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Optimization of the parameters for obtaining zirconia-alumina coatings, made by flame spraying from results of numerical simulation

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Abstract. The K-Sommerfeld values (K) and the melting percentage (% F) obtained by numerical simulation using the Jets et Poudres software were used to find the projection parameters of zirconia-alumina coatings by thermal spraying flame, in order to obtain coatings with good morphological and structural properties to be used as thermal insulation. The experimental results show the relationship between the Sommerfeld parameter and the porosity of the zirconia-alumina coatings. It is found that the lowest porosity is obtained when the K-Sommerfeld value is close to 45 with an oxidant flame, on the contrary, when superoxidant flames are used K values are close 52, which improve wear resistance.

1. Introduction

One of the most used materials to protect metal structures in aggressive temperature conditions and wear is zirconia (ZrO_2) due to its low thermal conductivity ($0.8 - 1.5 W/mK$), however, the low thermal conductivity of zirconia limits to a great extent its tribological applications, because of it reaches a high temperature of contact with another material, which induces thermal stresses in the coating reducing its mechanical properties. For this reason zirconia is mixed with alumina, which has high hardness as well as high thermal conductivity making it excellent for applications where there is wear, in order to give better structural properties to the coating rare earth oxides such as yttria and ceria are added, they stabilize the zirconia in the tetragonal and cubic phases at room temperature [1], [2].

The most used method for the protection of structures is the application of a thermal spray coating, with this technique it is possible to make coatings and repair worn parts by applying a wide variety of materials on substrates of different composition, this is generally done by plasma [3], however, the flame spraying can be used to project high melting point materials, when the temperature and length of the primary zone are known by different ($C_2H_2: O_2$) ratios (see Figure1) [4].

The software Jets et Poudres developed by the University of Limoges France, it allows to know all the thermal and kinetic history of the particle as it passes through the flame, by the values of temperature, melting percentage, and K-Sommerfeld number among others, data that facilitates the choice of parameters to obtain coatings [5-7].

K-Sommerfeld was described by Kappel and Mundo when they studied the impact of water droplets and ethanol on cold surfaces, the behaviour of a particle upon impact with a surface that may be the substrate or a previously deposited coating layer. Mundo et al, suggest that by number (K) it is



possible to predict the interaction between the particle and the substrate, they define that if K is between 3 and 57.7 [8], the particle sticks on the substrate to form a disk-shaped splat and if K is less than 3, the particle will bounce after impact with the substrate, while if K exceeds 57.7 the particle will splash after impact with the substrate, therefore, part of the material will not be deposited. The K -Sommerfeld is given by

$$K = We^{1/2} Re^{1/4} \quad (1)$$

Where We and Re are the dimensionless numbers of Weber and Reynolds, and which represent the relationship between the inertia of the molten particle with respect to its superficial tension and viscosity, expressed more specifically as:

$$K = [\rho v d / \mu]^{1/2} [\rho \mu^2 d / \sigma]^{1/4} \quad (2)$$

From where, v , d , μ , σ , are the density, velocity, diameter, viscosity and superficial tension of the drop (molten particle) that impacts the surface [8].

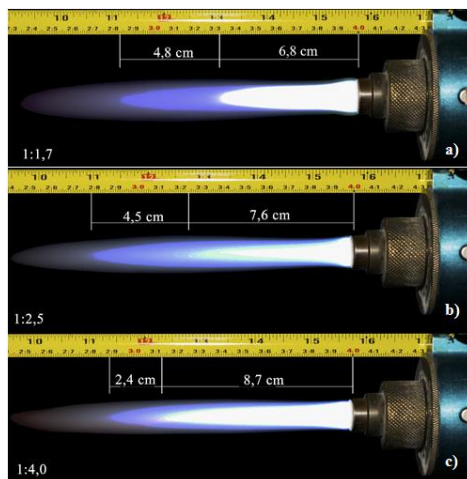


Figure 1. Length of the primary zone in a neutral oxyacetylene, oxidizing and super oxidant flame, respectively [4].

