Contact stress simulation problem in case of thermal spray coatings

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Abstract. In this study was addressed the problem of the contact stress simulation, generated in the case of the loads applied on thermal spray coatings, by finite element modelling. Starting from the characteristic lamellar morphology of this type of coatings, consisting of splats, voids, oxidized or unmelted particles, the studied layers were assimilated to an anisotropic material. Thus, it was tried to establish the parameters necessary for modelling, so that they define as accurately as possible the studied material. The purpose of this study was to identify the maximum value of the tension developed in the point contact, on the depth of the analysed layer. This value was subsequently used to determine the limit values for in practice use of the coatings.

1. Introduction

The widespread use, in many industrial fields, of the coatings made by thermal spraying, has required the finding of solutions to ensure their optimal operation functioning, when subjected to various types of stress: compression, wear (abrasive, adhesive, contact etc.), erosion, thermal shock, corrosion, fretting etc. [1-3].

As can be seen both in current practice and in many studies available in the literature, one of the most common types of destruction of thermally sprayed coatings is exfoliation (spalling, flaking) [4]. This is most often caused by a combination of characteristic factors of the assembly in which it operates, one of the most common being the operation in point contact mode (herzian contact). It is known that these working conditions lead to the accumulation of stresses in the layer, deformation of the coating and the appearance of contact fatigue [5,6].

Thus appears the need to study the way in which the generated forces are distributed, there being, at least from a theoretical point of view, several variants:
- accumulation of stresses in the sprayed layer (in the thickness of the coating);
- distribution of maximum stresses at the coating-substrate interface;
- accumulation of stresses in the substrate.

Another very necessary observation is related to the microstructural change produced by deformation under the influence of the contact force, this being directly related to the material characteristics [4], its degree of anisotropy [7], and the thickness of the coating.

Such an analysis, which indicates the optimal thicknesses of a coating made of a certain material by thermal spraying, is very necessary, because it could come to the aid of design engineers, who could thus...
accurately calculate the theoretical durability of the coating, in various operating conditions. However, the practical realization of such a study is very expensive and time and resource consuming, due to the large number of variables that must be taken into account.

A solution is the simulation with finite element of the behaviour of thermally sprayed coatings in different conditions. From the resulting data can be extracted solutions related to optimal layer thicknesses, respectively limit values of the stresses to which the coatings can be subjected in operation without being destroyed.

In this paper we addressed the issue of simulating the contact stress, generated in the case of various loads applied on thermal spray coatings, by finite element modelling, having as main variables the material characteristics (three different types of material were studied) and different thicknesses of layer (three different thicknesses were considered: 60, 80 and 100 μm respectively).

2. Materials and methods

2.1. Materials

For the analysis of the aspects related to the simulation of the contact voltage, three types of coatings made by thermal spraying were chosen. Table 1 presents the chemical compositions of the powders used to produce the coatings and the methods we used, two of them being obtained by the Atmospheric Plasma Spray (APS) method [8] and the third by Flame Spray (FS) method [9]. Low alloyed steel blades were used as the deposition substrate.

| No. | Powder | Coating method | Chemical composition | Commercial name (manufacturer) |
|-----|--------|----------------|----------------------|--------------------------------|
| 1   | Cr₂C₃-Ni20Cr | APS | 18.75wt% Ni, 9.95% C, < 2.25 wt% other elements, Cr balance | 81NS (Metco - Oerlikon) |
| 2   | ZrO₂-5CaO | APS | min. 91.5 wt% ZrO₂, 4.5 – 5.5 wt% CaO, the rest of the percents are represented by other oxides. | 201NS (Metco - Oerlikon) |
| 3   | NiCrBSi | FS | 0.7% C, 4% Fe, 15% Cr, 4.3% Si, 3.1% O, rest Ni | JK-586 (Deloro Stelite) |

2.2. Methods

2.2.1. Methods for thermal spray coatings characterization. The considered coatings were evaluated from a microstructural point of view by electron microscopy, for this purpose the Quanta 200 3D electron microscope was used, with the LV (Low Voltage) working mode and LFD (Large Field Detector) detector. The microstructural aspects of the surfaces of the coatings are presented in figures 1(a), (b), (c).

