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Experimental bending tests and numerical approach to determine the fracture mechanical properties of thin ceramic coatings deposited by magnetron sputtering

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Abstract

In this contribution, the fracture behaviour of a thin ceramic coating was investigated (Zirconia stabilized in its high temperature with Yttria was deposited by reactive magnetron sputtering, MS on high temperature Ni-based alloys substrate). A home-made bending apparatus was used to subject a thin small plate-like sample to a four-point bending test. An increasing bending moment was imposed in order to produce a set of crack patterns running right across the width of the sample bent. The bending apparatus is small enough to fit into the chamber of a scanning electron microscope (SEM) in order to measure the number and the crack positions along a selected portion of the sample length. The data was analysed under the assumption of a statistical Weibull distribution. A numerical computer simulation was performed to estimate the number of cracks, the cracks distribution, the fracture strength and the fracture toughness of the thin coating material. It was used an analytical model that assumes a stress relaxation, during cracking of the coating. It was observed that a selective choice of the Weibull distribution parameters has led to a good agreement between the experimental and the simulated data.

Keywords: Bending tests; Thin coatings; Fracture strength; Fracture toughness; Weibull distribution

1. Introduction

Advanced ceramic coatings deposited on metallic substrates are being used for high-temperature applications where a combination of strength, thermal stability and chemical inertness are needed. Ceramic coatings can be used as a protective coating to improve performance at high temperature of gas turbine components, diesel and aircraft engines. Pure Zirconia (ZrO_2) crystallizes in different polymorphs under different conditions of temperature and pressure. Zirconia, is a ceramic material which is known to have three low-pressure structural crystalline phases: monoclinic, tetragonal and cubic fluorite phase [1–3]. The system passes from the cubic phase to a tetragonal phase, and then to a monoclinic ground state with decreasing temperature. The cubic phase is stable (under thermodynamic point of view) between the melting temperature at 2708 and 2297 °C. Around 2297 °C a transition occurs to the tetragonal phase, which is a slightly distorted version of the cubic structure and is stable up to 1125 °C. Finally, decreasing again the temperature, another phase transition occurs to the monoclinic phase which is thermodynamically stable below 1125 °C. This last phase transition is accomplished by a volume increase of 3–5%. The result is a micro-cracking generation with a concomitant material damage [4] and thus, making impracticable the use of pure Zirconia as a protective coating for engine metal compounds subjected to thermal cycling. In this work we have added Yttria (Y_2O_3) to stabilize zirconia in its high temperature modification phases [5–8]. In order to

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obtain information about the mechanical properties of this coating system we have used the four-point bending test.

The four-point bending test has the advantage of imposing a bending deformation, giving a well-defined stress state on the composite system (substrate/coating system). If the bending deformation is high enough so that the stress in the coating exceeds the tensile strength, a set of cracks will be observed. As the bending deformation is progressively increased, then the number of cracks wills also increase and the cracks distributions will change over the length of the sample bent.

It is clear that the presence of cracks may influence the mechanical performances of tools or other coated engineering workpieces in real operating conditions. For example, in ceramic coatings used for high-temperature applications, an excessive tensile stress state (eventually exceeding the tensile strength) tend to promote crack propagation and therefore, affecting the thermo-mechanical integrity of the functional coated component which can result in a catastrophic situation for aircraft engines components.

In this contribution we have used a statistical distribution model to simulate the spatial distribution of cracks. In addition, we have developed a numeric computer program to estimate the coating tensile stress relaxation (once a crack is produced) and the coating tensile strength and fracture toughness.

2. Theoretical background

2.1. The four-point bending test: nominal applied stress

The relevant equations to determine the stress state installed (nominal stress) on a given substrate/coating system that undergoes bending from a four-point bending test is reviewed [9,10]. In the following, plastic behaviour is not considered as the onset of plastic deformation can easily be assessed from the deviation from linearity in the experimental load-deflection curve.

