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Evolution of thermal stress in a coating/substrate system during the cooling process of fabrication

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ABSTRACT

An analytical model is established for the thermal stress evolution in a film/substrate system during the cooling process of fabrication. Herein, heat transfer characteristics are incorporated which is critical for thermal spray coatings. The *in situ* temperature field solution is used to derive the instantaneous thermal stress field. Since the loss of thermal energy is account for, the new model may provide the basis for a more realistic prediction of the *in situ* thermal stress the fabrication process. The magnitude of thermal stress derived from the present model is lower than that of the classic one. The thermal stress is generated quickly and significantly during the initial seconds of the cooling process, and stabilizes later. The effects of several spray factors, such as the pre-heat temperature and the thicknesses of coating and substrate, are discussed and compared with a parallel experiment.

1. Introduction

Coating/substrate systems play important roles in almost every aspect of engineering. Very often, the deposition of coating is carried out at high temperature, and the system undergoes thermal cycles during use – the thermal stress upon cooling is of paramount importance for system integrity. For example, thermal spray is a widely employed coating process which is extendable to a wide range of coating materials, coating thicknesses and coating characteristics, applications include the WC/Co-based coatings deposited by HVOF (High Velocity Oxygen Fuel) method that are usually used for drilling as wear resistant coatings (Guilemany et al., 2006; Li and Christofides, 2006; Maiti et al., 2007), thermal barrier coatings (TBCs) fabricated by APS(Air Plasma Spray) method that are widely employed in gas-turbines (protect the metal engine blades from high temperatures) (Drexler et al., 2010; Thompson and Clyne, 2001; Xie et al., 2004; Zhang and Desai, 2005), Ti-Al intermetallic compound coatings prepared by wire arc spray method that are commonly applied in aerospace and automobile products (thanks to their good oxidation resistance, low density and strength retention at high temperature) (Liu et al., 2007; Watanabe, 2002). In all these examples, during the deposition process, the coating feedstock material is melted at high temperature before it can be deposited/sprayed successfully onto the substrate, and there is a significant temperature drop during the system cooling process, and a large thermal stress may be generated owing to the mismatch in coefficients of thermal expansion

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(CTE) between the coating and substrate (Bolcavage et al., 2004; Hsueh and Evans, 1985; Karaoglanli et al., 2013a,b; Li et al., 2010; Hutchinson, 1996), and be responsible for many failure mechanisms, such as crack initiation, propagation, and delamination, among others (Clyne, 1996; Drexler et al., 2010; Howard et al., 1994; Karaoglanli et al., 2011; Tsui et al., 1994).

One of the most important objectives of mechanics of thin films and multi-layers, is therefore, estimate the *in situ* thermal stress evolution during the cooling process, which has a significant value in evaluating the coating's performance and service lifetime. This topic has been intensively studied analytically in the past, and perhaps the most well-known method is the Stoney's equation (Clyne, 1996). When the coating's thickness is much smaller than that of the substrate, the stress in substrate is negligible, and this equation relates the system curvature to coating thermal stress. With the increase of ratio between the coating and substrate's thicknesses, stress gradients become more and more significant, and critical correction is needed (Freund and Suresh, 2003; Timoshenko and Gere, 1972; Tsui and Clyne, 1997a,b,c).

All these analytical models follow a conventional approach where the thermal stress is calculated solely based on the difference between the initial and final states of the system, and the details of the cooling process is ignored (see Appendix A for detail). Although some studies considered the variation of the coating and substrate's Young's modulus with temperature, the classic approach remained. Such a conventional method is incapable to analyze the evolution of thermal stress during the cooling process and thus lack the information for assessing of damage evolution, such as crack nucleation, propagation and fracture.

In fact, the conventional approach assumes no thermal loss, and the thermal energy difference of the entire system (between initial and final states) can be transferred into the thermal stress at the final state. However, the cooling process may take a significant time especially for air cooling, and the thermal energy lose is not negligible. An analytical model is needed which can account for thermal loss and *in situ* estimation of thermal stress development, which may be more effective in evaluating the system integrity at a given temperature.

In this paper, a coating/substrate model is established upon a semi-infinite thermal "sink" which is kept at a fixed temperature. To capture the temperature and thermal stress evolutions throughout coating and substrate, both space and time are discretized into infinitely small segments. Based on the *in situ* evolvement of temperature field, the thermal stress during each time step is computed during the cooling process. Effects of important parameters, such as the coating and substrate's thicknesses, substrate's pre-heating temperature, time step density, et al., are discussed. It is found that the conventional approach significantly overestimates the thermal stress in the system, owing to the part of the thermal energy that is transferred to the environment. The results may shed some lights on the damage evolution during cooling process, as well as that during service (within the thermal cycles).

2. Formulation of the model

2.1. Coating/substrate on a base sink

The system sits on a semi-infinite base sink which is maintained at an ambient temperature (e.g. 23 °C) throughout. A composite of "BC + Substrate" (100 μm for NiCrAlY + 500 μm for Incone l617) is firstly heated to a given level (such as 500 °C in Fig. 1(1)) prior to thermal spray. Initially, a hot coating of specified thickness (e.g. 250 μm) and temperature (e.g. 2680 °C) is deposited onto the substrate, as shown in Fig. 1(1). The system is stress-free in the original configuration shown in Fig. 1(5). Next, the coating/substrate system begins to cool as the heat is being transferred to the sink. With the varying of temperature field throughout the system shown in Fig. 1(2) and (3), owing to the mismatch of CTE, the thermal stress is developed whose magnitude also varies with time (see Fig. 1(6) and (7)) during the cooling process of fabrication. Finally, the entire system is cooled to ambient (Fig. 1(4)) and a final state of residual thermal stress is achieved (Fig. 1(8)).

We remark that in the present model, without losing generality, the thickness of coating and substrate, the temperature of ambient environment, substrate pre-heating temperature, as well as thermal spray temperature, take particular values and they can be easily changed for other working conditions. In addition, the heat sink is assumed to be placed below the substrate (e.g. a conductive "spray base" in Fig. 1), and one can improve the model by adding more heat sinks in other directions (such as that due to air) and revise the following heat transfer analysis accordingly. Moreover, by convention, the system is assumed stress-free in initial configuration, and we only consider the thermal stress caused by mismatch in CTE. Other sources of residual stress, such as epitaxial stress and initial stress generated during the deposition process, can be implemented into the model in a straightforward manner.

The time period of cooling process is discretized into N intervals, and N approaches infinity so as to obtain a converged result. For each interval, the *in situ* temperature field is calculated via heat transfer analysis (see below), and the corresponding thermal stress field is deduced (see below). Since the temperature field is non-uniform, the space is also discretized in the vertical direction: the coating and substrate are divided into I and J layers respectively, and both I and J are sufficiently large such that the result can be converged.

An equal biaxial in-plane stress state ($\sigma_x = \sigma_z$, and $\sigma_y = 0$) is assumed, with an effective Young's modulus $E^* = E/(1-v)$. Both the coating and the substrate are assumed to be isotropic and linear elastic. Their respective Young's modulus and CTE are (E_c^*, α_c) and (E_s^*, α_s), A nomenclature listing is provided in Appendix B.

2.2. Heat transfer analysis from state "K" to state "K + 1"

During the cooling process, the temperature distribution at each time interval (state) is first deduced through a simplified one-dimensional analytical model. We assume