2. Materials and methods

Castolin-Eutectic commercial reference powders MetaCeram 25088TM are used to make of the coatings. A ceramic powder of ZrO_2 -36 wt% Al_2O_3 is used to take the advantage of the good thermal properties of zirconia and the tribological properties of alumina. The chemical composition of the powders is obtained by X-ray fluorescence (XRF). The size distribution of the particles is determined by laser dispersion (Master Size 2000E); meanwhile, the porosity was determined by an optical microscopy images (OM) using Image-J software.

A numerical simulation was performed using the Jets et Poudres software [9], in order to find the parameters that allow to obtain homogeneous coatings with low porosity and good resistance to wear. A zirconia-alumina particle of less than $15\mu m$ to d_{10} of the distribution width of the powders used, which were made to interact with three flames, neutral, oxidant and superoxidant, for a projection distance of 8, 9 and 10cm. The thermal properties of the particles were obtained from the databases and taking into account the rule of the mixtures for compounds [10]. From the results of the simulation the parameter K -Sommerfeld and the melting percentage were given and they were used to choose the parameters to obtain the coatings.

The coatings are deposited using an Arete I chamber developed by the GIPIMME Group of the “Universidad de Antioquia (Colombia)”, which is equipped with a Castolin-Eutectic Terodyn 2000 torch and a RAYTEK infrared pyrometer to measure the surface temperature of the substrate, as well as the electromechanical systems that control the speed of the torch and the sample holder.

3. Results and analysis

3.1. Characterization of raw material

According to the chemical analysis performed on the starting powder, it is established that it is composed mainly of 59.72wt% - ZrO_2 , 35.7wt% - Al_2O_3 , 0.94wt% - HfO_2 , 0.25wt% Y_2O_3 and others.

The particle size distribution obtained by dispersion laser for the zirconia-alumina particles between 15 and $95\mu m$ with an average size of $50\mu m$, this shows a suitable average size to obtain ceramic coatings by flame spraying (FS) [11]. The analysis of the morphology of the powders is performed using SEM micrographs. In Figure 2, the powder morphology of zirconia (ZrO_2)-alumina (Al_2O_3) can be seen; it is made of spherical, micrometer, agglomerated and sintered particles, and also alumina nanoparticles (dark areas) and zirconia (light areas) can be seen [12], (see the cross section of a microsphere).

The analysis phase is performed by X-ray diffraction, (Figure 3) using the High Score Plus software, the presence of two phases is detected: the first with 63.5wt% of $m - Zr_4O_8$ and the second with 36.5wt% of $\alpha - Al_{12}O_{18}$.

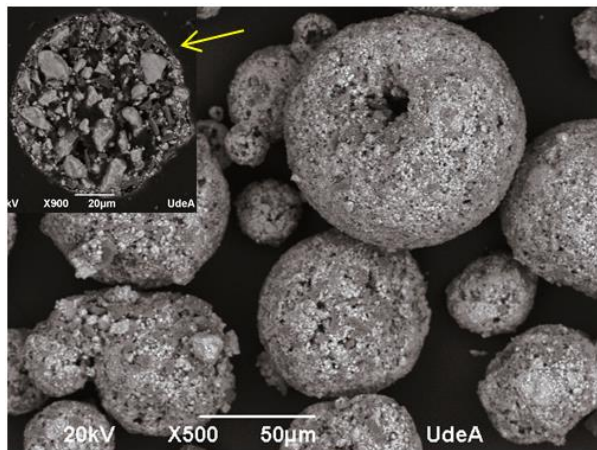


Figure 2. Micrograph powders zirconia (ZrO_2)-alumina (Al_2O_3).

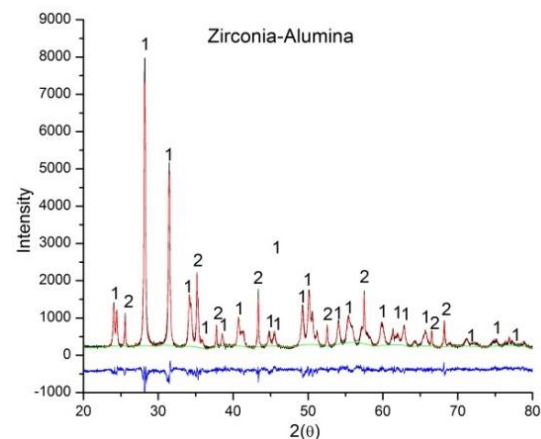


Figure 3. XRD spectrum of zirconia-alumina powders, used to make the coatings 1. $m - Zr_4O_8$, 2. $\alpha - Al_{12}O_{18}$.

