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TITLE MODELCOAT: FINITE ELEMENT MODELLING OF CERAMICS TBCS TO EXTEND THE OPERATIVE RANGE OF HEAT ENGINE COMPONENTS

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MODELCOAT:

FINITE ELEMENT MODELLING OF CERAMICS TBCS TO EXTEND THE OPERATIVE RANGE OF HEAT ENGINE COMPONENTS

Proposal No. BE -4272- “90
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Synthesis Report
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ABSTRACT

The industrial research project MODELCOAT has carried out a detailed investigation of some TBCS systems of industrial relevance to improve their reliability and lifetimes. The selected route to achieve the goal has been through the definition and application of a combined experimental and theoretical programme. The programme has compared experimental results and theoretical modelling at all stages of the work. The project has been focused to the modelling of thermal barrier coating microstructure, mechanical and thermal properties, and behaviour under service conditions.

A. INTRODUCTION

Thermal plasma spraying of ceramic materials offers interesting possibilities for the development of *new* engine components and for new processing routes to surface engineering in regard to the insulation of critical metal components. Thermal plasmas with temperatures typically on the order of 10,000 ‘K provide extremely high heating and quenching rates for particulate matter injected into such plasmas. Under these extreme conditions, unusual coatings may be produced with interesting properties.

Recent work has focused on the improvement, for selected powder composition, such as ZrO_2-Y_2O_3 on MCrAlY bond coat systems, of properties like thermal shock resistance, mechanical properties and lifetime. Most of the research work relating the thermomechanical properties of TBCS to the spraying parameters has taken an empirical approach. This has been due both to the lack of enough detailed experimental information about the microstructure of coatings and moreover the lack of adequate theoretical models.

Although thermal plasma processing attracted increasing attention over the past years, progress, especially in terms of industrial developments, is still hampered by serious gaps in the understanding of the correlation between spraying parameters and the corresponding microstructure and material characteristics so obtained. A synergetic interplay between experiment, theory and simulation have been indicated to be one of the key factors for faster progress in this field.

The present document describes on the main results obtained in the 36 months of activity of the BRITE/EURAM project MODELCOAT, Proposal No. BE-4272-W, Contract No. BREU-0535, title: “Finite element modelling of ceramics TBCS to extend the operative range of heat engine components".

A. 1. OBJECTIVES OF THE PROJECT

The MODELCOAT project has focused on the modelling of’ thermal barrier coating microstructure, mechanical and thermal properties, and behaviour under service conditions.

The overall programme consisted of five major tasks plus a management task.

(i) production, characterization and testing of state-of-the-art coatings (Task 1);
(ii) model development (Task 2) ;
(iii) assessment of model predictions (Task 3);
(iv) improvement of TBCS performance based on the global model for
  (a) reciprocating engine, and
  (b) gas turbine components (Task 4);
(v) assessment of project results (Task 5).

The first phase of the project has considered state-of-the-art coating production, characterization and testing, the set-up of specific tools for the numerical modelling and the evaluation of coating performance and model predictions. The second phase has seen the transfer of the complete set of acquired experimental data to the developed numerical model and their mutual integration for the definitions of improved process parameters. The improved process parameters have then been applied in a spraying of a novel generation of ceramic coating and their quality has been verified.

The central aspect of the project has been the combined experimental, theoretical and numerical effort on a number of' TBC on industrial components produced for well defined industrial coating production system under controlled conditions.

A.2. MEANS USED TO ACHIEVED THE OBJECTIVES

In order to achieve the planned objectives the project has been divided into five interdependent tasks and related subtasks. The different subtasks of the project and their main interrelations are schematically shown in Figure A. 1.

Within each of the defined tasks specific techniques and methods have been developed and used to achieve the desired results. These techniques and methods are collected and presented in detail in the Final Technical Report.

