On the estimation of strength properties of porous ceramic coatings

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A method for estimating the strength properties of a porous ceramic coating was proposed. The method is based on the analysis of preliminary test results on indentation of coatings with defects of varying size and depth of occurrence. The strength properties of the coating were studied by computer simulation combining the discrete description (the movable cellular automata method) and continuous description (the finite difference method). Relationships were found between the parameters of a pore such as its length and depth of occurrence in the coating and the critical stress corresponding to fracture of the coating. The proposed method can be used to study the strength properties of material surface layers and to predict the critical stress in a contact region.

Keywords: numerical simulation, movable cellular automata method, porous ceramic coating, strength properties of coatings

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1. Introduction

Today, rapt attention is focused on the issues that concern the coating deposition and modification of surface layers of materials for improving their performance [1–5]. This is especially urgent for various problems of contact interaction such as friction and wear, in which the interaction between surface layers governs the behavior of a unit or the whole mechanism. The most widespread methods of coating deposition, including wear resistant coatings, are thermochemical (thermodiffusion saturation of the surface) as well as chemical and physical deposition methods [1–5]. The above techniques provide a good combination of necessary physical and mechanical properties of friction surfaces (wear resistance, strength, microhardness, crack resistance, etc.) and saving on alloy additions, which enables the proper modification of the structure and properties of the substrate material. At the same time, friction units under actual operating conditions are exposed to a great number of influences. Cycle operation, high contact stresses and temperatures, a variety of active physical and chemical processes change the structure of wear resistant coatings and possibly cause the generation of various defects in them such as micro- and nanopores, cracks, etc. These factors can significantly change the performance characteristics of the coated materials, even to the point of their failure. In this connection there arises a need to check the quality of coatings not only in the course of friction unit operation but also immediately after the surface layer deposition or modification.

In recent years, along with the conventional quality control methods for surface layers, new approaches on the basis of nondestructive testing are being developed [6–8]. An important tool for the development of new quality control methods for surfaces and coatings is computer simulation. It makes possible to analyze the influence of various parameters (physical and mechanical parameters of the system, loading conditions, etc.) on the mechanical behavior of the coated material under loading.

In the present paper a theoretical study is carried out with computer simulation methods to investigate whether it is in principle possible to determine the form of the functional dependence of the strength properties of a coating with structural defects such as pores on the depth of their occurrence and characteristic sizes. The calculations are performed in the framework of a combined discrete-continuous approach that has proved to be very effective for the solution of this kind of problems [9–11]. The process of combining the discrete (the movable cellular automata method) and continuous (the finite difference method) approaches as well as each of the used methods is described in papers [12–14].

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2. Simulated system description

The mechanical properties of coatings with defects are estimated in a simulated indentation test. The test allows defining all the coating material characteristics necessary in practical use, such as microhadrness, detachment coefficient, crack resistance coefficient, Young's modulus and other [15, 16]. We simulate the indentation of a ceramic coating on a metal substrate (Fig. 1). The materials of the indenter, substrate and coating are respectively corundum, steel and zirconium dioxide. Zirconium dioxide is chosen because of its physical and mechanical characteristics necessary for the given problem (high wear resistance, the capability to increase many times the service life of parts, components and tools [18]). Besides, we have enough experience in correctly describing the behavior features of this material under quasi-static and dynamic loading [19]. The response functions of automata of the model materials are shown in Fig. 2. The elastic moduli *E* and Poisson's coefficients ν are listed in Table 1.

The lower layer of the metal substrate and the upper layer of the indenter undergo slight elastic deformation, they are simulated in the framework of the continuum mechanics method. The indenter tip and ceramic coating, i.e. the contact regions, subjected to severe deformation are simulated with the movable cellular automata method. The coating thickness is 91 nm. The substrate width and height are 1 200 nm and 2020 nm, respectively. The indenter tip size is 44 nm. The depth of occurrence of a pore (the distance from the coating surface to the upper edge of the pore) varies from 17.9 to 73.28 nm (from 19.7 to 80.5 % with respect to the coating thickness). The pore is a rectangular with rounded corners, its height is 17.9 nm and length varies from 44 to 324 nm in different problems.

