

Application of Multiscale Modeling in the Coating Formation Simulation of APS PYSZ TBCs

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The process parameters of atmospheric plasma spraying (APS) influence the coating formation and properties of partially yttria stabilized zirconia (PYSZ) thermal barrier coatings (TBC). Simulations can be used to investigate this dependency and to design the coating process for a targeted production of TBCs. A whole process simulation was realized by modeling the linked subprocesses: plasma torch, plasma free jet, powder particles characteristics, and coating formation. The coating formation can be described by model approaches with different physical assumptions and geometric scales. One approach is the simulation of single powder particles hitting the substrate surface. An alternative macroscale finite element model (FEM) model approach is applied in the coating formation simulation. A group of particles is pooled in a splash that is dependent on the precalculated particle distribution in front of the substrate. A third modeling approach is applied to calculate effective mechanical and thermodynamical properties of coatings dependent on the experimentally obtained or calculated microstructure of the PYSZ TBC, which is based on different homogenization methods. The application of three simulation approaches in the whole process simulation of APS is discussed; advantages and disadvantages are elucidated. Results based on simulation and experiments are presented for a variation of process parameters. Missing links in the multiscale approach are detected to make suggestions for future modeling and simulation work.

Keywords atmospheric plasma spray thermal barrier coatings, coating formation simulation, multiscale modeling, numerical homogenization

1. Introduction

Coatings produced by atmospheric plasma spray (APS) are used in several technological applications. Especially, nickel-base alloy components in gas turbines are protected by thermal barrier coatings (TBC) against heat and partially against corrosion during the gas turbine operation. The functional properties of the TBCs strongly depend on the coating material (partially yttria stabilized zirconia, or PYSZ), but also on the coating microstructure, which is determined by the APS process and the process parameters. Experimental runs with process parameter variations can be carried out to investigate this dependency. Modeling and simulation as an effective alternative to experiments have become more important for the last decade. This paper focuses on the coating formation simulation and coating characterization in the atmospheric plasma spraying process on different scales. It can be guidance for industrial users to apply

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process and coating simulation tools in the physical and structural characterization of PYSZ TBCs and to design and optimize the process based on it.

2. APS Subprocess Modeling Approach

The APS process has to be divided into subprocesses to realize an overall process simulation from the plasma forming in the plasma torch to the coating formation on the substrate, the component. This is due to the different physical characteristics in the process and also different geometric dimensions that cannot be considered by one suitable model and one numerical method in the simulation setup. The following processes are separately modeled: the process gas flow into the torch and plasma formation in the plasma torch; the plasma flow in the free jet outside the nozzle; the powder particle movement inside the jet and heating, melting, and evaporation; the coating formation on the substrate (Fig. 1) (Ref 2-4). Computational fluid dynamics (CFD) software tools (e.g., Fluent by Fluent Inc., Lebanon, NJ) based on the finite volume method are applied to calculate the velocity, pressure, and temperature field of the plasma torch and jet flow. A coupled thermodynamical, fluid dynamical, and electromagnetic dynamical approach is applied to simulate the dynamic electrical arc inside the torch and the energy and momentum transfer to the plasma flow (Ref 3). The heat and momentum transfer to the sprayed powder particles in the jet is calculated in a special software tool PLASMA2000 (Ref 5) or in a fully coupled approach in the CFD software tool, applying a discrete phase model approach. The PLASMA2000 software tool has advantages in the model description of the heat transfer from and to the powder particles. Melting, solidification, and evaporation as

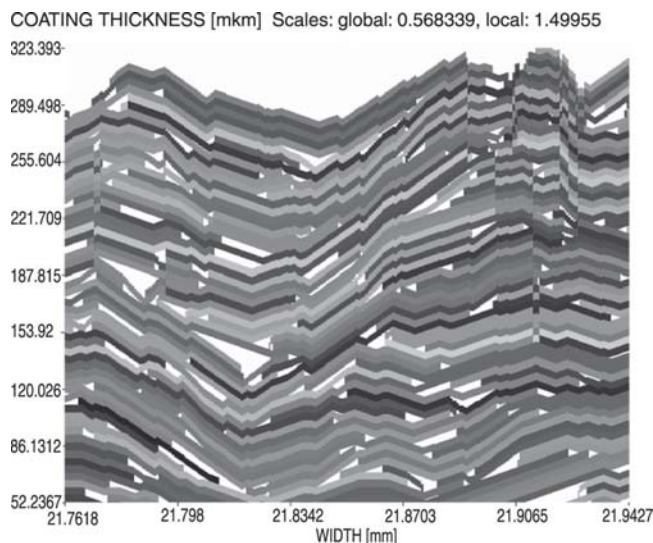


Fig. 1 Coating formation, an empirical approach (Ref 8)

well as different zones with different states of aggregation in the particle can be taken into account compared with standard discrete phase modeling in Fluent. The calculated physical quantities of one subprocess define boundary conditions of other subprocesses. The flow parameters at the nozzle exit of the plasma torch simulation define a boundary condition of the free jet simulation. A heat transfer model is developed to represent the substrate heating during the coating process (Ref 6). In this article, different approaches for the coating formation and coating characterization are elucidated.