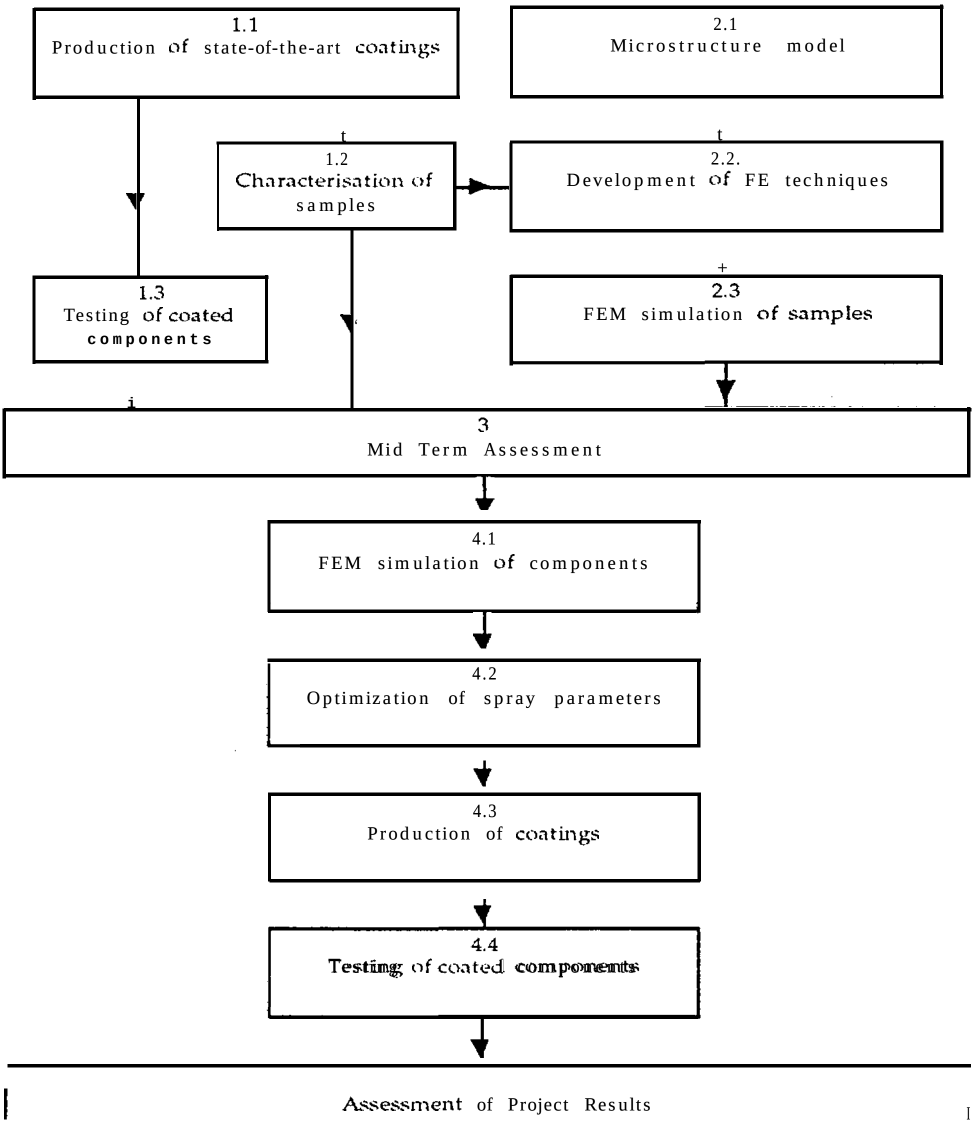

Figure A. 1: Program Flow Chart

B. SUMMARY OF MAIN RESULTS

Industrial applications of the present findings are summarized n the following points:

(1) Identification and application of a combined (experimental and modelling) strategy to extend operative range
(2) Failure mechanism identification
(3) Identification of key spraying parameters, proposal for improvements and assessment of improvements
(4) Development and applications of new manufacturing technologies (ATCS) and general control of quality of manufacturing processes

B. 1 IDENTIFICATION AND APPLICATION OF A COMBINED STRATEGY TO EXTEND OPERATIVE RANGE

A general framework for the development and application of numerical models based on experimental characterisation have been defined. In brief it consists of the following blocks:
(1) production of coatings under controlled conditions. The development of the models have indicated the needed monitoring of specific process variables as important to the final properties of the coating; the main selected process parameters are the substrate temperature and substrate temperature gradients.
(2) the measured variables are then used in numerical models to assess the initial mechanical state of the coatings to predict the degree of damage present as well as the distribution of the residual stresses. Validation of these predictions are obtained by experimental characterisation techniques specifically developed within the project.
(3) the different coatings (corresponding to different initial states of the coating i.e. microstructure and distribution of stresses) are then tested in thermal cycles designed within the project. Again the experimental tests have been extended to monitor variables following the needs and the indications coming from the numerical models of the simulation of the tests. The selection of the “best” coating are at present assessed by direct measurement of the life time during the them-ml cycle. Models to indicate the state of stress and indication of localization of stresses as a function of loading conditions and initial mechanical stste has also been developed and contribute in the identification fo the “best” initail state for the coating wit preference to the specific operative condition that the cycle wants to reproduce.