In the paper we accept the restriction that the symmetry axes of the pore and indenter coincide. Such an assumption allows us to estimate the minimum critical stress at which the coating material is damaged. Loading is performed by applying equal force to all grid nodes of the upper indenter layer and thus we simulate the action of a uniformly distributed compressive stress σ. In order to eliminate dynamic effects and achieve a specified load value, the stress grows from 0 to σ by a sinusoidal law. The lateral surfaces of the specimen (coating and substrate) are free. The velocities of the nodes of the lower grid layer are set equal to zero to simulate a fixed substrate.

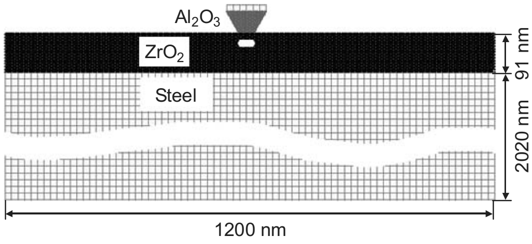

Fig. 1. Simulated indentation of a ceramic coating on a metal substrate

Table 1

Parameters of model materials [20]

Material	*E*, GPa	ν
Al$_2$O$_3$	416	0.3
ZrO$_2$	172	0.3
Steel	206	0.28

For the simulation of nanoscale pores, the diameter of a movable cellular automaton is 4 nm. The grid spacing in the continuous description is 16 nm. The problem is solved in the plane strain approximation. The strength of the coating with a defect is defined by the minimum value of the indentation stress σ_c at which a crack between the pore and the indenter initiates. This characteristic can also be an estimate of the critical stresses in a contact pair at which the friction mode is changed.

The procedure of finding σ_c is the same for all problems and consists in the following. At the first stage we estimate roughly the value of σ_c by the indentation test results for a specimen with a pore of a given size. At this stage the indenter moves with constant velocity *V*. The obtained estimate of the coating strength (the stress corresponding to crack initiation between the indenter and the pore) is designated as σ_V. Two values of the loading velocity are used: $V_1 = 0.5$ m/s and $V_2 = 1.0$ m/s. The value of σ_V is determined as an arithmetic average of the σ_{V_1} and σ_{V_2} values. At the second stage the value of σ_V is refined in a series of calculations, so that in the *i*-th calculation the stress σ_i is applied to the indenter whose value is found from the relation

$$\sigma_i = \sigma_V \pm \Delta \cdot i, \text{ where } \Delta = 0.01\text{–}0.1 \text{ GPa}.$$

The sought value of σ_c is determined as $\sigma_c = \min \sigma_i$, at which macrocracking occurs in the coating between the indenter and the pore.

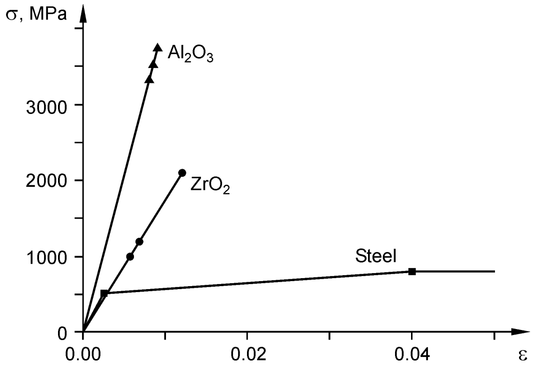

Fig 2. Response functions of movable cellular automata

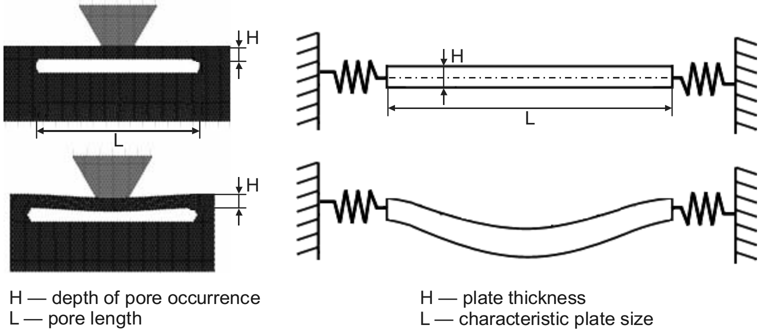

Fig. 3. Part of the indented model coating which corresponds to a bended plate with elastically fixed edges

3. Preliminary estimate of the coating strength on the basis of the geometric parameters of a plate in a bending test

A part of the model coating above the pore is, in the limiting case, a rectangular plate with two elastically fixed edges (Fig. 3). Indeed, the material of the studied coating exhibits linear elastic behavior [20], and the ends of the "plate" under bending are affected by the elastic forces acting from the "surrounding" coating material. The pore length *L* can be interpreted as the characteristic size of the plate and the depth of occurrence of the pore *H* as the plate thickness. The bending deflection of the considered part of the coating which occurs under indentation loading corresponds to the deflection of the plate.