3. Powder Particle Impact Simulation

3.1 Particle Impact Simulation—Overview

The impact of single powder particle at the substrate, the deformation, and solidification of the (partially) melted particle can be modeled by different approaches. Coatings are built up layer by layer. The arriving particles form splats at the substrate depending on their velocity, temperature, and viscosity. The process of particle splashing is physically complex. For example, physical phenomena such as the temperature-dependent material behavior (e.g., viscosity) of the splashing particle, the surface tension between particle and the ambient fluid, and the contact behavior between particle and substrate surface have to be considered. During the splashing process additional phenomena such as (micro) crack formation in the ceramic coating can be observed. A lamellar, porous (micro) cracked microstructure is characteristic for APS PYSZ TBCs.

3.2 Particle Impact Simulation—Empirical Approach

The particles arriving at the substrate spread and form a splat. They are supposed to be in a (partially) molten state before they solidify during and after the splat formation. The form of a splat is assumed to be a cylindrical disc in some empirical approaches (Ref 7, 8). The ratio of a particle diameter prior to impact and the

final splat (disc) height depends on the Reynolds number of the particle and varies according to different empirical descriptions. The complex physical behavior of the ceramic particle cannot be described by this approach. Nevertheless, properties such as the coating porosity and local coating growth rates and thickness distributions can be investigated by this mesoscale approach (Fig. 1).

3.3 Particle Impact Simulation—Physical Modeling

The most sophisticated models for the coating formation simulation were developed based on the physical description of the particle impact (Ref 9-11). One approach is to consider the arriving particle as a fluid with temperature-dependent fluid properties. This assumption can be made because the arriving ceramic particles are in a fluid or semifluid state. The numerical method to calculate the relevant field quantities is based on CFD and additionally a volume-of-fluid (VOF) modeling to simulate free surface flow. The VOF model is a multiphase approach where two or more fluids (or phases) exist in a calculation domain and do not interpenetrate. A sharp interface between the different phases is characteristic for this method. In the case of particle impact, the particle forms one fluid (one phase) and the ambient gas (air, process gas) defines a second phase. The particle can be tracked, and the impact behavior (deformation, flattening, cooling, solidification) can be calculated on the basis of physical laws.

A variable is introduced for each phase of the model: the volume fraction α_i of the phase i in the computational cell. The volume fractions of all phases are summed to unity in each computational cell. There are three possible states for the volume fraction of a phase: $\alpha_i = 0$ (the cell is empty of the phase i), $\alpha_i = 1$ (the cell is full of the phase i), $0 < \alpha_i < 1$ (the cell contains the interface between phase i and other fluids). The tracking of the interface between the phases is calculated by solving continuity equations for the volume fraction of the phases. In the case of two phases (first phase, ambient gas; second phase, particle), only one continuity equation has to be solved:

$$\frac{\partial}{\partial t} (\alpha_2 \rho_2) + \nabla \cdot (\alpha_2 \rho_2 \underline{v}_2) = S_2 + (\mu_{12} - \mu_{21}) \quad (\text{Eq 1})$$

where ρ_2 is the density, \underline{v}_2 is the velocity, S_2 is the mass source term for phase 2, μ_{12} is the mass transfer from phase 1 to phase 2, and μ_{21} is the mass transfer from phase 2 to phase 1. The volume fraction of the first phase (ambient gas) is calculated for each computational cell based on the sum of volume fractions to unity rule: $\alpha_1 = 1 - \alpha_2$.

Single particle impact simulations were carried out for different initial conditions (particle velocity, particle temperature). The commercial software FLUENT (Fluent Inc.) was used for this purpose. The ceramic powder particle material is $\text{ZrO}_2 + 7\% \text{Y}_2\text{O}_3$. The properties for surface tension, heat transfer parameters, the temperature-dependent viscosity (based on Ref 10), and contact parameters are implemented. Examples for this simulation of the impact of a PYSZ particle with a diameter of 40 μm, an initial velocity of 250 m/s, and an initial temperature of 3300 K are illustrated in Fig. 2 and 3. The ambient medium is air