3.2. Results of the simulation

The results of the simulation performed with the Jets et Poudres software for each of the conditions are shown in Table 1. As can be observed, for the neutral and oxidant flames at the projection distances of 8, 9 and 10cm and for the superoxidant flame at a distance of 10cm we obtain Sommerfeld values that are in the range between 3-57.7 condition in which the particle is deposited without bouncing, or forming splashes [5]. However, the melting percentage reached for the particles in the neutral flame is very low with respect to that reached for oxidant and superoxidant flame at a distance of 9 and 10cm. It is important to keep in mind that the particles are composed mainly of zirconia having a low coefficient of thermal conductivity of 0.8-1.5W/mK, making it difficult to diffuse the heat and its melting. In addition, in a neutral flame obtained from a ratio of oxygen and acetylene ($C_2H_2: O_2$) equivalent to 1:1.9 by volume, a maximum temperature of $3113^\circ C$ is reached, with a length of the primary reaction zone of about 6.8 cm, whereby the particles do not melt when the substrate is placed at 8, 9 or 10cm. On the other hand, to obtain an oxidizing flame an excess of oxygen is added in a ratio of 1:2.9 by reducing the flame temperature meanwhile having a longer primary reaction zone of about 7.6cm in length, then the particles spent a longer time in the hottest area of the flame and a short time in the secondary zone, reaching a higher melting percentage. In the case of a superoxidant flame where a greater amount of oxygen is added in the ratio 1:4.2, the flame temperature decreases and the length

of the hot zone reaches a distance of about 8.7cm [4], thus, particles traveling 8cm in this flame do not reach a sufficient melting percentage to generate a homogeneous coating. According to this, it can be concluded that the condition in which the zirconia-alumina particles are best melted is when an oxidizing flame is used, where, the particles have a longer time in the hot zone, and this is why an increase in projection distance increases in the melting percentage of the particles. For the zirconia-alumina coatings it is evident that the K-Sommerfeld number is influenced by both the flame type and the projection distance.

Table 1. K- Sommerfeld number and melting percentage from the results of the simulation.

Flame	Parameters	Projection distance		
		8 cm	9 cm	10 cm
Neutral (1:1.9)	K-Sommerfeld	36.8	32.7	32.9
	Melting %	4.6	28	26
Oxidizing (1:2.9)	K-Sommerfeld	49	45	45
	Melting %	31	78.2	78.2
Super-oxidant (1:4.2)	K-Sommerfeld	75.2	63.3	52.1
	Melting %	37	100	83.4

3.3. Projection parameters

In order to create the coatings three flames were chosen, and three projection distances. The torch moves with a linear velocity of 0.59cm/s, the sample holder rotates at 116rpm, the flow of the powder remains constant at 9g/min. The coatings are called N8, N9 and N10, for those obtained with neutral flame at 8, 9 and 10cm in length, O8, O9 and O10 for those obtained with oxidizing flame and SO8, SO9 and SO10 to those obtained with superoxidant flame.

3.4. Validation

It is important to keep in mind that the materials given have wide distribution range in its size, which varies from about 15 to about 95 μ m, making it difficult to melt all the particles. Figures 4, 5 and 6 show SEM images of the surface of the coatings, where the obtained results in the simulation for both the K Sommerfeld and the melting percentage are show. The coatings N8, N9 and N10 (Figure 6) have a surface with non-melted particles and very few partially melted particles, which agrees with the melting percentage of the particles and the value of K-Somerfeld obtained in the simulation. The melted particles with an acceptable value within the range of Sommerfeld are the smallest that reach the melting temperature. The coatings O8, O9 and O10 (Figure 5) whose K-Sommerfeld is in the range of 45 to 49 and their melting percentage between 31 and 78.2% have a structure with well fused splats and some splashes due to excessive thermokinetic energy reached by the particles. The SO9 and SO10 coatings show a surface with melted particles and many splashes as a result of larger number of small particles achieved enough thermokinetic energy to melt and produce splashes at the time of impact. The SO8 coating, on the other hand, has large number of unmelted particles joined by smaller, well-fused particles. This is because the temperature and residence time of the particles in the flame are not enough for the larger ones to melt, these results are in agreement with those predicted in the simulation where the percentage of fusion is 37%.

