the level of softening of the structure, the permissible value of the relative error, the initial distribution of the mechanical properties of the structure under study, and the parameters of their modification are defined to optimize the value of the softening of the structure;
- block of calculating the stress-strain state of the structure and the magnitude of its softening (according to steps 6-8 of the algorithm);
- block for establishing optimal parameters of surface layers (according to the step 9 of the algorithm), condition (3) is checked in the block, and if it is satisfied, then the optimal solution is derived, if not, then the distribution functions of the parameters of surface layers are modified, and the algorithm returns again to execution of the previous one;
- block for outputting the optimal results, in which the found solutions that satisfy condition (3) are displayed.

An advantage of the proposed algorithm is its ability to provide a searching for the desired quantities for setting problems of any dimension with an arbitrary initial distribution of mechanical properties.

A generalized scheme of the research object with the presence of stress concentrators is shown in Figure 2.



Fig. 2. Schematic presentation of the object of study: X – the area that the body occupies,  $\partial X$  – the body limit,  $x \in X \cup \partial X$ ;  $Y_1, \ldots, Y_n$  – stress concentrators;  $\partial X_1^i, \partial X_2^i, \partial X_3^i$  – the areas of the body where the specified boundary conditions are;  $\vec{F}_1^i(x)$  – the vector of force loads;  $\vec{u}_2^i(x)$  – the vector of displacements,  $i = 1 \ldots k$ ; K = K(x) – a compression bulk modulus, G = G(x) – modulus of shear,  $\sigma = \sigma(x)$  – strength parameters of the material

The object of study consists of a body that occupies an area of space X, which is limited by the surface  $\partial X$ . There are stress concentrators in the body  $Y_1, \ldots, Y_n$ , which can be both internal and external. Areas are given on the surface of the body  $-\partial X_1^i$ , where there are power loads  $\vec{F}_1^i(x)$ ,  $\partial X_2^i$ , in which the movements are specified  $\vec{u}_2^i(x)$ , and unloaded areas  $\partial X_3^i$ ,  $i = 1, \ldots, k$ . The distribution of mechanical properties of the material in the body is as follows:K = K(x), G = G(x),  $\sigma = \sigma(x)$ . The task of the study is to establish such an optimal distribution K, G,  $\sigma$  in the body X under which condition (3) is fulfilled.

To solve problems (1)-(3) by using the finite element method, let us use its "weak formulation". This results in the following ratio [15]:

$$\int_{O} (\vec{\nabla} \cdot \hat{\sigma}) \cdot \vec{v} dx = 0, \tag{4}$$

where  $\vec{v}$  is the weighting vector,  $\Omega$  is the integration domain,  $\hat{\sigma}$  is the stress tensor, which according to model (3), equals to

$$\hat{\sigma} = \vec{\nabla} \cdot \left( \frac{K(x)}{1 - \sqrt{Z(x)}} (\vec{\nabla} \cdot \vec{u}) \hat{I} + \frac{2G(x)}{1 - \sqrt{Z(x)}} (\vec{\nabla} \otimes \vec{u} - \frac{1}{3} (\vec{\nabla} \cdot \vec{u}) \hat{I}) \right).$$

In this paper, in order to simplify the calculations, parameters  $\alpha_1$ ,  $\alpha_2$ ,  $\alpha_3$  are assumed to be zero, since the distribution of damage rate in the body will be taken into account using the elastic characteristics (K(x), G(x)) of the model under consideration.

The integration by parts of expression (4) results in the following:

$$\int_{\Omega} (\vec{\nabla} \cdot \hat{\sigma}) \cdot \vec{v} dx = -\int_{\Omega} \hat{\sigma} \cdot \cdot (\vec{\nabla} \otimes \vec{v}) dx + \int_{\partial \Omega} (\hat{\sigma} \cdot \vec{n}) \cdot \vec{v} ds, \quad (5),$$

where  $\vec{n}$  is the vector over the body surface  $\partial \Omega$ .

Equation (5) is basic for stress-strain analysis of a structure using the FEniCS software.

# 3. Example calculations for establishing the optimum distribution of properties in the near surface layers of parts with hete-rogeneous mechanical characteristics

By way of modelling illustration let us consider a 2-dimensional contact problem for a body with gradient mechanical characteristics and containing a surface stress concentrator (Fig. 3a).

Such setting of the problem is a classic one for the analysis of body behaviour under friction single or distributed multiple contact conditions and ensures high designed accuracy in real structures working under friction conditions [1].

The gradient distribution of mechanical properties, in particular microhardness, shown in Fig. 3b, can be achieved by various targeted technological processes aimed at hardening the part surface.