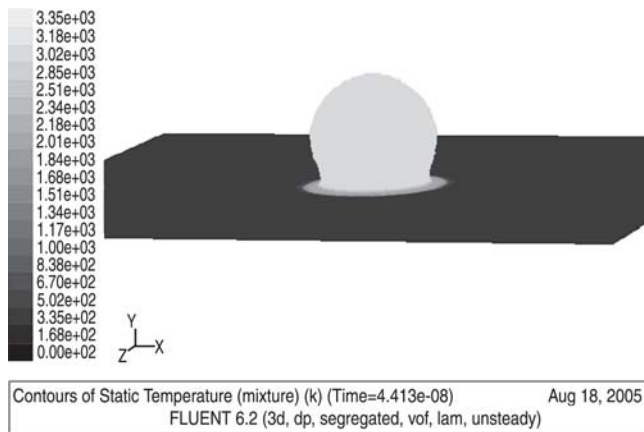


Fig. 2 PYSZ particle impact simulation 44 ns

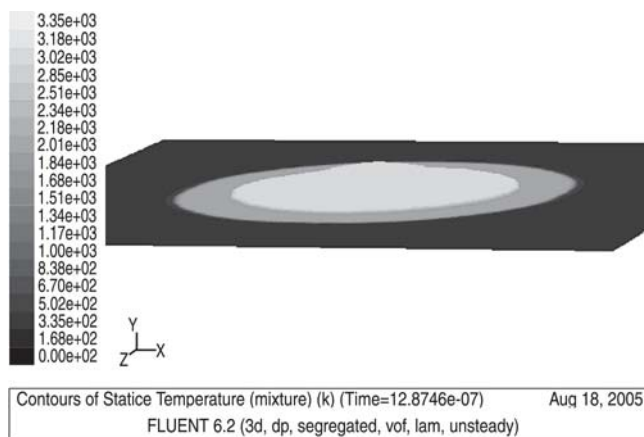


Fig. 3 PYSZ particle impact simulation 0.19 μ s

at rest and room conditions. The temperature dependency of the viscosity is taken into account in this model (Ref 10). The substrate is aluminum with convective heat transfer conditions to the medium in this case. Surface tension at the interface between the ambient medium and the particle is considered. For these test simulations constant values for other material parameters are defined.

This simulation approach represents the behavior of the particle impact most correctly if all physical phenomena are taken into account in the models. However, only a few particles can be simulated with the available hardware resources in a reasonable calculation time. Therefore, this simulation approach is a simulation in the microscale domain. A full coating buildup on complex components cannot be calculated by this method. This methodology is very suitable for the local investigation of the particle splashing. Some phenomena such as crack formation, crack propagation after cooling, and the contact behavior between the splashed particles have to be investigated more deeply to be considered in this physical modeling. The CFD modeling might be not the best method to represent these phenomena immediately after cooling. Particle behavior is then closer to a solid than to a fluid. A coupled fluid-solid approach can be an alternative for the ceramic particle impact simulation.