Fig. 1 schematizes the geometry of a four-point bending test performed on a coating/substrate system, in which it is considered that the substrate thickness, t_s is much higher than that of the coating t_f, (i.e. $t_s+t_f \approx t_s$).

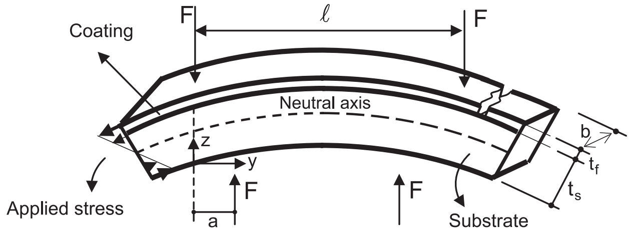

Fig. 1. Four-point load bending geometry.

In the Euler-Bernoulli beam theory, it is assumed that plane cross-sections perpendicular to the axis of a beam remain plane and perpendicular to the axis after deformation. In this theory, the transverse deflection w of the beam is governed by the following differential equation:

$$\frac{d^2w}{dy^2} = \frac{M(y)}{EI} \tag{1}$$

where d^2w/dy^2 is the beam curvature, y is the position along the beam axis, w is the beam deflection, $M(y)$ is the bending moment, EI is the product of the substrate elastic modulus E and the moment of inertia I of the beam. For a rectangular beam, $I \cong bt_s^3/12$ since that the total thickness of the composite system is almost equal to the thickness of the substrate.

In the four-point load bending geometry, the absolute value of the bending moment is $M=Fa$, being constant and reaching its maximum absolute value for the beam region, $a \leq y \leq \ell/2$. In order to verifying Eq. (1), w must satisfy appropriate boundary conditions to solve it:

$$\begin{aligned} &\text{If } y = 0 \Rightarrow w = 0 \\ &\text{If } y = \ell/2 \Rightarrow dw/dy = 0 \\ &dw/dy\big|_{y=a}^{-} = dw/dy\big|_{y=a}^{+} \quad \text{(derivative continuity)} \end{aligned} \tag{2}$$

Integrating Eq. (1) and using the boundary conditions in Eq. (2), the beam deflection ($u=w|_{y=a}$) at the position of load application can be written as:

$$u = \frac{M}{6EI}\left(3a\ell - 4a^2\right) \tag{3}$$

From the Euler-Bernoulli beam theory the maximum strain ($\varepsilon_{\max}$), occurs in the fibres positioned at a maximum distance $z_{\max} \cong (t_s - z_{na})$ from the beam neutral axis, z_{na}. Since the film thickness is much less than that of the substrate ($t_f \ll t_s$), then $z_{na} \cong t_s/2$. Thus, the maximum strain is written as

$$\varepsilon_{\max} = \left[\frac{3t_s}{a^2(3f-4)}\right]u \tag{4}$$

where $f=\ell/a$ is a constant for each four-point bending geometry. The normal stress in the substrate (σ_s) is calculated using the plate bending theory [11]. This is plain strain and requires that the elastic modulus of the substrate (E_s) is replaced by $E_s/(1-v_s^2)$, where v_s is the substrate Poisson's ratio in the usual beam formulae [9]:

$$\sigma_s = \left[\frac{3E_s t_s}{a^2(3f-4)\left(1-v_s^2\right)}\right]u \tag{5.1}$$

The nominal stress in the coating (σ_N), is calculated from Eq. (5.1) where the elastic modulus and Poisson ratio of the substrate are respectively substituted by the elastic modulus (E_f) and Poisson ratio (v_f) of the coating.

$$\sigma_N = \left[\frac{3E_f t_s}{a^2(3f-4)\left(1-v_f^2\right)}\right]u \tag{5.2}$$

The above equation has as main advantage to allow the calculation of the nominal stress in the coating from an imposed external deflection. However, it is important to note