Fig. 3. Problem setting: a) study object: AB is the contact spot (regions of contact interaction),  $\vec{T} = (T_1, T_2)$  is the load vector, d is the thickness of hardening zone, R<sub>1</sub> is the radius of stress concentrator, Z<sub>1</sub> is the distance between contact zone and stress concentrators; b) diagram of the microhardness distribution by depth: HV<sub>1</sub> is the value of microhardness at the surface, HV<sub>0</sub> is the value of microhardness at the material depth

However, the sound implementation of these technological solutions regarding ensuring an optimal distribution of mechanical properties requires a calculated justification.

Let us take the microhardness value, which describes the condition of a material in the local area, as a basic characteristic of the distribution of mechanical properties. The transition from microhardness values to strength properties is undertaken according to [17].

For direct calculations let us assume that  $HV_l$ = 3900 MPa,  $HV_0$  = 2600 MPa, d=2 mm, output physical load value is 12.5 · 10<sup>4</sup> H, friction coefficient is 0.25,  $R_l$  = 3 mm,  $Z_l$ =10 mm, which corresponds to the working conditions of railway equipment parts following plasma hardening [18,19]. The result will be a stress field that looks like the one shown in Figure 4.

The analysis of the stress state in fig. 4 shows that the highest stress levels occur directly in the contact region and at the stress concentrator. At the same time, the distribution of mechanical characteristics in the body enables managing the stress-strain state of the structure to a wide extent.

Since the stress-strain state unambiguously doesn't define the strength properties of an object let us take the structural softening as a characteristic of its operational properties according to ratio (2).



Fig. 4. Distribution of stresses in the studied structure given the presence of a concentrator, Pa

The distribution of softening value presented in Figure 5 shows that the greatest loss of strength parameters is in the area of the stress concentrator.

As it can be seen in Figure 5, the biggest value of softening of the investigated structure is in the area near contact loads and the stress concentrator.

Let us examine the effect of the stress concentrator size on softening of a structure depending on the depth of strengthening of the material layer.

For this purpose, let us select functional (3) as the optimization criterion, and let us treat the thickness of the strengthened layer d as a control parameter. The thickness of a hardened metal layer can be varied, in particular by controlling technological modes of the plasma hardening process.

Let us change the value of d from 0 to 10 mm and the stress concentrator radius  $R_1$  from 1 to 3 mm. When



Fig. 5. Distribution of the value of softening in the body given the presence of a stress concentrator

calculated, the friction coefficient was as follows: 0.06, 0.125, 0.25, 0.5.

As a result, the following dependence of the maximum softening zone from d is received (Figs. 6, 7, 8).

As can be inferred from the calculations done, depending on the surface stress concentrator size and the friction coefficient, there exists a certain value of the strengthened layer depth d\*, which is approximately three times greater than the stress concentrator radius, upon reaching of which the softening parameter does not change significantly. If the concentrator radius  $R_1$  is 1 mm, the value of d\*= 3 mm, if  $R_2$ = 2 mm the value of d\*= 6 mm, if  $R_3$  = 3 mm the value of d\*= 9 mm.

Further increasing of strengthening depth is not feasible, as at the same operational strength parameters the energy costs of the processing increase.



Fig. 6. Softening zone values at normal load  $12.5 \cdot 10^4$  N and stress concentrator radius  $R_I = 1$  mm



Fig. 7. Softening zone values at normal load  $12.5 \cdot 10^4$  N and stress concentrator radius  $R_1 = 2$  mm



Fig. 8. Softening zone values at normal load  $12.5 \cdot 10^4$  N and stress concentrator radius  $R_1 = 3$  mm

An increase in the softening parameter along with the increased friction coefficient indicates a change in the strength parameters of parts depending on the specific processes taking place in the friction contact zone.

The proposed approach is a further development of works [14,20] and makes it possible to select technological strengthening to manage operational parameters of parts bearing stress concentrators in order to ensure their hardness and durability.

#### 4. Conclusions

1. Based on computational and applied mechanics approaches, the problem of optimising operational

parameters of parts bearing stress concentrators upon technological strengthening has been considered.

- 2. Using FEniCS software for FEM-analysis and its Python implementation the stress state of structure under loads close to the operational ones has been analysed.
- 3. It has been determined that, depending on the stress concentrator size, strengthening must be performed to a different depth, which should be approximately three times greater than the concentrator radius. If the concentrator radius  $R_1$  is 1 mm, the depth should be strengthened up to  $d^* = 3$  mm, if  $R_2 = 2$  mm the depth should be strengthened up to  $d^* = 6$  mm, if  $R_3 = 3$  mm the depth should be strengthened up to  $d^* = 6$  mm. Further increasing of strengthening layer depth is not feasible, as at the same operational strength parameters the energy costs of the processing increase.

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