The predominant phases are monoclinic zirconia and alpha alumina which are given from the starting powders, indicating that there were particles that did not reach the melting point, however, the cubic and tetragonal phases of zirconia are also there, which are retained due to the presence of yttrium and hafnium oxides. The alpha and beta phases of the alumina correspond to particles that melted and solidified (metastable or transition eta phase). There are two areas corresponding to the amorphous part, the first in 22-37 (20) and the second in 52-65 (20). According to Fauchais *et al.* [13], the amorphous phases are always presented and are formed by the high cooling rates up to 600×10^6 K/s, in a conventional plasma spray process using micron sized particles (see Table 2).

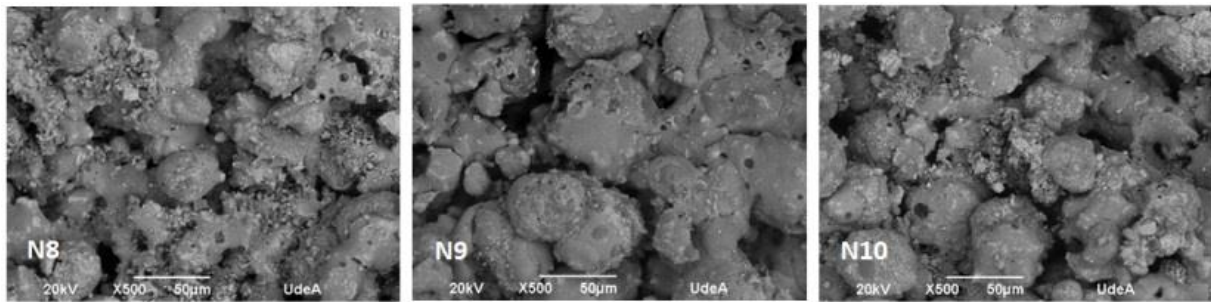


Figure 4. The morphology of the surface view of the coatings obtained with neutral flame.

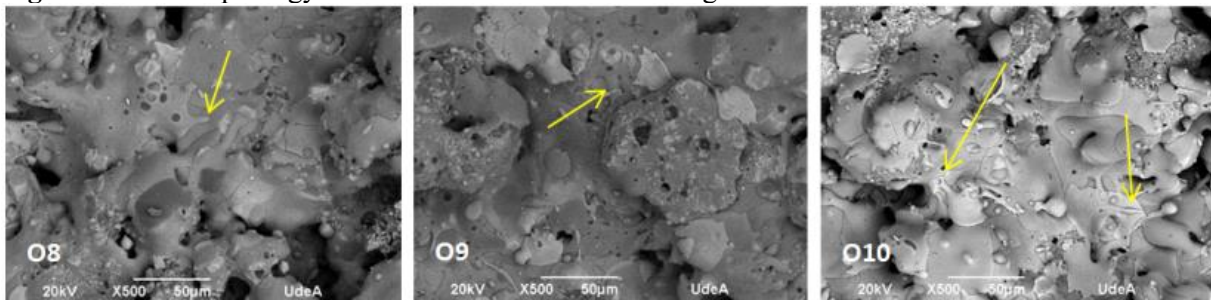


Figure 5. The morphology of the surface view of the coatings obtained with oxidizing flame.

