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To cite this article: L Rodríguez *et al* 2017 *J. Phys.: Conf. Ser.* **935** 012022

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Projection parameters for zirconia-alumina-ceria coatings made by flame spraying from results of numerical simulation

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Abstract. A numerical simulation was performed with the software Jets et Poudres, the results let choose the parameters to deposit zirconia-alumina-ceria coatings of different composition on substrates of red clay, by thermal spraying with the oxyacetylene flame to obtain homogeneous coatings with good adhesion to the substrate. The effect of the projection distance (7, 10 and 12cm) between the substrate and the torch, the fusion percentage of particles and the K-Sommerfeld number was determined. This number is dimensionless and is affected by the projection distance and by the chemical composition of the particles. For a projection distance of 9cm, the fusion percentage of the particles varies between 83.8% and 100%, and the K-Sommerfeld number between 47.3 and 50 for the different compounds. This makes possible to obtain uniform coatings with good wettability, therefore, good adhesion to the substrate, while for the distance of 7cm the fusion percentage varies between 22% and 38%, due to the short time of the particles in the flame which causes low adhesion, when the projection distance is 12cm the particles do not have sufficient kinetic energy to reach the substrate and therefore the coating is not deposited.

1. Introduction

With the purpose to protect the surfaces of structures made of different materials alumina, zirconia and ceria coatings among others are used, which enhance their thermal, tribological and corrosive properties[1,2]. The zirconia ZrO_2 is used due to its stability to high temperatures and its low conductivity (0.8–1.5W/mK) [3]. At room temperature the zirconia is in its monoclinic phase, which does not allow it to be used in structural applications, that is why it is mixture with oxides from rare lands like the ceria which promote the retention in the cubic and tetragonal phases in room temperature. The aluminium oxide is used due to its low friction coefficient, that is why it is used in applications against wear and corrosion it also shows a low electrical and thermal resistance allowing it to be used in high temperatures [3].

One of the techniques used to obtain the coatings is by flame spraying (FS), which consists in melt a material (dust) and deposit it on a substrate. The oxyacetylene flame gets its energy of oxygen and acetylene combustion reaching temperatures close to 3100°C, which allows different of high-melting compounds to be used. The particles are adhered to the substrate by means of a mechanical anchor where the molten material in the form of droplets moistens the irregularities of the substrate and adheres while cooling simultaneously [4]. The morphology of the coatings obtained depends on the physical, chemical and morphological properties of the raw material and the projection parameters such as the type of neutral or oxidant flame, the distance between the torch and the substrate, the preheating temperature of the substrate and the flow of powders among others.

To predict the behaviour of the particles in the flame and his interaction with the substrate is rather difficult, that is why one resort is the numerical simulations that allow me to study the thermo kinetic behaviour of the particles in the flame. The software Jets et Poudres developed by the university of Limoges (France) allows to know the temperature, the melted percentage, and the dimensionless K-Sommerfeld number of the particles [5]. The K-Sommerfeld number was described by Mundo and Kappel, in the study of the impact of water drops and ethanol on cold surfaces, they found that the value of K is in the range from 3 to 57.7, where for minor values of 3 the particle bounces and does not stick fast to the substrate and if it is major of 57.7 the particle will splash on having struck with the substrate. This parameter is used in thermal projection since it allows to predict the behaviour of the particles when interacts with the substrate which determines the wettability and the homogeneity of the deposited splats, which is related to the anchorage of the coating [6].

The K-Sommerfeld value is given by the dimensionless numbers Weber (We) and Reynolds (Re), which relate the inertia, tension surface and viscosity of the molten particles and is determined for:

$$K = We^{1/2}Re^{1/4} \quad K = [\rho v d/\mu]^{1/2}[\rho\mu^2 d/\sigma]^{1/4} \tag{1}$$

Where: ρ, v, d, μ and σ, are the density, the speed, the diameter, the viscosity and the superficial tension of the melted particle that strikes on the substrate[7].

2. Materials and methods

A numerical simulation is made with the software Jets et Poudres to determine the melted percentage and the K-Sommerfeld number of agglomerated particles of zirconia-alumina-ceria, after they have crossed a oxyacetylene flame, in order to know the conditions under which the melted or partially melted particles stick fast to the irregularities of the substrate and form a homogeneous coating, preventing the particles from bouncing or on the contrary they form splashes, aspects which prevent the proper ordering of splats, giving rise to porous coatings due to stacking defects and problems of adhesion or cohesion due to poor wettability.