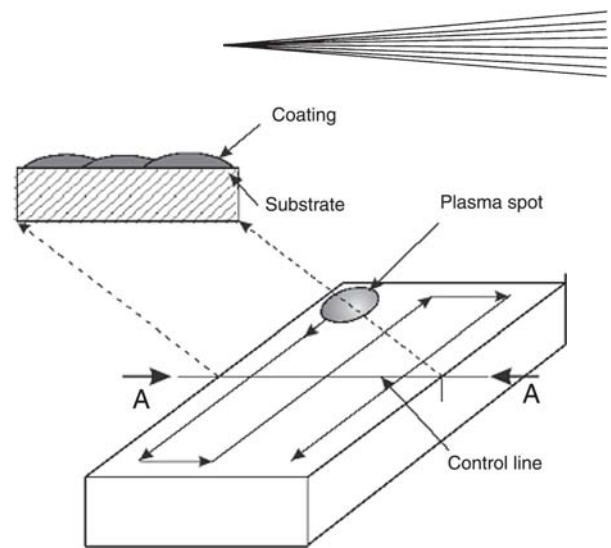


Fig. 4 Scheme of plasma torch

4. FEM Coating Formation Simulation

4.1 The Modeling Concept

In this section, a simulation methodology for the coating formation simulation is described that is different from the previously described single particle impact simulations. This methodology was developed by the authors in the framework of the research work in the collaborative research center of “Integrative Modeling of Materials” (Ref 12). This approach is applied in the investigation of the coating formation during APS on arbitrary and complex components by simulation methods. The aim is to investigate the physical behavior (thermal, stress-strain state) of the coating/substrate system during the APS coating production process. This method can also be applied to simulate and investigate the coating growth rate and thickness distribution on arbitrary components and arbitrary traverse paths during the process. This combination of the simulation of coating thickness distribution and the thermomechanical behavior of the coating/component compound is an advanced approach compared with the described empirical particle impact simulation approach. The finite element method (FEM) macroscale approach allows ones to apply continuum elements representing the coating microstructure influence in the material model (homogenization strategies). The microstructure formation (pores, cracks, etc.) and the macroscale coating formation are completely separated in this approach. This is also a main difference to the physical and empirical particle impact modeling approach. The FEM macroscale coating formation simulation makes more effective and faster calculations for the most complex components and traverse paths possible than the empirical and physical particle impact simulations can realize. This simulation setup based on the FEM takes the time dependence of the APS process into account. The plasma torch moves relatively to the substrate/component. This process of torch moving is separated into discrete time steps. After every time step, the plasma torch changes its position and thus the position of the plasma spot at the surface changes too. A discrete movement of the torch and the plasma spot is created for the coating formation simulation. The order of magnitude of such time steps is about 100 μ s. All other time dependencies in the process such as the instable arc root move-

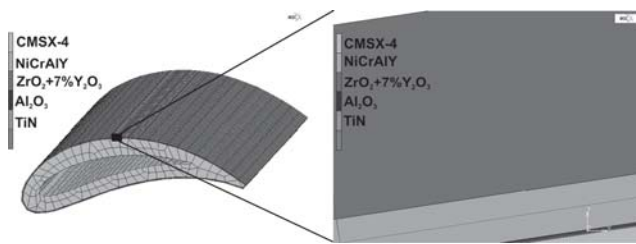


Fig. 5 FE model of a coated turbine blade model (FEM tool: MARC2003/MSC)

ment are considered in the related subprocess modeling approaches such as the plasma torch simulation in this case. However, the time scales of subprocesses are different, and the influence of the arc root movement on the particle flight in the free jet is then considered in the coating formation approach by the calculated *integrated* (over the time step of the plasma torch movement!) particle distribution in front of the substrate. Due to the moving plasma spot, the *splatwise* coating formation is done layer by layer in this process (Fig. 4). This simulation approach is aimed to model this process in the geometric scale of the substrate dimension.

This macroscale FEM simulation approach can be applied by industrial users as a fast simulation methodology in the APS process design and control to minimize the thermal stresses in the substrate/coating compound or to obtain a uniform coating thickness distribution on special components. Predictive parameter studies by a numerical optimization using this simulation approach can be carried out for this purpose. The use of the single particle impact modeling for this macroscale coating formation simulation would lead to a very high consumption of computer resources and calculation time. For example: if the tracking of one particle by physical particle simulation from arriving at the substrate until the complete solidification would take 1 h (optimistic assumption), then the simulation of the formation of a 200 μm coating on a 4 by 4 cm quadratic specimen would take about 110 days.

4.2 The FEM Modeling Algorithm

The macroscale coating formation approach is based on a predefined meshed model of the coated component (Fig. 5). The predefined mesh for the TBC elements is created based on a maximum coating thickness for this coating. Models were used with predefined layers in the range from 200 μm to 1 mm. The perpendicular (to the coating surface) initial dimension of the elements is 10 μm and the lateral 100 μm (parallel to coating surface). An adaptive mesh refining and roughening procedure can be optionally applied during the algorithm. In Fig. 5, the base nickel (Ni) alloy material (CMSX-4, Cannon Muskegon Corporation, Muskegon, MI), and a set of functional coatings is defined. The APS PYSZ TBC is the final red-marked coating in this figure.

All TBC coating elements are deactivated at the beginning of the coating formation simulation. The elements are activated in the way that they represent the calculated powder particle distribution in the plasma spot in front of the substrate (Fig. 6) (Ref 4). The plasma torch and thus the plasma spot move along the turbine blade surface. This plasma spot location has to be calculated for every time step of the coating period in the algorithm.

The position of the plasma torch is determined by the position of the nozzle exit of the torch $x(t)$ and the direction of the plasma jet from the nozzle $dx(t)$ for every increment of the coating time (Fig. 6). The realization of every plasma torch and substrate movement is possible in the algorithm described in Ref 12.

The powder particle distribution (coating thickness profile) in front of the substrate is obtained by the simulation of powder particle acceleration and heating in combination with the plasma free jet simulation (Fig. 7) (Ref 4). In Fig. 7 different scaled coating distributions for different injection velocities (v_{mi}) and particle diameter distributions (d_{mi}) are shown. The coating profiles perpendicular to the plasma torch movement are scaled dependent on the mass flow μ of the particles and the coating porosity U :

$$H(x) = \alpha * h(x) \quad \alpha = (\mu * \Delta t) / \left(\rho * v_{pl} * U * \int_{-\infty}^{\infty} h(x) dx \right) \quad (\text{Eq 2})$$

where h is the coating thickness profile distribution, H is the scaled profile, α is the scaling ratio, Δt is the simulation time increment, and v_{pl} the relative plasma torch (to the substrate) velocity. Differences in the coating buildup and the thermal behavior for different particle distributions are presented in Fig. 8.