B.2 FAILURE MECHANISM IDENTIFICATION

Thermal cycle tests were carried out on semi-components to investigate failure mechanisms and in particular crack propagation processes for both applications considered in the project: pistons and turbine blades. In parallel numerical procedures have been developed for the thermal cycling of coated structural components based on the finite element modelling of coating, bond layer and substrate- or core material. The numerical models have proved capable to indicate the critical locations and to assist in the explanation of the failure mechanism, therefor indicating possible route to improvements.

Piston$s
The work of DB was devoted to the characterisation of macro-cracks due to thermal stresses in the standard zirconia TBC's for diesel engine applications (pistons). These macro-cracks are initiated at thermal shock and they are regarded to be the important failure mechanism for the TBC.

Special attention was therefore paid to the time (number of cycles) until this macro-crack was initiated and to the propagation of the crack until spallation of the coating, leading to a failure curve. In order to follow the crack path until the final spallation a Spectrotherm instrument based on laser induced thermal waves in the touted component was used.

The results show with good accuracy that for the coated components investigated in this project and for which the numerical model has been developed the failure is caused by a macro-crack initiated in the edge of the interface bond coat and top coat. This crack propagates stress-dependent in the top coating about 10 - 30 mm horizontal. The spallation of the coating and thus the, failure of the component is completed when the crack joins the surface of the top coating. The crack initiation was correlated with the component failure. For a total of five tests it was found that the macro-crack causing failure is initiated when on the average 90% of the final life- time has been reached. The numerical calculation may thus be interrupted at macro-crack initiation

Blades
The work of MTU was devoted to the characterisation of macro-cracks due to thermal stresses in the standard zirconia TBC's for aeronautics engine applications (turbine blades).

The result of the thermal cycling of the coated blade conforms with the failure patterns observed in the coating after a few cycles (typically 1 to 5). The photographs of magnified images investigated by MTU indicate cracking across the coating on both the pressure and the suction side at the stress maximum behind the last cooling hole and at the transition of curvature at the trailing edge. Cracking across the coating is observed also in the middle between the maximum where the flat stress profile maintains the high intensity. Although at this early stage we may rather speak of fissures across the coating, in the main, two open segmentation cracks appear each on either side of the tail. On the pressure side, the segmentation crack is definitely located at the curvature transition, whilst on the suction side, segmentation may alternatively occur at the middle location with a fissure then visible at the rear stress maximum. Ultimately, segments of the coating are detached from the profile around the trailing edge.

Modelling
Computer simulations of thermal cycling tests on pistons and on turbine blades (carried out by ICA and UNI-TN) provide detailed information on the nature of strain and stress, their distribution and intensity as a function of time. Thereby critical locations have be identified in the coating and were confirmed by the experimentalists to be prone to failure. In addition, numerical analysis indicated the reversals from heating to cooling in the cycle as a critical instant inducing a cooling shock in the blade coating. Variations of the manufacturing conditions underline the positive effect of an increasing deposition temperature and/or a diminishing temperature gradient, both reducing the stress level during thermal cycling. The temperature dependence of the properties of the core material may be significant and is of primary importance for the blades exposed to higher temperatures than the pistons.

The predictions based on the numerical modelling reasonably interpret the observations in the testing laboratories for both pistons and blades. The knowledge evolving on the results of the numerical modelling and computer simulation work has been utilized for proposing modifications in the manufacturing and the operation of the coatings in order to delay failure thus increasing lifetime.

B.3 IDENTIFICATION OF KEY SPRAYING PARAMETERS, PROPOSAL FOR IMPROVEMENTS AND ASSESSMENT OF IMPROVEMENTS

Following the results of the numerical modelling of the manufacturing process for the coating on the blades and on the pistons, and of the thermal cycling tests (see subsection 4 in Section D), the following route for improvements have been identified:

Pistons

Since the critical stress fields experienced by the ceramic coating during thermal cycling are generally tensile in the radial direction and tensile in the axial direction close to the lateral edge at the ceramic-substrate interface it seems reasonable to try to search for spraying parameters that produce coatings that have compressive radial residual stresses after production.