The carried-out simulation of agglomerated particles of zirconia-alumina-ceria of 8, 10 and 12μm of diameter from different chemical composition, named as Composite 1 (C1), Composite 2 (C2) and Composite 3 (C3). A particle of powder of different chemical composition interacts with a oxidizer flame in the relation 1:3.2 and is projected to 7, 9 and 12cm, these distances are chosen according to [8,9], in order to evaluate how it affects the percentage in volume of the compounds in the k-Sommerfeld number and in the melted percentage of the particles [10]. The physical, chemical and thermal properties of the particles needed for the simulation are taken from the databases and calculated by the law of mixtures bearing in mind its composition in volume.

In order to validate the results of the simulation the coatings are done using commercial powders, one composite of zirconia-alumina ZrO_2, 36 % in weight Al_2O_3, from a commercial brand called Metaceram 25088 from Eutectic Castolin® and another of cerium oxide, which are placed in a ball mill to homogenize the size of the particles for his later agglomeration. The agglomeration is done in an agglomerating drum developed by the group GIPIMME of the university of Antioquia, like a binder a polyvinyl alcohol to 2% is used, which was selected in agreement to the results reported by [11], then they are left to dry during an hour in a stove to 70°C, finally they are sifted in a rotap, gathering the resulting particles in a 400 mesh and retaining them in a 500 mesh, the agglomerated powders are characterized morphologically by images SEM and his microstructure by refinement Rietvel DRX difractograms.

The coatings are done in the thermal projection chamber of the "Universidad de Antioquia", on substrate of red clay [12], in order to improve the structural properties of the tiles with the coating. The evaluation of the results is done by SEM, DRX and Pull Off.

3. Results and analysis

3.1. Composition of the raw material

In the Table 1 is named like C1, C2 and C3 to each one of composites of the powders obtained after the agglomeration, the concentration of every composite is given in percentage of volume, increasing the concentration of oxide of cerium. The results of diffraction of X-rays allows us to see three zones of amorphicity mainly between 10 and 20, 27-38 and 46-58 (2Θ) [13], as evidenced in Figure 1, for the named composite as C1. The refinement Rietveld allow find the percentage in weight of the present phases in each of the powders, as it appears in the Table 2, where from it is important to highlight that the zirconia is in its in monoclinic phase and the alumina in alpha or corundum.

Table 1. Composition of the particles for three powders of contribution.

Composite	Name	ZrO_2	Al_2O_3	CeO_2
		Volume percent (%)		
Composite 1	C1	48.83	41.03	10.14
Composite 2	C2	46.85	39.37	13.78
Composite 3	C3	44.79	37.64	17.57

Table 2. Phases in the starting powders (%).

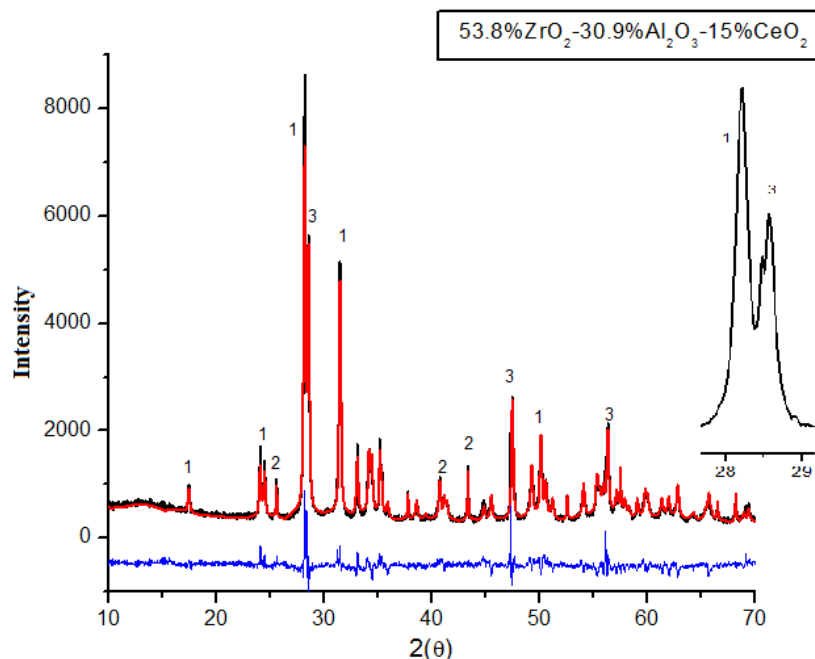| Compound	Phase		
	m $- Zr_4O_8$	$\alpha - Al_2O_4$	c $- Ce_4O_8$
C1	59.2	26	14.8
C2	51.9	28.4	19.7
C3	47	24.4	28.6

Figure 1. Phases presents in C1 $1. m - Zr_4O_8$ $2. \alpha - Al_2O_4$ $3. c - Ce_4O_8$.