The whole simulation process chain from the plasma torch to the coating formation simulation is realized by this approach. The finite elements to be activated represent a group of particles, the so-called *coating spot*. Initial conditions related to their thermal and mechanical state have to be applied to them just before their activation in this algorithm. This is the most crucial point in this macroscale coating formation simulation approach. Initial conditions are obtained from the physical single particle simulation on one hand and from the powder particle flight simulation on the other hand. An averaging has to be carried out because some solidifying powder particles in such a *coating spot* are in different states and others are still in flight. The thermo-mechanical behavior of the coating/substrate compound during the coating process depends on the material properties of the APS-PYSZ-TBC. One (continuum) finite element in the coating spot already represents a part of the coating with solidified particles and interfaces between them. A link between the particle impact simulation and this FEM macroscale coating formation simulation is the representation of the coating microstructure (calculated in the microscale approach) in the material model description for the TBC elements. Special homogenization methods (presented in the next section) were developed and applied to represent these microstructural effects in continuum material models. The coating microstructure can be calculated for different sets of basic process parameters of the APS process (process gas mixture, torch power, torch current, selected ceramic powder, injection parameters, spraying distance, angle of attack of the plasma jet to the substrate surface) and stored in a database. Thus, the microstructure (including the porosity) of the TBCs is predicted by microscale particle impact simulations. These microstructural data can be loaded then from the database for different traverse paths and plasma torch positions during the macroscale FEM coating formation simulation. During the macroscale coating formation simulation, parameters such as the coating formation distribution and the thermomechanical behavior of the coating/substrate compound are predicted. If the calculation of the coating microstructure cannot be carried out dur-

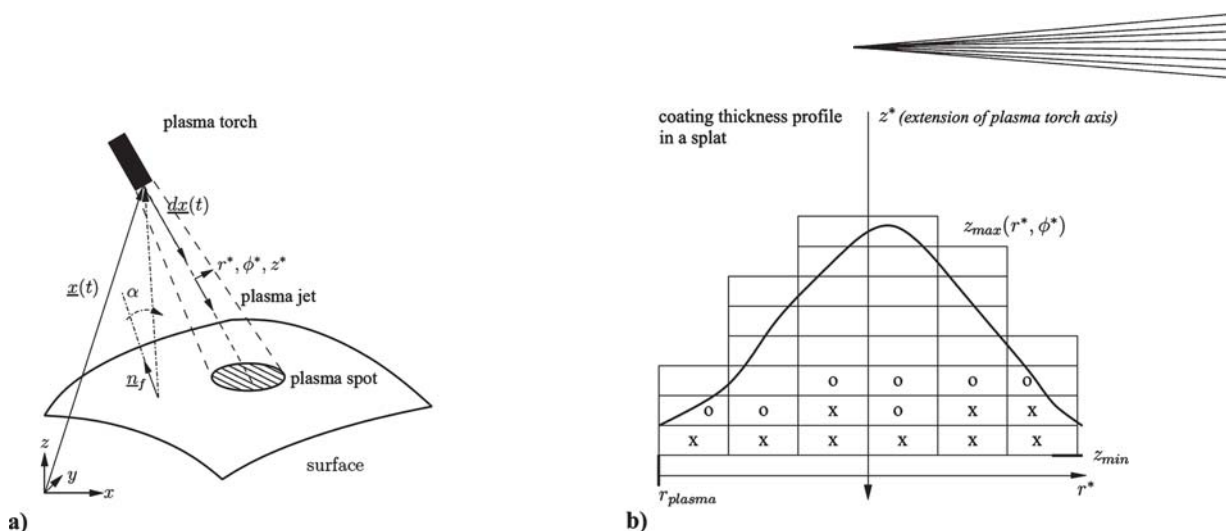


Fig. 6 Sketch of the coating formation algorithm. The “x” marked elements represent the activated FEM elements forming the coating in the plasma spot step by step. The “o” marked elements are candidates under the precalculated coating profile for the activation in the next loop of the algorithm. One of the “o” elements will be selected for activation. It becomes an “x” element. The activation stops during one time increment if the coating elements fill the calculated profile.