In the literature plates are classified on the basis of their length to height ratio L/H. The mechanical behavior of a plate, including its capability for bending resistance, strongly depends on to what class it belongs [21]. There is a class of thick $(L/H \le 8\div10)$ and thin $(8\div10 \le L/H \le 80\div100)$ plates. Thick plates are large bodies, for which calculations are performed with regard to all stress state components with the use of general equations of a spatial problem. For thin plates, apart from bending forces, membrane forces and deformation in the median surface of the plate are essential [21]. In the given sense, the model plates considered in the paper correspond both to the class of thick and thin plates. Therefore, even before performing model calculations we may state that the strength properties of the coating with a pore, particularly σ_c, are defined by the ratio of the pore length to the depth of its occurrence in the coating L/H. Besides, for coatings corresponding to different classes of plates the form of this dependence will most probably be different.

4. Numerical study of the porous coating fracture and search for the functional dependence of the coating strength properties on the defect parameters

Analysis of the simulation results has shown that only the L/H ratio exerts influence on the coating fracture pattern, because this quantity determines the type of the forces dominating in the loaded part of the coating. A change of the *L* or *H* value alone does not influence the fracture pattern, given that the L/H ratio value lies within a certain range (for the considered coatings $0.6 \le L/H \le 18.1$).

The fracture of the coatings with $0.6 \le L/H \le 8.3$ occurs due to the formation of macrocracks propagating directly from the indenter tip at angles of 30º and 150º from the surface line (Figs. 4(*a*, *b*)). The coatings with $8.3 \le L/H \le 18.1$ fracture due to the formation of vertical cracks in the material above the pore propagating upward from the pore edges as well as due to the formation of a symmetric system of inclined cracks in the center of the given fragment which propagate at angles of 30º and 150º from the surface line (Figs. 4(c, *d*)). In the coatings with $8.3 \le L/H \le 18.1$, as distinct from the coatings with $0.6 \le L/H \le 8.3$, cracks are initiated both directly in the contact points of the corners of the indenter tip (Fig. 4(*d*)) and under the indenter at a distance from its tip (Fig. 4(*c*)). The fracture pattern observed in these coatings (Fig. 4(*c*, *d*)) is not typical for isotropic monolithic solids under indentation loading. This allows us to consider them as a construction whose fracture is governed by its geometry. In all the studied coatings cracks are initiated in the points of maximum shear stresses as the fracture criterion for automata links in the MCA method is calculated by the stress intensity in a pair of interacting automata [8, 22].

In the context of the above-drawn analogy these results agree well with the engineering evaluation of the behavior of plates [21] both by the type of the forces arising in bending and by the value $L/H = 8.3$ that separates the class of thick and thin plates.

The simulation results show that the value of the critical indentation stress σ_c for the considered coatings is determined by the size of the pore and depth of its occurrence as well as by the ratio of the two values. Particularly, an increase of the defect length *L* as well as a reduction of the depth of its occurrence *H* causes a decrease in the strength properties of the coating. The dependences demonstrating these tendencies for the model coatings are given in Fig. 5.