These conditions should:

provide a method to counter-balance the tensile stresses during thermal cycling;

provide also compressive axial residual stresses close to the lateral edge at the ceramic-substrate interface, that could be useful to delay the creation of a localised macrocrack at this critical location;

provide a peak of tensile residual stresses in the substrate close to the substrate-ceramic interface that could be used to lock the ceramic in place during operation loading.

The extensive investigations of different temperature profiles in order to identify good initial conditions to produce residual stress fields that fulfil the above request have provided the following indications:

- from the model the spraying conditions that produce such compressive (on the average) radial residual stresses in the ceramic (i.e. average tensile stresses in the substrate) are high substrate temperature and/or low substrate temperature gradients
- the same conditions (high substrate temperature and/or low substrate temperature gradients) assure also compressive axial residual stresses close to the lateral edge at the ceramic-substrate interface.

Turbine Blades

- During the course of thermal cycling - under testing or service conditions - the ceramic coating is as a rule exposed to higher temperatures than the core. Since the thermal expansion coefficient of the core material, however, is an increasing function of temperature approachingultimately almost twice the value of the constant one of the ceramic coating, the elevated operation temperatures induce tensile circumferential stresses in the ceramic layer. The magnitude of the cycling stress can be reduced by increasing the stress-free temperature of the coating at deposition. This diminishes the stress-inducing part of the thermal expansion of the coated blade- The effect corresponds to a fictitious production of compressive circumferential stresses in the coating after cooling-down from the deposition temperature. These stresses would appear if the thermal expansion coefficient of the core material would possess throughout the temperature range the value it assumes at high temperatures in the cycle.

- The stress in the coating is highest around the nose of the profile and at the tail excepting the curved part of the trailing edge. Both regions are characterized by the absence of cooling holes in the core material. A modified cooling system might reduce temperature and thermal strain in the blade material there, thus leading to a more homogeneous distribution of the cycling stress in the coating.

- The numerical simulation of the cycling tests by finite elements and the analysis of the results in conjunction with micromechanics modelling, indicate that spontaneous failure of the coating by segmentation cracks might not occur if straining does not exceed the stage at the end of the heating phase. This requires a smooth transition to cooling. If the cooling shock is unavoidable during operation, thermal straining of the coating might be diminished by altering the conditions of deposition. In this connection, a higher deposition temperature seems to be beneficial only as long as it does not imply an increase in the elastic modulus of the sprayed material. Laboratory measurements by DB indicate, however, that the modulus of elasticity is in fact an increasing function of the deposition temperature. Therefore, a preferable alternative is to diminish the temperature gradients in the cross- section by appropriately adjusting the cooling conditions during spraying, whilst maintaining the deposition temperature of the coating unchanged.

A first application of the above guidelines have been carried out at DB and MTU in th spraying of new coated components with improved spraying parameters, in particular high deposition temperatures and controlled temperature gradient during deposition. The most interesting results have been obtained at DB where drastic incresed of life-times of coated pistons have been obtained. Table I compares the best two series of results obtained at the beginning of the project and at the end of the project

State-of-the-art		**End of proj :ct**	
Series	No. of cycles before failure	Series	**No.** of cycles before failure
1	297	3	1350
2	**767**	**4** "	**2400"**

B.4 DEVELOPMENT AND APPLICATIONS OF NEW MANUFACTURING TECHNOLOGIES (ATCS) AND GENERAL CONTROL OF QUALITY OF MANUFACTURING PROCESSES

In the course of the project:

(1) new spraying manufacturing technology like ATCS, have been applied;

(2) innovative methods of characterization of thermal barriers coatings have been developed and applied; these methods can have a direct industrial applications as new methods of process control. In particular :
improved Rietveld methods to enhance the quantitative analysis of phases;
- X-ray microdiffration methods for analysis of residual strain fields;
- transverse scratch test techniques for the assessment of mode of tooting failure
transient thermography techniques relevant for measurements (of coating thermal properties), defect detection and hence quality control;

(3) numerical procedures have been developed for both the manufacturing and thermal cycling of coated structural components based cm the finite element modelling of coating, bond layer and substrate- or core material. The numerical models have proved capable to indicate the critical locations and to assist in the explaination of the failure mechanism, therefor indicating possible route to improvements.