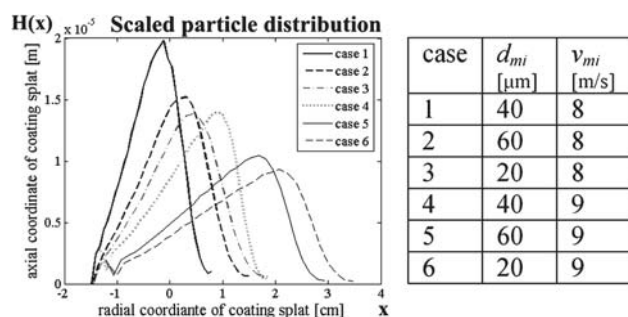


Fig. 7 Calculated particle distributions (coating thickness profile of a splat) in front of the substrate

ing the particle impact simulation due to missing material data of the powder particles for example, experimentally obtained microstructures (SEM images) for different process parameters are the basis for the homogenization strategies to calculate the material models. These experimentally obtained microstructures can be stored in the database as well, and the macroscale coating formation simulation can be carried out. The prediction of the coating thickness distribution and the thermomechanical behavior of the component during the coating process is still possible.

The advantage of this macroscale FEM coating formation approach in combination with the single particle impact simulation compared with stochastic coating formation approaches (Ref 13) is the physical basis of the simulation. All models are based on the physics of the coating process. There is no assumption about the distribution of process parameters except the particle injection parameters. The presented approach is more consequent and integrative (from the plasma torch to the coating). For this reason, it is more flexible if installation design or process parameters are changed, and it can be applied to other thermal spraying processes as well. The coating formation algorithm does not need to be changed. The disadvantage is the higher effort in the model preparation and partially also the higher calculation effort, especially the single particle impact simulation. The challenge here is also the determination of all relevant material properties and models for the single particle impact simulation.

5. APS-PYSZ-TBC Coating Properties Characterization

The material properties of the APS-PYSZ-TBC depend on the coating microstructure. The material modeling for the APS PYSZ TBC layer has to be taken into account in the macroscale FEM coating formation simulation as well as in operation simulations of the coated turbine blades. Homogenization methods were developed and implemented to represent the influence of the microstructural defects on the physical coating behavior in continuum models (Ref 14, 15). Homogenization means neither a physical nor a technological homogenization in this context. It is a method to calculate effective material properties or estimate the effective material behavior in a representative area of the inhomogeneous structure. The structural characteristics such as pores and cracks are not implemented in the homogeneous model of the representative calculation area. However, the influence of these microstructural defects on the material behavior is taken into account in the material models and properties. The microstructure of APS PYSZ TBCs is an input for this methodology. It can be obtained either from experiments or from results of single particle impact simulations. If these microscale coating formation simulation results are used, then a link between the single particle impact simulation and the macroscale coating formation simulation is created. Scanning electron microscopy (SEM) images of polished APS PYSZ TBC samples (Fig. 9a) are two-dimensional (2D), but give a realistic input for the homogenization of extended calculation areas. These images are black and white (B/W), digitalized to define two phases: white ceramic PYSZ and the black “void” (pores, cracks), as shown in Fig. 9(b). The methodology for the calculation of material properties and models using homogenization strategies is the same for experimentally obtained microstructures and for calculated microstructures. Experimentally obtained microstructures are used in the following overview of the developed homogenization strategies. The procedure for calculated microstructures by single particle impact simulation is equivalent.

Two alternative homogenization strategies are applied. The first method is called homogenization based on the physical

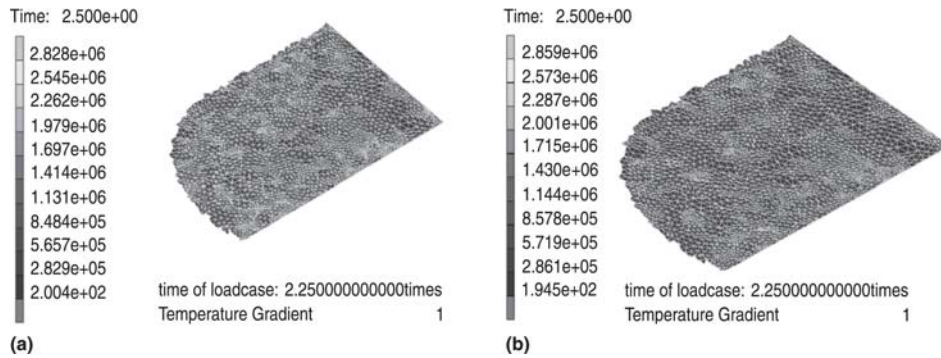
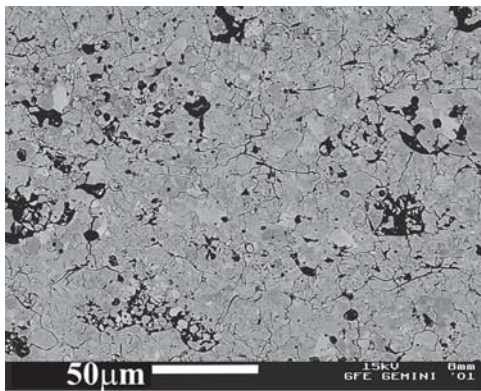


