Information system “Graded coatings”

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Abstract. Functionally graded coatings are widely used to protect structures and machine parts from damage caused by mechanical and thermal loads. The information system “Graded coatings” was developed to help the researchers to design such coatings and also for expanding the availability of tools for calculating and analysing of experimental data. The system was constructed for interactive data preparation and multi-parametric analysis of the results of numerical-analytical solution of mixed boundary value problems of crack theory and theory of elasticity and thermoelasticity for continuously inhomogeneous coatings of complex structure.

1. Introduction

The advantages associated with an increase in the service life of products with continuously varying depth properties stimulate the process of designing of so-called functionally-graded materials and functionally-graded coatings. High cost and long duration of field tests of materials and products directly at the stands and the need to properly interpret these results support a high interest in the construction of mathematical models and solving thermomechanical problems in the case of the variable physical and mechanical characteristics of material [1, 2].

J. R. Barber [3-5] paid serious attention to solving thermoelastic problems. In studies by Z.H. Jin [6] and H.M. Shodja [7] the problems of thermoelasticity for functionally-graded materials were considered, however, in these works the thermal conductivity coefficient was assumed to be constant. Investigations of the effect of temperature on functionally graded materials were carried out by N. Noda. [8]. The influence of inhomogeneity parameters in functionally-graded materials during thermoelastic steady-state contact is studied in the paper by S.P. Barik [9]. Thermoelastic contact between a flat punch and the functionally-graded coating was reviewed by H.J. Choi and G.H. Paulino [10]. Y.H. Jang in [11] presented a numerical solution for a steady thermoelastic contact for a Hertz-type problem. Thermomechanical analysis for heterogeneous two-layered coatings was given in the papers [12, 13]. A number of works [14-16] are devoted to predicting behavior of the mechanical characteristics of functionally-graded coatings during crack formation using the extended finite element method. In addition to objects of artificial origin, natural materials are actively investigated to assess the distribution of mechanical characteristics by their depth, for example, when optimizing materials for implantation [17-20] or when assessing the efficacy of medical intervention [21]. Note that studies of the problem of thermoelastic contact taking into account an independent change in the coating according to an arbitrary law of the thermal conductivity coefficient, linear expansion coefficient, heat capacity coefficient, Young’s modulus and Poisson’s ratio are absent in the known literary sources. One of the reasons is the absence of known analytical solutions to inhomogeneous problems of thermoelasticity with general independent laws of variation of thermomechanical characteristics by depth [22, 23].
2. The purpose of the information system “Graded coatings”

A prototype of the information system was developed using Fortran Powerstation 4.0 to carry out numerical calculations that implement the original technique developed by us for solving mixed boundary problems of static axisymmetric thermoelasticity for continuously inhomogeneous coatings of complex structure. The prototype can also preserve results of calculations and subsequently carry out their multiparametric analysis along with visualization of stress-strain state of inhomogeneous coating and its thermomechanical characteristics.

For its development the database was created and maintained in the environment Visual FoxPro. The database stores the calculation results, preceded by key attributes containing the task code and the calculation information descriptor code. In addition, it contains fields for storing information about the ratio of the coating thickness to the radius of the contact area, the radius and depth of the calculated points and the calculated characteristics themselves. To carry out multiparametric analysis, a module was developed that allows the user to create analytical queries to the database and visualize their results using the Gnuplot package. The initial information about each calculation contains information about the thickness of the coating, the thermoelastic characteristics of the substrate, as well as a description of the laws of independent change in the thermoelastic characteristics in the coating. In addition, there is a description of the parameters of the surface effect and individual parameters of the calculation itself (the type of the problem being solved, the set of nodes in which the kernel is being built, etc.). The information is saved to the database, the key attribute is a composite key from the codes of the impact descriptor, coating and calculation parameters.

The values of the components of the fields of displacements, deformations, stresses, temperature, and heat flux are constructed using numerical integration at the given points of a half-space inhomogeneous by depth.

3. Description of the website “Graded coatings”

Currently, the web-interface of the information system “Graded coatings” is being developed for interactive data preparation and multiparametric analysis of the results of the numerical-analytical solution of mixed boundary value problems of the theory of cracks and the theory of elasticity and thermoelasticity for continuously inhomogeneous coatings of complex structure. The database was ported to PostgreSQL, and the server side of the web interface is developed in Python using the Django library. The project of the website assumes the opportunity to familiarize with the description of the purpose of the information system and the list of tasks to be solved without registration. When registering, the user gets access to the mode of forming a description of the properties of the graded coatings (laws of change in Young’s modulus, etc.) and other components of the task for calculating the problem of interest. After sending the form with the task for processing and carrying out the calculation, the user can conduct a multiparametric analysis of the results obtained.

