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Glass–alumina composite coatings by plasma spraying. Part II: Microstructure-based modeling of mechanical properties

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Abstract

The mechanical properties of composite glass–alumina coatings produced by plasma spraying, as described in Part I, were numerically characterized with relation to the peculiar microstructure. Finite element meshes were created for the most significant coating typologies, starting from SEM acquired microstructures. The coatings elastic properties and fracture behaviour were characterized as a function of relevant microstructural features. The results confirm that the coatings are anisotropic, with a lower elastic modulus in the direction perpendicular to the substrate plane (spray direction), because of the lamellar microstructure; increasing the alumina volume fraction increases the elastic modulus value both in the spray and transverse direction. Moreover, it is found that cracks start from large, irregular pores, and propagate easily through the glass areas, but are stopped by alumina. Smaller individual glass areas hinder crack propagation. The post-deposition thermal treatment described in Part I produces tensile residual stresses in the glass and compressive ones in the alumina; thus, the arresting effect of the latter on cracks propagation is greatly enhanced.

Keywords: Plasma spraying; Ceramic composites; Scanning electron microscopy (SEM); Finite element modelling

1. Introduction

The present works aims at modelling the elastic and fracture behaviour of composite alumina–glass coatings as a function of their microstructural features. In fact, it is well know from literature that the peculiar microstructure of thermally-sprayed materials deeply affect the resulting properties. Their unique and intermingled splat microstructure originates from the processing conditions; it is straightforward that the resulting micro-defects govern the overall performance. Moreover, the coatings investigated in this work are composite, i.e., two different constituents materials are used to build the system. Therefore, the intrinsic characteristics of each material will influence the effective properties proportionally to the respective volume fraction.

In recent years, the need for the development of computational modelling tools able to relate microstructure with properties has greatly increased [1,2]. As a matter of fact, for an optimal design of materials, it is demanding to establish microstructure-properties correlations. Several analytical approaches and numerical techniques have been proposed to quantify such relations [3–8]. Among the others, finite element methods have proven to be an effective tool. Complex and heterogeneous materials, such as composites, have been analysed and the role of different constituents in terms of amount and morphology has been quantitatively established. Porous materials have been thoroughly investigated in order to detect the detrimental effect of porosity on the resulting properties. Recently, also plasma sprayed systems have received a great deal of attention, due to their technological interest as thermal barrier and wear resistance protective coatings.

However, in representing materials microstructures, most works deal with the so-called RVE, namely the representative volume element; this means that the smallest portion of the material which is significant for the whole is investigated, i.e., it is assumed that such portion is periodically repeated through the entire material. While this assumption may suffice for the determination of average homogenised properties, in some cases it is essential to probe the influence of the real microstructure on phenomena occurring at the microscale level.

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In this work, we adopt a microstructure-based computational approach which allows to analyse actual microstructures. In fact, previously acquired images via scanning electron microscopy can be utilised to directly build finite element models of the coatings experimentally analysed and described in Part I. In such a way, the effect of the real coating microstructure can be assessed on the final properties.

It is worth noting that, to the best of the authors' knowledge, the number of works treating the accurate modeling of the actual plasma-sprayed coating microstructures is still very limited [7].

The final goal of this paper is the identification of the contribution of each constituent, namely glass and alumina, to the final properties; moreover, since the pores and cracks are known to have a detrimental effect on mechanical properties, the reduction of materials performances with respect to ideal fully dense coatings are analysed. The numerical results are also compared to the experimental ones, where available, in order to validate the computational tool.

Finally, the potentials as well as the limitations of the computational approach are evaluated.

2. Materials and methods

The experimentally obtained coatings have been investigated in terms of elastic and fracture properties. Only the systems that were demonstrated to be of technological interest were considered; therefore, coatings such as as-sprayed glass coating were not analysed since their too defective microstructure prevented the usage as engineered materials. On the other hand, coatings of pure alumina were studied for comparison with the other alumina–glass coatings, even if the production of pure alumina samples is not the purpose of the present work. Table 1 summarizes the peculiar characteristics of the studied composite coatings.

An efficient and accurate numerical tool (called OOF = Object Oriented Finite elements simulation) for the correlation of effective mechanical properties to the microstructure was used to model the composite coatings. OOF [9,10] is a microstructure-based finite element code which is able to map digitised images of the material onto FEM grids. Thus, this method relies on direct image elaboration of real microstructures obtained, for example, using scanning electron microscopy (SEM). Therefore, the microstructure of thermally sprayed composite coatings is taken into account with all its significant features, such as phases distributions, porosity and defects.

Table 1
Principal features of the investigated coatings

Sample	Al_2O_3 volume fraction (nominal %)	Al_2O_3 volume fraction (real %)	Porosity (%)
SCH	40	40	As-sprayed: 7 thermally treated: 10
SF40	40	50	As-sprayed: 6 thermally treated: 10
SF60	60	63	As-sprayed: 7 thermally treated: 4
SF80	80	86	As-sprayed: 7 thermally treated: 7
SA	100	100	As-sprayed: 5 thermally treated: 13

The SCH sample was obtained by using the coarse glass powder, the SF series by using the finer glass powder, as described in Part I.

Table 2
Thermomechanical properties of composite coatings constituents

	Alumina	Glass
E [GPa]	300.0	69.2
Poisson's ratio	0.27	0.24
CTE [°C^{-1}]	$8.2*10^{-6}$	$9.0*10^{-6}$
K_{IC} [MPa m$^{1/2}$]	2.486	0.659

The use of the OOF code for the determination of complex materials properties is well documented in literature. For example, the problem of thermal residual stresses has been deeply investigated by various authors [11–13], as well as the internal stress distribution in composites [14,15]. Crack propagation mechanisms and reliability of heterogeneous systems have been analysed [16–20]. Thermal barrier coatings have been studied, correlating the microstructure to residual stresses—in particular with reference to interface asperity—[21,22] and to elastic moduli and thermal conductivity [7]. Moreover, glass matrix composites reinforced with alumina particulate, obtained via powder technology, have been thoroughly investigated in terms of elastic and fracture properties [23–25].

In this work, cross-sections of the thermally sprayed glass–alumina coatings were used to generate microstructure-based finite element meshes, starting from previously acquired SEM images (see Part I). The grid can be refined as appropriate to capture microstructure details. Even if an adaptive meshing strategy is available, in this work a very fine mesh is constructed (i.e., two triangular elements per pixel) due to microstructural complexity. In this way, the computational grid should capture the relevant details of the coating morphology.

Moreover, it should be noted that the SEM image from which the mesh is created should be carefully chosen. In fact, the selected image should be representative of the investigated coating, in order to obtain average results significant for the description of the whole system. On the other hand, the image should reproduce with sufficient accuracy the details of the microstructure (e.g., pores and cracks), if the effect of such features has to be analysed; otherwise, for example, the effect of pores on crack propagation cannot be detected. Usually a compromise between meshing accuracy and computational time is found.

The grids were constructed attributing to each phase the corresponding materials properties, which are summarised in Table 2. As regards the alumina, it should be noted that properties of γ-alumina were used [26], since the experimental analysis pointed out that this was the main phase. As regards the glass, the mechanical properties were experimentally determined on glass bars produced ad hoc. Fig. 1B reports an example of a so-constructed mesh. By using the finite element solver, the elastic properties were calculated by reproducing tensile tests. All simulations were performed