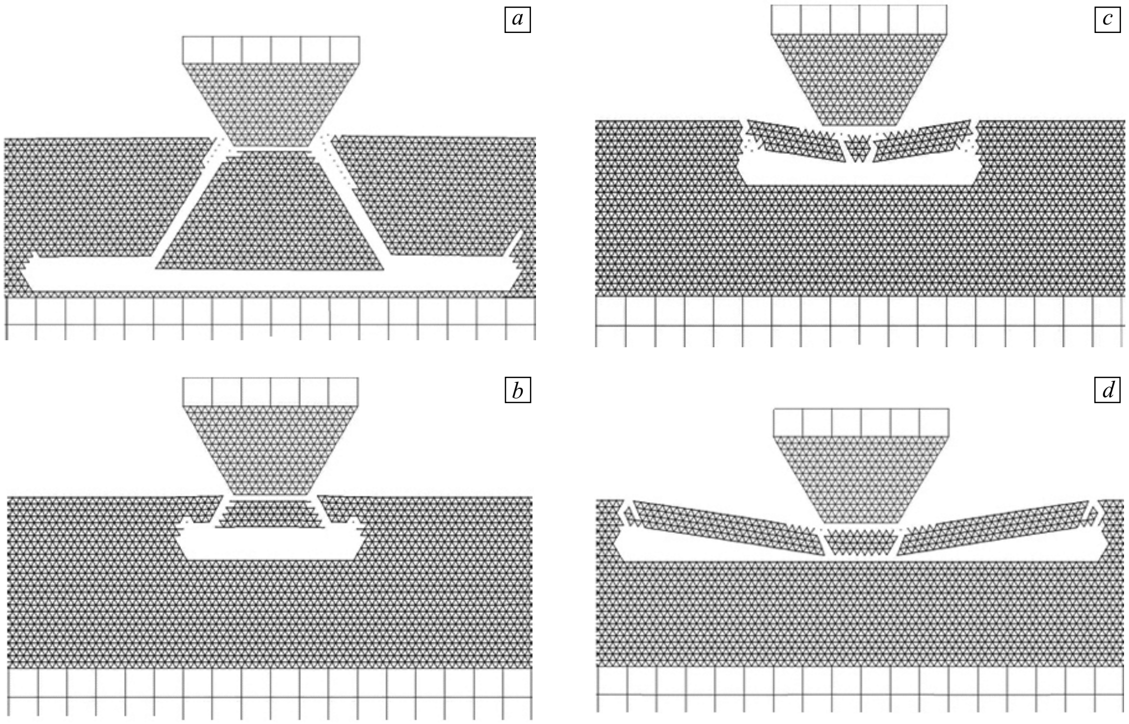

Fig. 4. Schematic coating fracture in the zone of a defect at the moment of crack initiation in the coatings with different values of L/H = 3.76 (*a*), 5.8 (*b*), 8.3 (*c*), 16.9 (*d*). Automata links are shown

The calculations are performed for the case of the minimum, maximum and intermediate depths of pore occurrence in the coating.

The construction of the above dependences in the logarithmic coordinates has shown that they are exponential (Fig. 6), and their general form can be written as

$$\sigma_c = A_H L^{-n}, \quad (1)$$

where A_H is a coefficient possessing an individual value for each depth of occurrence *H*, and *n* is the function of *H*.

It is seen from the diagram (Fig. 6) that some points corresponding to H = 17.9 nm deviate from the dependence. They lie below the approximation line and can also be described with the exponential relationship, but with other values of A_H and *n*. Notice that for these points the condition $8.3 \le L/H \le 18.1$ holds true. For other $0.6 \le L/H \le 8.3$. This very fact suggests that the strength properties of the model coatings, apart from *L* and *H*, are also determined by the ratio L/H. The conclusion also agrees with the above-drawn analogy that a coating with a pore behaves like a bended plate. Since for the majority of the model coatings the condition $0.6 \le L/H \le 8.3$ holds true, only these coatings will be further considered. This will make it possible to exclude the influence of the parameter L/H on σ_c and to consider σ_c only as $\sigma_c = \sigma_c(L, H)$, and hence to define more precisely the form of the relationship sought.

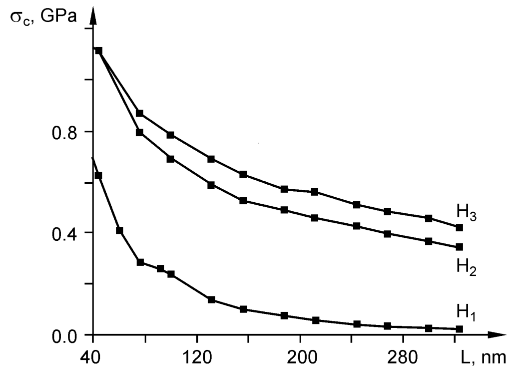

Fig. 5. Critical indentation stress σ_c versus pore size *L* at different depths of pore occurrence *H*: H_1 = 17.9 nm, H_2 = 59.4 nm, H_3 = 73.3 nm