In figures 1(a) and (b) can be observed the specific aspect of the coatings produced by thermal spraying, being visible on the surface some semi-molten particles, some agglomerations of particles but also a partially porous aspect, with deeper areas at the boundaries of some splats. Figure 1(c) shows the morphology of the NiCrBSi coating surface, in the processed state (sanding with abrasive paper), a necessary operation due to the remelting to which the coating was subjected after the deposition by the FS method. It is characterized by the presence of a large number of phases, coloured with different shades of grey: eutectic matrix consisting of Ni solid solution with spheroidal precipitates L12 type (light grey), coarse crystals type Ni₃Si₁₂ (medium grey), columnar crystals (dark grey) of M₇C₃ (M = Cr) and M₃B₂ (M = Ni, Cr) type.
For a complete characterization, a sample of each type of coating was cross-sectioned and metallographic prepared by grinding with abrasive papers of different granulations, followed by polishing with abrasive paste and etched with specific reagents. The microstructural aspects of the samples in cross section are presented in figures 2 (a), (b) and (c).

Figures 2(a) (on the right side of the image) and 2(b) (on the left side of the image) show the cross-sectional appearance of the coatings, with layered lamellar structure, formed by successive deposition of the accelerated splats to the substrate, structure specific to coatings produced by APS. Also, in figure 2(c) is presented the cross-section aspect of the NiCrBSi coating, on the surface prepared from a metallographic point of view being visible the same structures specified in the case of figure 1(c).

The material characteristics necessary for the simulation of the contact tension were obtained by micro-indentation with the help of the UMTR 2M-CTR Microtribometer, being extracted the values of the modulus of elasticity, respectively the microhardness. The test configuration consisted of a Rockwell type diamond tip, with a radius of 5mm, the maximum loading force used during the tests being 20N. Three tests were performed for each sample, the results obtained being summarized in table 2.

2.2.2. Methods for contact stress simulation. In order to study the problem of simulating the contact stress generated when applying some loads on the thermal spray coatings considered in this paper, the CATIA V5 program was used. Starting from the lamellar structure of the coating and taking into account other studies in the literature, the premise was addressed that the analyzed coatings are anisotropic materials.
They were used for the discretization network the parabolic tetrahedron elements. In the contact area, the local discretization network has the following dimensions: local mesh size = 0.015mm and sag = 0.01mm. Otherwise, the global discretization network has the following dimensions: global mesh size = 0.1mm and sag = 0.05mm. This resulted in a total number of 55072 nodes and 43882 elements.

The Gauss R6 mathematical method (fast Gauss method) was used to solve the finite element static analysis.

The following aspects were considered:
- smooth contact between a ball and a plane,
- ball radius = 8mm (ball radius R),
- loading Q = 72.6153N (normal load).

The material parameters that were not obtained experimentally were taken from the literature: the Poisson's ratio [10, 11], respectively the density [12]. Regarding the Coulomb module, it was analytically obtained with the calculation formula (1), based on some previously established parameters.

\[ G = \frac{E}{2(1 + \nu)} \]  

where: \( E \) - Young's module, \( \nu \) - Poisson's ratio.

It was considered that the ball is made of low alloy steel, as well as the substrate, their material parameters being: Young's modulus \( E = 210 \text{ GPa} \), Poisson's ratio \( \nu = 0.30 \), density \( \rho = 7.86 \text{ g/cm}^3 \).

