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Multi-scale modeling and analysis of an industrial HVOF thermal spray process

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Abstract

A hybrid (deterministic/stochastic) fundamental model is proposed for the major physico-chemical processes involved in an industrial HVOF thermal spray process (Diamond Jet hybrid gun, Sulzer Metco, Westbury, NY, USA). The model includes continuum type differential equations that describe the evolution of gas and particle temperature and velocity, and a rule-based stochastic simulator that predicts the evolution of the coating microstructure. Regarding gas/particle dynamics, the Reynolds- and Favre-averaged Navier–Stokes equations and the energy balance equations are solved with the renormalization group (RNG) k–ε turbulence model, and the particle trajectories, temperature histories and melting degrees are determined using the fourth-order Runge–Kutta method. On the microscopic particle deposition process, the formation of coating microstructure is captured by the Madejski deformation model and several rules that govern splat formation, solidification and coating growth. Based on the proposed model, a detailed comprehensive parametric analysis is carried out to study the relationship between the key process parameters and the particle in-flight behavior as well as the resulting coating properties.

Keywords: HVOF thermal spray; Coating microstructure; CFD; Modeling; Analysis

1. Introduction

Currently, there is a great interest in the field of nanostructured (also called nanoscale, nanophase or nanocrystalline) materials, whose grain sizes are typically less than 100 nm (Cheng et al., 2003). This interest is motivated by the discovery that such materials have properties superior to those of conventional bulk materials including greater strength, hardness, ductility and sinterability, size-dependent light absorption, and reactivity. With the recent advances in the production of high quality nanoscale powders, including atomization, colloidal precipitation, mechanical milling, and vapor phase nucleation and growth (see, for example, Mueller et al., 2003, 2004; Wegner and Pratsinis, 2003; Xun et al., 2004), the focus of nanostructured materials research is now shifting from synthesis to processing, for example, the fabrication of nanostructured coatings using the high velocity oxygen-fuel (HVOF) thermal spray process (He et al., 2000; Ajdelsztajn et al., 2002). The nanostructured coatings are extensively tested in many industries as thermal-barrier and wear-resistant surface layers to extend product life, increase performance and reduce production and maintenance costs.

The physical and mechanical properties of HVOF sprayed coatings are strongly influenced by the nano- or microstructure of the deposit, which, in turn, depends to a large extent on the physical and chemical states of particles at the point of impact on the substrate, such as velocity, temperature, degree of melting and oxidant content. These variables, however, are strongly dependent on several key process parameters including the fuel/oxygen ratio, total gas flow rate, spray distance and powder size distribution (Li et al., 2004b). In order to improve coating performance, much experimental work has been done in the last decade to study the effect of these key process parameters on the physical

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and mechanical properties of HVOF sprayed coatings (e.g., de Villiers Lovelock et al., 1998; Lugscheider et al., 1998; Gourlaouen et al., 2000; Hearley et al., 2000; Lih et al., 2000; Gil and Staia, 2002). The optimization of process parameters involved in these works usually relies on cost intensive trial and error procedures, for example, the conventional Taguchi method, which uses a set of orthogonal arrays that stipulates the way of conducting the minimal number of experiments that could give the full information of all the factors affecting the coating performance parameters (de Villiers Lovelock et al., 1998). This approach is expensive but reliable for a specific HVOF thermal spray process. However, a lack of fundamental understanding of the dynamics of the gas and particle behavior as well as of the microscopic deposition process significantly restricts its applicability because the experimentally derived "optimal" solution is not directly applicable to other thermal spray processes in which some important parameters, such as nozzle configuration, powder or fuel type, etc., are different (Cheng et al., 2003). It is in this context that the computational fluid dynamics (CFD) analysis of gas dynamics and particle in-flight behavior in HVOF thermal spray systems is of great importance. Coordination between theoretical CFD modeling and experimental efforts is expected to be mutually beneficial for both investigations.