The website menu includes the following items: Home page; The laws of heterogeneity; Impacts; Coatings; Calculation parameters; Calculation; Processing of results; Log off. The first item is informational, the rest call up interactive forms that allow you to get acquainted with the lists of objects stored in the database:

1. descriptions of the laws of change in thermomechanical properties;
2. descriptions of thermomechanical loads (indentation, expansion of disc cracks, etc.);
3. descriptions of various coatings;
4. descriptions of additional calculation parameters;
5. descriptions of tasks for the calculation, indicating specific coatings, effects and additional parameters;
6. descriptions of tasks for processing results.
Lists of the laws of inhomogeneity, coatings, impacts and calculation results contain graphic thumbnails to help users to navigate through the selection. Each item in the list includes buttons "Change" and "Delete", in the header of the table there is an item "Add". Thus, the user has the ability to add, modify and delete any objects in his configuration, but does not possess access to other people's objects.

**Figure 2.** List of laws of change of thermo-mechanical characteristics
4. An example of using the "Gradated coatings" website

Let us consider the simplest case of a continuous change in properties by depth - a monotonic decrease. We suppose that the Young's modulus can change by a factor of 2 in comparison with the substrate. Figure 1 shows 4 different cases of its change.

![Figure 3. Laws for the Young's modulus change](image)

For materials with coatings in case of modelling nanoindentation experiment, it is possible to determine the elastic modulus that is relevant for a certain contact zone [28-30], and therefore is a certain average value between the modulus of elasticity of the surface and deep layers of the material. This characteristic will be called the stiffness function of inhomogeneous base [31]. In case of spherical indentation, the stiffness function has the following form:

$$E_c \left( \frac{a}{H} \right) = \frac{3}{4} \frac{P}{a \delta} \frac{1}{1 - \nu_0^2}$$  \hspace{1cm} (1)

where $a$ – contact area radius, $\delta$ – indenter displacement, $\nu_0$ – Poisson’s ratio of the layer on the surface, $H$ – layer thickness. For an inhomogeneous material, the stiffness function or effective modulus is a function of the dimensionless geometrical parameter $a/H$.

We introduce descriptions of the corresponding coatings, impact parameters (spherical punch), additional calculation parameters and then send the task for calculation. Let us switch to the calculation results processing mode.

![Figure 4. Calculation results processing mode](image)

Figure 4 shows the values of the stiffness function presented depending on $a/H$ for the combinations of laws of change of elastic parameters described above. Analysis of the behavior of the curves (Figure 5) shows that the curves of the stiffness function 2 and 3 are barely distinguishable.
However, if we introduce the function
\[
S_l \left( \log_2 \left( \frac{a}{H} \right) \right) = S \left( \frac{a}{H} \right)
\]
and numerically differentiate it by \( \log_2 \left( \frac{a}{H} \right) \), then according to the obtained curves we can separate the linear decrease (laws 1, 3) from the step one (laws 2, 4) and thus determine the real thickness of the inhomogeneous layer.

**Figure 5.** Stiffness function values depending on \( a/H \)

**Figure 6.** Derivative values of the stiffness function in a logarithmic scale
5. Conclusion
The original numerical-analytical method was used to model the behavior of functionally graded coatings under the thermomechanical load. The method implemented made it possible to successfully construct an approximate solution of static thermoelasticity problems for a continuously inhomogeneous medium. The solution of mixed problems of the action of a heated or cooled punch on a continuously inhomogeneous half-space is reduced to solving systems of paired integral equations. The kernel transforms are approximated by expressions of a special form, which made it possible to obtain an analytical solution. For the practical application of the developed methods for the numerical and analytical solution of a wide range of mixed and unmixed boundary value problems of the axisymmetric static theory of thermoelasticity, taking into account an arbitrary combination of the laws of change in thermomechanical properties (Young's modulus, Poisson's ratio, thermal conductivity and linear expansion coefficients), a program complex in the Fortran language has been developed. The initial data for the calculation was collected in the form of a set of text files that contains tables of values of the laws of inhomogeneous changes in thermomechanical properties, a description of the types of influences (distributed pressure, various punches, temperature or heat flow), a set of design parameters that affect the accuracy and time of calculation.

To generate the initial data, save the results of calculations and carry out their further multiparametric analysis, a database has been developed. The database was created and maintained by data under the control of the PostgreSQL database management system. The Gnuplot package was used to visualize the calculation results. The information system web interface was developed on the basis of the Django cross-platform system and the Python language. A brief description of the site was given and an example of its usage was provided. From November 1, 2020, the website will be available at http://109.195.227.87/.

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