**Table 2. Material characteristics of the analysed coatings.**

| Sample / test          | E (GPa) | Poisson ratio (\( \nu \)) | Hardness (GPa) | Coulomb's modulus (GPa) | Density (g/cm\(^3\)) |
|------------------------|--------|----------------------------|----------------|-------------------------|-----------------------|
| NiCrBSi / 1            | 90.253 | 0.25                       | 5.2965         | 40.112                  | 6.53                  |
| NiCrBSi / 2            | 97.792 | 0.25                       | 4.9933         | 43.463                  | 6.53                  |
| NiCrBSi / 3            | 90.883 | 0.25                       | 5.8741         | 40.392                  | 6.53                  |
| Cr\(_2\)C\(_3\)-Ni20Cr / 1 | 65.540 |                           | 1.2972         | 28.745                  |                      |
| Cr\(_2\)C\(_3\)-Ni20Cr / 2 | 50.846 | 0.28                       | 0.9388         | 22.300                  | 6.0                   |
| Cr\(_2\)C\(_3\)-Ni20Cr / 3 | 64.420 |                           | 1.3067         | 28.254                  |                      |
| ZrO\(_2\)-5CaO / 1     | 74.987 |                           | 1.3698         | 33.476                  | 2.3±0.5               |
| ZrO\(_2\)-5CaO / 2     | 84.605 | 0.24                       | 1.5150         | 37.770                  | 2.3±0.5               |
| ZrO\(_2\)-5CaO / 3     | 56.669 |                           | 1.0380         | 25.598                  |                      |

**3. Results and discussions**

Starting from the aim of this study, namely to identify the maximum value of the stress developed in the contact point, on the depth of the analysed layer, different variants of the layer thickness were analysed by finite element modelling.

Thus, for the simulation performed in this study, three different layer thicknesses were considered optimal, for each of the three coatings: 60 \( \mu \text{m} \), 80 \( \mu \text{m} \), respectively 100 \( \mu \text{m} \). After setting all the parameters and running the simulation routines, data were obtained regarding the displacement of the specimens in the contact area, respectively on the distribution of the contact pressures and von Misses stress appeared for each of the 9 situations. These data are presented in graphical form in figures 3-8, but also in numerical form, comparatively, in table 3.

Figures 3 and 4 show the results obtained in the case of NiCrBSi coating. Figure 3 show the displacement of the coating and of the substrate for the thickness of 60\( \mu \text{m} \), whose values are between 0.00224 mm (maximum - red) and 0.000224 mm (minimum - blue), this aspect being considered representative for all three layer thicknesses.

In figure 3(a), the movements of the points in the discretization network are represented by arrows, and in figure 3(b) are presented the uniform aspect of the deformation. Figure 3(a) shows more clearly the delimitation between the deformation of the coating that is observed in the upper part of the image.
and is characterized by the production of maximum deformations (red colour), respectively the substrate deformation visible in the lower part, characterized by medium and small deformations represented by colours ranging from yellow to blue.

Figure 4 shows the distributions of the contact pressures at the contact with the ball (figure 4(a)), respectively the von Misses stresses developed for each of the three layer thicknesses considered (figure 4(b)). Regarding the pressure distribution, it is observed that the maximum values were developed in the thickness of the thermal sprayed layer, as expected, but maximum values are also observed at the interface with the substrate, respectively in it, characterized by a punctual distribution. Analysing the colour variation (maximum stress is represented by red), it becomes clear the difference between the maximum stress between the thinner and the thickest layer, the latter seeming to successfully take over the maximum stresses produced.

Figure 3. The displacement of the 60μm thickness NiCrBSi coating: (a) arrow representation of the discretisation points; (b) uniform displacement representation.

Figure 4. The distribution of pressures (a) and Von Misses stresses (b) for NiCrBSi
Figure 5. The displacement of the 60μm thickness Cr$_2$C$_3$-Ni20Cr coating: (a) arrow representation of the discretisation points; (b) uniform displacement representation.

Figure 6. The distribution of pressures (a) and Von Misses stresses (b) for Cr$_2$C$_3$-Ni20Cr coating.