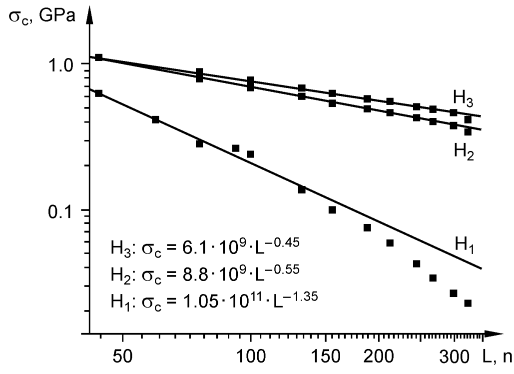

Fig. 6. Critical indentation stress σ_c versus pore size *L* at different depths of pore occurrence *H* (H_1 = 17.9 nm, H_2 = 59.4 nm, H_3 = 73.3 nm) and approximating exponential functions in the logarithmic coordinates. The points correspond to model calculations

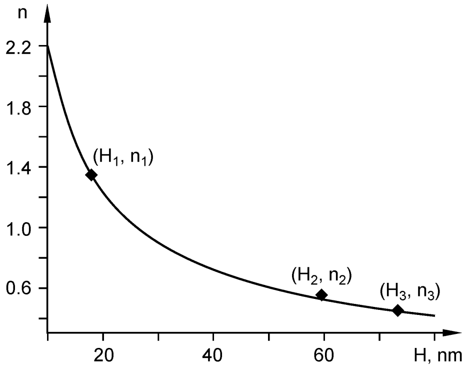

Fig. 7. Graphical representation of the exponential function $y = \dfrac{13.5}{x^{0.795}}$ approximating three calculation points (H_i, n_i) that satisfy the sought function $n = n(H)$: (17.9 nm, 1.35), (59.4 nm, 0.55), (73.3 nm, 0.45)

A way of finding the functional relationship $n = n(H)$ is to perform a series of calculations to determine σ_c for coatings with different L and H values from the considered range. The way, however, requires substantial computing resources. We propose a different way of finding $n = n(H)$. An approximation line in the logarithmic coordinates is selected by three points $(H_i, n_i) = (17.9$ nm, 1.35), (59.4 nm, 0.55), (73.3 nm, 0.45), which satisfy the sought relationship and correspond to the depths of pore occurrence, and thus the form of the relationship $n = n(H)$ is defined. Then, the approximation accuracy is checked by performing two additional test calculations. The best approximation of the given points is obtained with the use of the following exponential function (Fig. 7):

$$n = 13.5/H^{0.795}, \tag{2}$$

where H is measured in nanometers. We can therefore infer that it is precisely the relationship that we sought for the studied model coatings. So, the strength properties of coatings with a pore of different length L and depth of occurrence H are described by the following relationship (here, L and H are in nanometers):

$$\sigma_c = A_H L^{-n}, \text{ where} \tag{3}$$
$$n = 13.5/H^{0.795}, \;\; 0.6 \le L/H \le 8.3,$$
$$44 \le L \le 324, \;\; 17.9 \le H \le 73.3.$$

5. Accuracy check of the found relationship

At the next stage of investigating how the mechanical properties of coatings depend on the defect characteristics we check the accuracy of the found analytical relationship (3). The intermediate value $H_t = 38.7$ nm was chosen from the considered range of the depths of pore occurrence 17.9 ≤ ≤ H ≤ 73.28 nm, and the parameter $n_t = 0.74$ corresponding to it was found from relationship (2) (Fig. 8).

For the coating with the chosen $H_t = 38.7$ nm and a pore of the length $L = 244$ nm lying in the considered range 44 $\le L/H \le$ 324 nm the corresponding value $\sigma_c =$ = 0.256 GPa was found in a computer-based calculation. By the obtained values of n and σ_c we found from (1) the value $A_H = 1.5 \cdot 10^{10}$ and the assumed analytical relationship for describing the strength properties of a coating with pores of different length L at depth of occurrence 38.7 nm:

$$\sigma_c = 1.5 \cdot 10^{10} L^{-0.74}. \tag{4}$$

Relationship (4) was verified in an additional calculation in which the critical stress σ_c was estimated for the case of a brittle coating with a pore of the length $L = 156$ nm occurring at the same depth H_t. The two calculation points found and the corresponding analytical dependence for H_t as well as the dependences obtained for other depths of pore occurrence are represented in Fig. 9. As is seen, the analytical estimates agree qualitatively and quantitatively well with the simulation results. The analytical straight line corresponding to H_t belongs explicitly to the class of straight lines (corresponding to H_1, H_2, H_3) constructed by the calculation results, and its deviation from the simulation result (from σ_c corresponding to $L = 156$ nm) is less than 1 %.