Fig. 8 Coated PYSZ layer after 2.25 s on an invisible flat substrate for particle distributions (a) 1 and (b) 6 (FEM tool: MARC2003/MSC. Software Corporation, Santa Ana, CA)



(a)



(b)

Fig. 9 (a) SEM image APS-PYSZ-TBC. (b) B/W digitalization

equivalence (PE homogenization). This method is based on the assumption that a physical quantity integrated over the inhomogeneous calculation area is equivalent to this quantity in the homogeneous model with the same area dimensions (Ref 14). The physical quantity can be the integrated heat flux to calculate the thermal conductivity, for example (Fig. 10). The PE homogenization method could successfully be applied for the determination and fitting of nonlinear material laws (Fig. 11). The obtained material law parameters such as the Young's modulus and the yield strength could be validated by experimental measure-

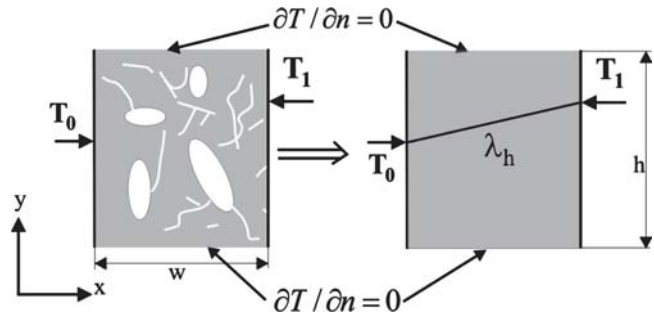


Fig. 10 Scheme of thermal PE homogenization

ments (Ref 14). This indicates the applicability of the homogenization method as a link between the microscaled structure and the macroscale (effective) coating behavior in a system.

A second homogenization strategy was applied as an alternative to the PE homogenization. It is based on the periodicity of the material structure and thus material properties. This common theory of the homogenization method for periodical structures (PS homogenization) was developed by Sanchez-Palencia (Ref 15). A multiperiod approach was developed based on this theory by the authors to take microstructural defects of different orders of magnitude into account. Spectral analysis of the digitalized microstructure is applied to investigate the periodicity of the structure and to implement this in a multiperiod model (Fig. 12a and b) (Ref 16). The PS homogenization is a suitable and faster method for the calculation of material properties (e.g., Young's modulus), and the PE homogenization is applicable for the determination of nonlinear material models.

The determined material models and properties are implemented in a sophisticated macroscale coating formation simulation where the thermal and mechanical behavior of the coating/substrate system during the coating process is investigated (Fig. 13).

6. Summary and Conclusions

In this article, a concept for a multiscale coating formation simulation of APS PYSZ TBCs is presented. This concept is based on research work of different groups in this area of mod-

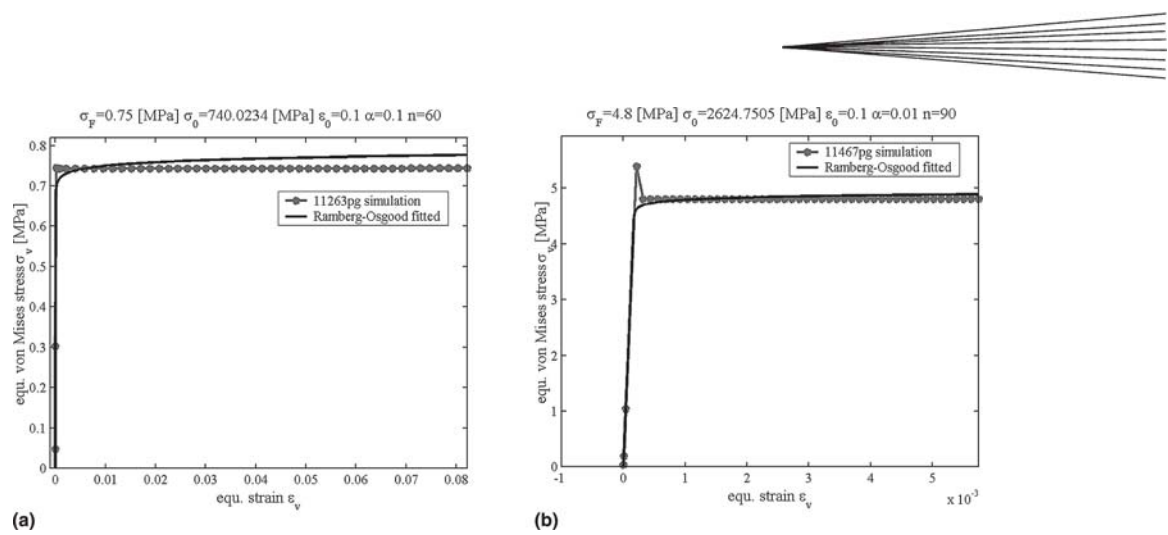


Fig. 11 PE homogenization: developed mechanical material models for APS-PYSZ-TBCs