The HVOF thermal spray process is very complex regarding description in a theoretical model, because it involves combustion, turbulence, compressible flow, multiphase interactions, subsonic/supersonic transitions and droplet deformation and solidification. There are four main physicochemical processes occurring in the thermal field and flow field: transformation of chemical energy into thermal energy of the gas by fuel combustion, conversion of thermal energy into kinetic energy of the gas jet by expansion through the nozzle, transfer of momentum and heat from the gas to the powder particles, and conversion of particle kinetic and thermal energy into internal energy at coating deposition. It is widely acknowledged that the higher the particle velocity, the denser the coating (Cheng et al., 2001b). In order to transfer as much kinetic energy as possible to the particles, the gas jet is typically maintained at supersonic conditions outside of the torch. This is realized by a convergent–divergent nozzle (Cheng et al., 2003). As long as a sufficiently large nozzle pressure ratio (NPR) is maintained, the gas will be accelerated to achieve sonic velocity at the throat of the nozzle and supersonic velocity in the divergent section. However, depending on the values of the pressure at the gun exit and ambient pressure, the flow condition at the exit of the gun may be underexpanded ($P_e > P_a$), ideally expanded ($P_e = P_a$) or overexpanded ($P_e < P_a$). The Diamond Jet hybrid HVOF thermal spray process (Sulzer Metco, Westbury, NY, USA), which is of interest in this work, is designed to have overexpanded flow conditions at the exit of the torch in order to achieve a higher gas velocity (Mills, 2003). In the past decade, extensive CFD work has been done to obtain an in-depth understanding of the physio-chemical behavior involved in various HVOF thermal spray processes (Power et al., 1991; Chang and Moore, 1995; Oberkampf and Talpallikar, 1996; Yang and Eidelman, 1996; Hassan et al., 1998; Lopez et al., 1998; Gu et al., 2001; Cheng et al., 2001b; Dolatabadi et al., 2003). However, most of HVOF systems in these studies have underexpanded flow conditions. Moreover, the particle melting behavior, which plays a very important role in the formation of the coating microstructure (Li et al., 2004b; Shi et al., 2004), has never been studied by existing CFD investigations. Finally, multi-scale modeling of the HVOF thermal spray process, which includes the macroscopic two-phase flow and the microscopic particle deposition process, has not been addressed in the existing literature.

In a previous work (Li et al., 2004b), a comprehensive control-relevant parametric analysis of the industrial Diamond Jet hybrid HVOF thermal spray using a simplified one-dimensional model was performed and a feedback control system targeting the control of volume-based average of particle velocity and melting degree at the point of impact on the substrate by manipulating the feeding gas flow rates was proposed. In this work, we focus on multi-scale modeling and analysis of gas dynamics, particle in-flight behavior and coating microstructure evolution in the industrial Diamond Jet hybrid HVOF thermal spray process, using a comprehensive model. The thermal and flow fields of the gas are solved by Eulerian approach and the particle velocity, temperature and degree of melting by Lagrangian approach. On the gas dynamics side, we solve the Reynolds and Favre-averaged Navier–Stokes equations. Due to high Reynolds numbers and large pressure gradients in the nozzle, the renormalization group (RNG) k–ε turbulence model is used with the non-equilibrium wall function treatment to enhance the prediction of the wall shear and heat transfer. The eddy dissipation model, which assumes that the reaction rate is limited by the turbulent mixing rate, is employed to model the chemistry. The governing mass, momentum and energy balance equations together with the ideal gas state equation are solved at first using a first-order upwind scheme to get to a convergent solution and then a second-order upwind scheme to capture the shock diamonds that occur in the external flow field. On the particle dynamics side, we solve the equations that describe the particle trajectories, temperature histories and melting degrees using the fourth-order Runge–Kutta method. The formation of coating microstructure is modelled by stochastic simulation, in which certain basic rules are applied to encapsulate the main physical features involved in the deposition process. Based on the proposed model, a detailed comprehensive parametric analysis is carried out to study the relationship between the key process parameters and the particle in-flight behavior as well as the resulting coating properties.