C. CONCLUSIONS

During the course of the MODELCOAT project the knowledge of the con-elation between spraying parameters and the quality and duration of the coated componets has been improved in three main areas:
identification of important spraying parameters
identification of failure mechanisms
identification (via numerical analysis) and assessment (via testing) of possible route for improvements of coaling life-times

The detail comprehension of the influences of the relevant process parameters (such as substrate temperature,deposition temperature gradients, oxidation level, etc.) does indicate ways to advance coatings quality and properties. The impact of such indications have been tested for diesel engine applications. The aim of the project has thus in the main being reached.

The following comments can be made at the conclusion of this project:

- The combination of production, experimental and numerical effort has proved to be an effective approach for the optimization of spraying parameters for specific industrial applications. In particular the use of models relating the residual stress levels to experimental life-time evaluation has been identified as an efficient route to achieve the desired optimization goals.

- The development and the application of innovative experimental techniques (such as micro X-ray diffraction for residual strain measurements, alternative measurements of coating adhesion by a fracture mechanics approach, heat pulse techniques to quantify thermal diffusivit y as well as the identification of failed areas) have permitted to improve the monitoring of the manufacturing process as well as the monitoring of the overall quality of the produced coatings.

The concerted development of these innovative tools and their applications have represented the central aspect of the present project.

D. ACKNOWLEDGEMENTS

This work was supported by the BRITE/EURAM programme of the Commission of European Communities (Brite/Euram Contract BREU -0535, Proposal BE -4272- 90)

E.' ANNEX: PROJECT'S PUBLICATIONS

A list of publications, conferences and Ph.D thesis concering part of the research carried out in the present project follows.

Publications

- P. Scardi, M. Leoni, L. Bertamini, "Residual Stress in Plasma Sprayed Partially Stabilized Zirconia TBCs: influence of the deposition temperature, submitted in Thin Solid Films.

- M. Leoni, L. Bertamini, P. Scardi, "Influence of phase stability on the residual Stress in Partially Stabilized Zirconia TBCS produced by plasma spray", submitted in to Surf. and Coat .Tech.

- L. Bertamini, G. Campana , R. Dal Maschio and M. Mw-these, "Characterization and Modelling of a Burner Rig Test for a Thick Thermal Barrier Coatings for Automotive Applications", submitted to Surf. and Coat .Tech.

Conferences Presentations and proceedings

Results of the project have been presented at:

- I. St. Doltsinis, R. Handel and G. Noetzel, " Some thoughts on the constitutive modelling of brittle materials undergoing microcraking ", Meeting of the Committe of Expert on " Physical and Mathematical Aspects in Material Theory ", April 1992, Stuttgart, Germany

- T. Cosack and W. Hinreiner, " Volumenverminderung an plasmagespritzten Wärmedämmschichten auf Grund von Sintercorgängen in teilstabilisiertem Zikonoxid, TS 93, Aachen (Germany), March 1993, DVS-Berichte Band 152 p. 123-127

- P. Adam and T. Cosack, "Thermal Barrier Coatings - their Functional Benefits, Problems and Improvements in Manufacturing and Quality", 1993 European Propulsion Forum, Bath (United Kingdom) June 1993, p. 13.1 - 13.8

- L. Bertamini, S. Sturlese and P. Beber, " Atmosphere and temperature controlled spraying (ATCS) of thermal barrier coating on aluminum alloys ", International Symposium on Automative Technology and Automization, Aachen 13-17 September 1993.

- M. Marchese, T. Cosack and I. St. Doltsinis, "Improvements of reliability of heat engine components under service conditions using Finite. Element Analysis of ceramic TBCs", Brite/Euram Workshop on Surface Techniques in Mechanical Engineering, Garmish-Partenkirchen, Germany, September 19-20, 1994.

Thesis

- Fredin Carl, "Versagen von Plasmaspritzschichten aus Y_2O_3-stabil isierten ZrO_2 zur Wärmedämmung im Motor unter Thermoschockbeanspruchung", PhD-Thesis, University Stuttgart, 1993

- Giorgio Campana, "Caratterizzazione e modellazione di test di shock termico mediante "burner rig" di barriere termiche ceramiche spew per applicazioni automobilistiche", tesi di Laurea in Ingegneria dei Materiali, Università di Trento, 1995.

- Matteo Leoni, " Determinazione sperimentale degli stress residui in rivestimenti ceramici", tesi di Laurea in Ingegneria dei Materiali, Università di Trento, 1995.