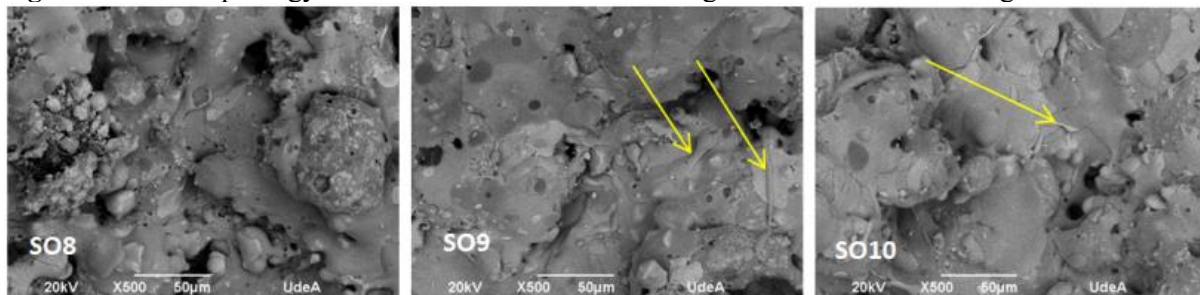


Figure 6. The morphology of the surface view of the coatings obtained with superoxidizing flame.

Table 2. Phases in the zirconia (ZrO_2)-alumina (Al_2O_3) coatings.

Sample	Phases present in the coatings					
	m - ZrO_2	t - ZrO_2	c - ZrO_2	α - Al_2O_3	γ - Al_2O_3	η - Al_2O_3
O8	51.7	6.4	21.9	15.4	3.2	1.4
O9	51.6	4.8	26.9	13.9	2.3	1.5
O10	49.0	15.6	9.6	15.2	9.8	1.7
SO8	55.3	14.7	4.8	16.8	2.3	6.1
SO9	48.7	9.2	23.7	11.3	6.2	0.8
SO10	47.1	7.0	27.2	6.1	12	0.7

The porosity percentage and the mechanical properties of hardness and wear resistance of the coatings were evaluated for samples O8, O9, O10, SO8, SO9 and SO10 which show a K-Sommerfeld value between 45 and 75.2. Table 3 shows the porosity of the coatings evaluated, where it can be observed that the samples O8, O9 and O10 corresponding to a K-Sommerfeld value between 45 and 49, they have a lower percentage of porosity. The SO8, SO9 and SO10 coatings with a K-Sommerfeld between 52.1 and 75.2 have a higher percentage of porosity due to the presence of splashes predicted by the value of Sommerfeld. With regard to microhardness it is important to keeping mind that this is affected by both the porosity and the presence of hard phases as the corundum [5,11], for example the coating SO8 is the most porous and is the one with the highest percentage of the phase $\alpha - Al_2O_3$, 16.8%. In the case of the SO10 coating, it shows the lowest porosity percentage, and has the lowest

percentage of $\alpha - \text{Al}_2\text{O}_3$ of 6.1%, this makes the hard phase with porosity and the effective hardness similar in all the Cases studied.

Table 3. The mechanical properties of the coatings zirconia (ZrO_2)-alumina (Al_2O_3).

Sample	Porosity [%]	Microhardness Vickers [GPa]	Wear rate $\times 10^{-4}$ [$\text{mm}^3/\text{N.m}$]
O8	5.3 ± 0.9	7.8 ± 0.6	1.3 ± 0.07
O9	5.1 ± 0.9	8.4 ± 0.9	2.1 ± 0.20
O10	5.4 ± 1.2	8.6 ± 0.3	2.1 ± 0.46
SO8	9.1 ± 1.1	8.0 ± 0.4	1.2 ± 0.13
SO9	6.9 ± 1.1	8.3 ± 0.4	1.7 ± 0.31
SO10	5.8 ± 0.9	8.2 ± 0.6	1.3 ± 0.20

4. Conclusions

The simulation developed with the software Jets et Poudres allows to predict the thermokinetic behaviour of a particle of zirconia-alumina when interacting with an oxyacetylene flame, by means of the value K-Sommerfeld and the melting percentage. From these results it is possible to establish the most suitable projection parameters in order to obtain coatings with certain characteristics intended for specific applications, which makes the simulation a useful tool that optimizes the time, energy and materials needed to obtain homogeneous coatings with good mechanical properties.

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