Figure 7. The displacement of the 60μm thickness ZrO$_2$-5CaO coating: (a) arrow
representation of the discretisation points; (b) uniform displacement representation.

Similar observations were made in the case of the other two types of coatings, where the deformations produced at the level of the deposited layers of Cr$_2$C$_3$-Ni$_2$0Cr (figure 5), respectively of ZrO$_2$-5CaO (figure 7) could be analysed. It is observed in both cases that the displacement is mostly produced in the coating, being marked by the presence of red - yellow colours, while the substrate suffered very slight deformations, marked by the yellow - green colours. In a comparative analysis, we can highlight the fact that the NiCrBSi coating allowed the deformation of the substrate to the greatest extent, followed in descending order by the coating made of Cr$_2$C$_3$-Ni$_2$0Cr, respectively that made of ZrO$_2$-5CaO.

Regarding the contact pressure distributions, we can make similar comments in the case of Cr$_2$C$_3$-Ni$_2$0Cr coatings (figure 6(a)), respectively ZrO$_2$-5CaO (figure 8(a)). It is obvious the same behaviour of developing the maximum values of the ball contact pressures inside the coating, simultaneously with the existence of maximum points at the interface with the substrate. The latter are very harmful due to the probability of their transformation into points of exfoliation initiation of the coating, having a cumulative effect with the other types of stresses to which the coating can still be exposed during use.

In addition to this evaluation, the distributions of von Misses stresses must be analysed, and similar comments can be made in the case of Cr$_2$C$_3$-Ni$_2$0Cr coatings (figure 6(b)), respectively ZrO$_2$-5CaO (figure 8(b)). Thus, it is observed, as in the case of the first analysed layer (NiCrBSi), the fact that the stresses are concentrated inside the layer the more its thickness is greater, but there are also maximum stresses at the interface between the coating and the substrate.

Table 3 presents, synthesized, the data obtained after the simulation, compared for the three types of coatings, respectively for each of the three thicknesses taken into account.
From the obtained data it is observed that the maximum stresses were recorded, for all three types of coatings, in case of the layers with a thickness of 60μm, the highest value being recorded in case of NiCrBSi coating, followed in descending order by the values recorded in case of Cr2C3 - Ni20Cr and ZrO2-5CaO coating, respectively. The same trend of the values registered for the maximum stresses is maintained in the case of layer thicknesses of 80μm, respectively 100μm, the lowest value registered for the maximum stresses developed at the contact with the ball being 971.44MPa, in the case of ZrO2-5CaO coating.

Regarding the influence of the material characteristics on the deformation of the coatings, it is observed that, with the increase of the material density, a decrease of the degree of deformation is registered.

4. Conclusions
Following the simulation of the contact stress generated when applying some loads on the thermal spraying coatings, performed in this paper, the following conclusions can be drawn:
- the lamellar morphology characteristic of the coatings deposited by thermal spraying, formed by splats, voids, oxidized or incompletely melted particles, imposes the consideration of the coating material as anisotropic material;
- to perform the simulation of the contact voltage generated upon contact with a ball, the following material parameters were used: Young's modulus, Poisson's ratio, Coulomb's coefficient and density;
- the results showed that the coating largely takes over the maximum stresses, respectively the displacements of the material produced at the contact with the ball, but there are also maximum stress points at the interface with the substrate, which can become, by cumulative effect with other types of stress (in operation conditions), points of exfoliation initiation of the coating;
- another observation resulting from the simulation is that the stresses decrease with increasing thickness of the layer subjected to stress, due to the effect of taking over a larger number of stress points that no longer reach the substrate.

We can thus say that the simulation of the contact stress generated when applying stresses on the layers deposited by thermal spraying can be used to design various applications of these coatings, both in terms of required material characteristics and in terms of optimal thickness of the considered coating. This aspect is of major importance because it is known that one of the problems of the coating durability in real use is given by finding the optimal balance between the thickness of the layer and the stresses to which it is subjected.

5. References
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