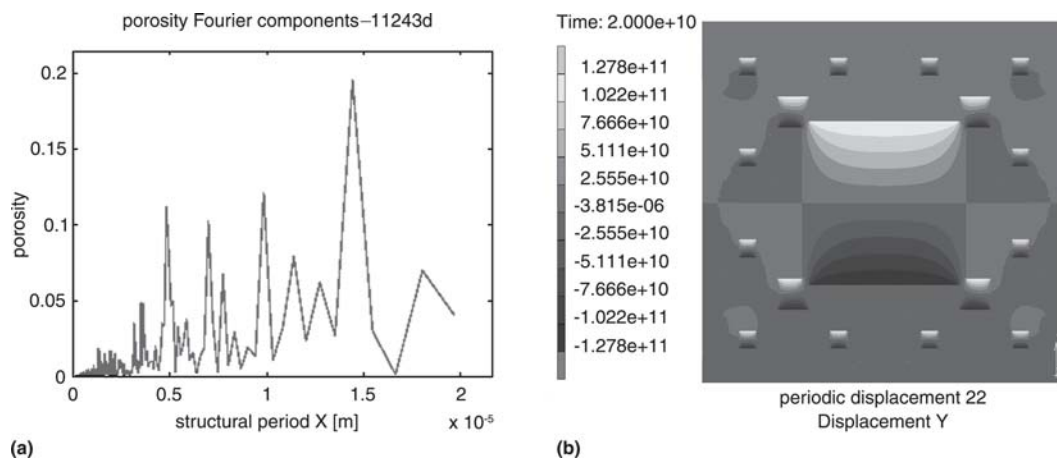


Fig. 12 PS homogenization: (a) spectral analysis; (b) calculation of periodic displacements (FEM: MARC/MSC)

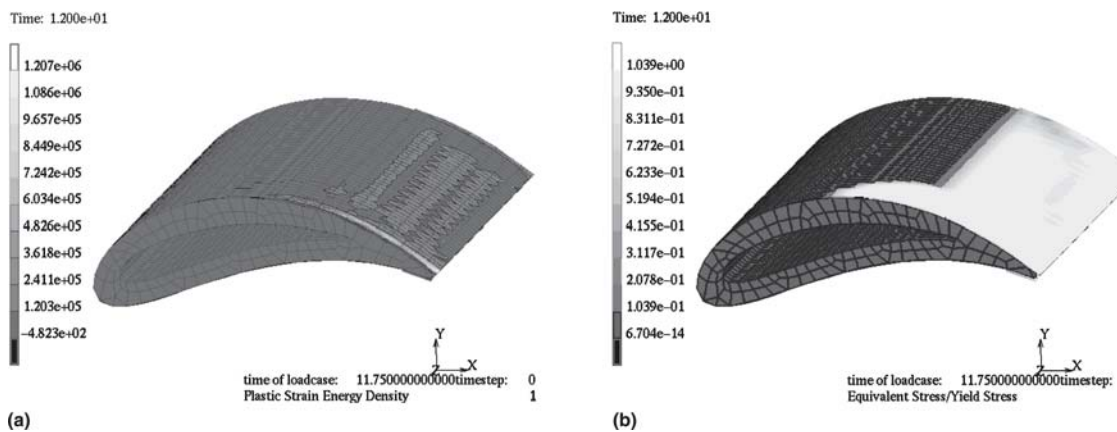


Fig. 13 FE macroscale coating formation simulation with developed material models. (a) Plastic strain energy and (b) Equivalent stress/yield stress (FEM tool: MARC2003/MSC Software Corporation, Santa Ana, CA)

eling and simulation. The authors place their research work in the area of the development of macroscale coating formation simulation approaches and the application of homogenization strategies for the coating characteristics in this context. This

multiscale approach is a guide for industrial users to apply modeling and simulation in the process design and optimization of thermal spraying processes. The developed macroscale approach is especially useful for the investigation of process pa-

parameter and component geometry that are dependent on coating characteristics such as the coating thickness distribution and the thermal and mechanical behavior of the coating/substrate system during the APS process. The presented homogenization strategies form a link between the microstructural characteristics of the coatings and the macroscopic physical coating/component system behavior. The physical modeling of the single particle impact behavior is suitable for the coating structure formation simulation on the microscale. This approach has to be improved related to the implemented temperature-dependent material behavior for the ceramic particles and other phenomena such as inner structural contact and the crack formation and propagation during the solidification.

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