This result confirms our assumption about the exponential form of the relationships $n = n(H)$ and $\sigma_c = \sigma_c(L)$, and consequently relationship (3) can be used for finding the strength properties of a coating with a pore in the given variation range of the parameters L and H. Thus, only one model calculation for each value of H and arbitrary L is enough to find σ_c for coatings in the entire range of values of the defect parameters using negligible time and computational resources.

It should be noted that the considered model is multiparametric, namely, it is characterized by the width of the indenter tip, the height and length L of the pore and depth of its occurrence H. The validity of the proposed estimates is shown only for the case of the two varying parameters L and H and only for the considered range of their ratios, because only these quantities were of primary interest for our investigation. In order to find the limits of the range of the parameter values, in which the derived relationships hold true, as well as to account for the influence of two other

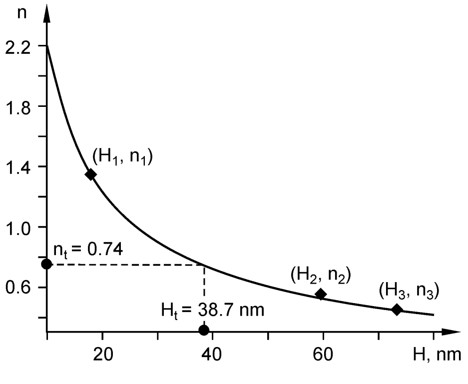

Fig. 8. Determination of the exponent n of relationship (1) which corresponds to the depth of pore occurrence $H_t = 38.7$ nm

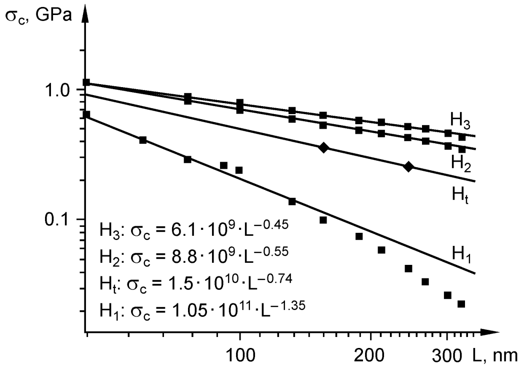

Fig. 9. Critical indentation stress σ_c versus pore size L at different depths of pore occurrence H ($H_1 = 17.9$ nm, $H_2 = 59.4$ nm, $H_3 = 73.3$ nm) for the considered model coatings (logarithmic scale). The points correspond to the computer-based calculation, approximating functions — to their analytical estimates

parameters on the strength properties of coatings with a defect, an additional investigation must be carried out.

6. Conclusion

The paper puts forward a new method of estimating the strength properties of a brittle coating with defects such as pores. The approach is based on the calculation of the critical stress that causes porous coating fracture in preliminary indentation tests, in which the depth of occurrence of pores and their characteristic length vary. Using the obtained values we plot the dependence of the critical stress on the length and depth of occurrence of a defect in the surface layer in the entire range of values of the varying parameters. This relationship, together with the available data about the characteristic depths of occurrence and sizes of pores in the coating, allows the estimation of critical stresses without additional investigation. The given approach actually provides a basis for nondestructive testing methods and can be used to study the strength properties of material surface layers and coated materials. The accepted restriction that the symmetry axes of the pore and indenter coincide does not reduce the significance of the proposed method because it nevertheless allows the estimation of the minimum critical stresses that cause coating fracture. The deviation of the indenter from the line passing through the center of the pore will lead to an increase of σ_c. Hence, if the stresses achieved in the contact region are lower than the assessed values obtained in the proposed method, the coating will not fracture. The investigation results can be used in various applied problems, particularly, to predict critical stresses in a friction pair.

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