3.2. Morphology of the powders

The SEM images (Figure 2), allow seeing that the powder particles are formed by agglomeration of smaller particles of nanometric order. The composite C2 shows a more uniform agglomeration where see oval particles with smaller added particles. In the composite C1 and C3 the agglomerated particles are smaller; nevertheless, they are formed also by nanometric particles.
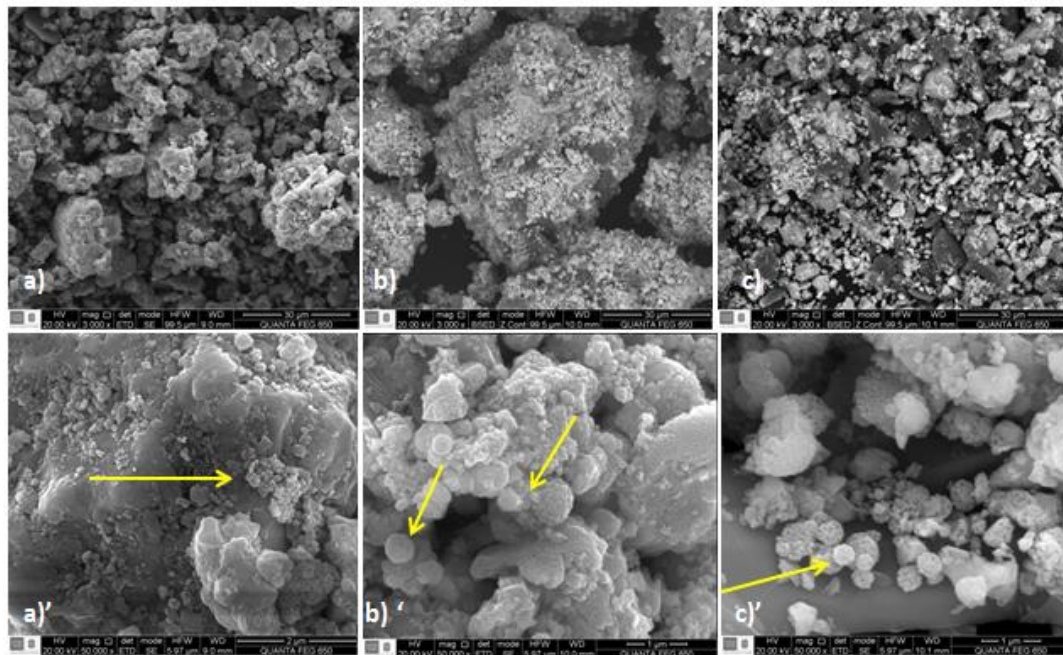
Figure 2. Morphology of the powders, where (a), (b) and (c) correspond to C1, C2 and C3 to a magnification of 3000X, (a'), (b') and (c') they are approximations to 50000X of them.

3.3. The simulation

The results of the simulation let us conclude that the parameter K-Sommerfeld depends on the projection distance and the size of the particles, as well as the melted percentage depends on the time of these in the warm zone of the flame. The parameter K-Sommerfeld, the melted percentage and the reach of the particles, for the different projection conditions are shown in the Table 3. For a distance of 9 cm conclude that the K - Sommerfeld vary between 43.7 and 50 and the melted percentage between 83.8 and 100%, whereas for a distance of 7cm the value of K overcomes the limit of 57.7 and finally for a distance of 12cm they do not have the sufficient energy to reach the substrate. In conclusion to obtain homogeneous coatings the particles must be projected to a distance of 9cm, with an approximate size of 8μm.

3.4. Projection parameters

According to the simulation results and the conclusion of some authors, the coatings are made with an oxidizer flame in a relation of 1:3.2 (acetylene: oxygen), to a distance of 9cm. The torch moves to a linear speed of 0.72cm/s, the sample holder is rotated at 116rpm. The flow of the powders was kept constant to 12.6g/min, three warm up and six projection passes are made.

3.5. Morphology and microstructure of the coatings

The coatings are named like R1, R2, and R3, obtained from the composite C1, C2 and C3 respectively. The superficial morphology of the coatings is see in SEM images. In the Figure 3(a), (b) and (c), there see the melted particles of a splat shaped like a disk, partially melted particles, splashes and cracks generated in the moment of solidification of the particles. In the images (a'), (b') and (c') the morphology of the coatings appears in a transverse cut, it can be seen that the particles in all the cases have good wettability with the substrate.

The coatings R1 and R3 have a uniform morphology with the presence of lamellas corresponding to fully melted particles, on the other hand in R2 where addition to the lamellas their unmelted particles due to the agglomerated particles of the composite C1 and C3 are smaller in comparison with C2, the results of the simulation show that the size particles influences the melting percentage.

Table 3. K- Sommerfeld, melting percentage, scope of studied particles.

| Compound	Size Particle (μm)	Parameter	Projection distances		
			7cm	9cm	12cm
C1	8	K-Sommerfeld	80.78	47.9	41.35
		% Melted	27.1	100	100
		Scope (cm)	7	9	9.5
	10	K-Sommerfeld	151.1	100.7	76.88
		% Melted	10.7	59.2	100
		Scope (cm)	7	9	10.9
	12	K-Sommerfeld	220.8	167.3	126.5
		% Melted	1.4	26.4	100
		Scope (cm)	7	9	11.9
C2	8	K-Sommerfeld	89	50.0	44.6
		% Melted	15.8	100	100
		Scope (cm)	7	9	9.6
	10	K-Sommerfeld	84.6	104.9	79.9
		% Melted	20.3	44.5	100
		Scope (cm)	7	9	11
	12	K-Sommerfeld	227.18	173.6	110.2
		% Melted	1.1	19.3	91.2
		Scope (cm)	7	9	11.9
C3	8	K-Sommerfeld	90	47.3	44.6
		% Melted	15.8	83.8	100
		Scope (cm)	7	9	9.6
	10	K-Sommerfeld	162.2	110	76.79
		% Melted	6.1	34.5	100
		Scope (cm)	7	9	11.1
	12	K-Sommerfeld	234.45	180.1	115.7
		% Melted	0.8	15	70.8
		Scope (cm)	7	9	11.9
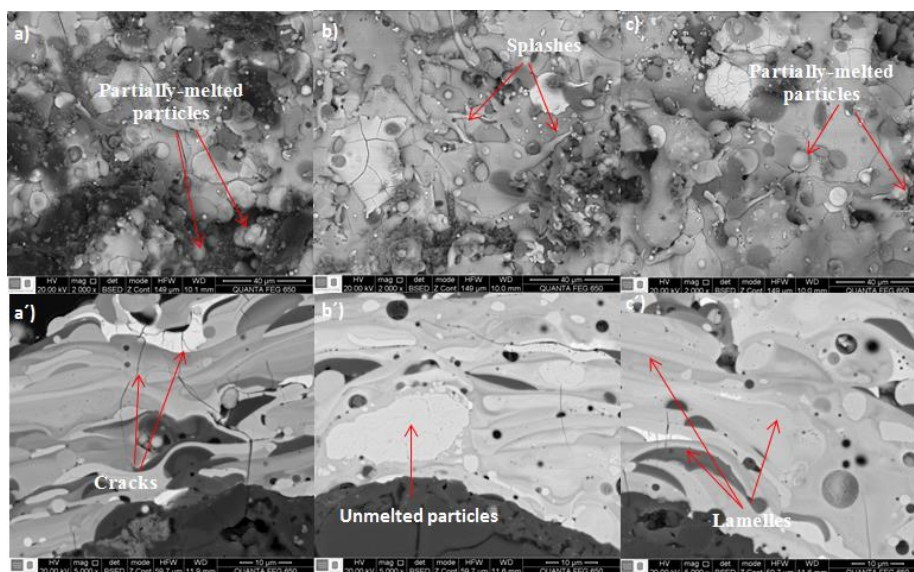
Figure 3. Morphology of the coatings. (a), (b) and (c) correspond to R1, R2 and R3 with a magnification of 2000X in the superficial part of the coatings. (a'), (b') and (c') it corresponds to a magnification of 5000X of the transverse surface of them.

The thickness of the coatings and his adhesion are recorded in the Table 4. The adhesion results show cohesive faults taking away part of substrate.

Table 4. Physical properties of the coatings.

Coating	Thickness (μm)	Adhesion Lb/in^2 (Psi)
R1	340 ± 27	1060 ± 183
R2	371 ± 87	1130 ± 60
R3	395 ± 66	1060 ± 162

4. Conclusions

The Software Jets et Poudres, allows a good approximation to obtain the coatings projection parameters of agglomerated powders of zirconia-alumina-ceria, for oxyacetylene flame. The conditions that predict the obtaining of homogeneous coatings and well adhered to the substrate correspond to a distance projection of 9cm, using an oxyacetylene flame oxidizer. The optimum K-Sommerfeld value for this type of coatings varies between 47.3 to 50 according to the results of the software and its validation.

Acknowledgments

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