Multiscale Features in Surface Engineering: Matching the Appropriate Length Scale for Coating Simulation and Development

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Surface engineering is a critical technology for the competitiveness of many European and non European countries. A possible definition to be adopted is "t*he design of surface and substrate together as a functionally graded system to give a cost effective performance enhancement of which neither is capable on its own*". It is an interdisciplinary activity whose successful implementation requires an integrated approach at the design stage, based on the cooperation between design and surface engineers to achieve desired performance and suitable added value. The final aim is to select appropriate technologies to obtain cost effective and optimal surface property designs for specific applications. Surface engineering thus can act as a bridge, transferring technology and expertise between various end-user sectors. The interaction between design, properties, surface engineering technologies, and industry sectors has been widely represented by a 'road map' scheme such as that reported in Fig. 1.

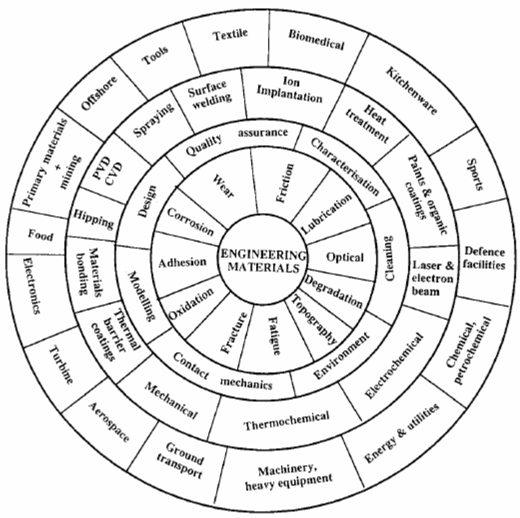

Fig. 1 Surface engineering road map scheme

The contribution of surface engineering to key industry sectors is wide: as an example the performance of aircraft and motor vehicles is critically dependent on surface engineered components and some 80% of both industries is affected by coatings. Other examples can also be mentioned, such as the use of modern PVD multilayer coatings for high performance cutting tools to allow for dry machining, reducing the need to dispose of coolants at the same productivity level; the use of duplex surface engineering treatments on titanium alloys to increase wear resistance thus allowing their use for lightweight components in advanced applications (Formula One, offshore, biomedical and sports sectors); use of surface engineered components for biomedical devices (prosthetic joints, substrates for tissue regeneration, advanced biosensors) which need tailored surfaces for both functionality and biocompatibility, etc.
In the power generation area for aero gas turbines, surface engineering is essential to increase competitiveness and to achieve reliability, cost and performance targets. Actual needs are placed on:
- the development of new materials, advanced coatings and novel design concepts to achieve the future performance;

- the optimisation of current coating systems, to offer the desired performance, managing cost and environmental impact;
- the integration of surface engineering into the design process for strategic performance benefits.

Critical components are those operating in high temperature conditions, associated with the combustion process and the downstream hot gas path for which service life depends on materials degradation. Coatings are applied to combat surface degradation mechanisms such as wear, corrosion and oxidation. The aim is to develop new, advanced coating systems, capable of extending the materials performance range, together with customized technologies and reliable models for materials behaviour for both life predictions and process/material optimization. Increase of operating temperature, increase of component life, increase of inspection intervals are the main requirements. Aero-engine manufacturers are the biggest users of thermally sprayed coatings, both at the original equipment manufacturing stage and during the subsequent repair and overhaul and thermal spray coatings are still to remain an important technological feature in this area (Fig.2).

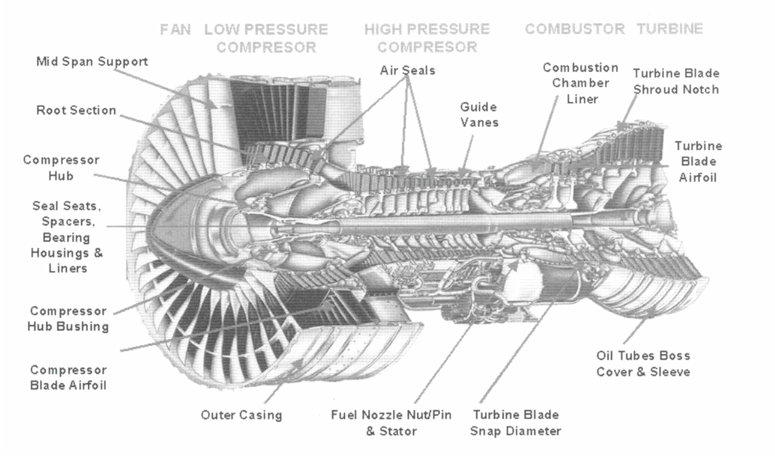

Fig. 2 Examples of surface treatable components in aero-engines

How the new trends in materials development can match the industrial and engineering requirements needs? Looking at the European White Book on Fundamental Research in Materials Science (Max Plank Insitut fur Metallorschung, Stuttgart), in the section Future Directions and Research Priorities it can be found ".. *particular attention should be given to understanding a material's behaviour from the atomic/nano-level via microstructure to macrostructure levels using advanced analytical techniques and computer modelling*…". Mesoscopic features, with characteristic scale between the atomic and macroscopic, can be crucial on how materials perform.

This introduces the importance of computational mechanics in which, generally speaking, simulation methods include the broad areas of quantum mechanics, molecular dynamics and multiple-scale approach, based on coupling the atomistic and continuum models. But the fastest supercomputer in the world can handle up to a billion of atoms today in molecular dynamics simulations, which correspond only to a small cube of 1μm in size. Even with the rapid advance in computer power, if the Moore's law is followed, in the next 15 years the size can increase to only about 10μm. Thus a possibility to overcome this aspect is to follow a top down approach to adjust continuum theory and correct as necessary some approximations, such as for example elastic anisotropy. In exploiting mesoscopic modelling it is fundamental to understand what controls materials behaviour: obtaining a suitable image of a mesostructure in not enough. It must be considered wheter the property of interest is an average property of the system or it is a property depending on special features. For an average property such as an elastic constant, a medium theory could be adopted or average out some timescale. If special features are essential, as microcracks for fracture initiation, many reconstructions of a mesostructure can be required and it is essential to obtain a correct morphology but also a good statistical description of correlated properties. The appropriate scale for a proper modelling has thus to be selected and this could involve both time and length. As an example, in the field of thermal barrier coatings for turbine blades or combustion chambers, designed to reduce materials temperature and resist to spalling and corrosion, a typical microstructure is shown in Fig.3 in the case of a plasma-sprayed coating.

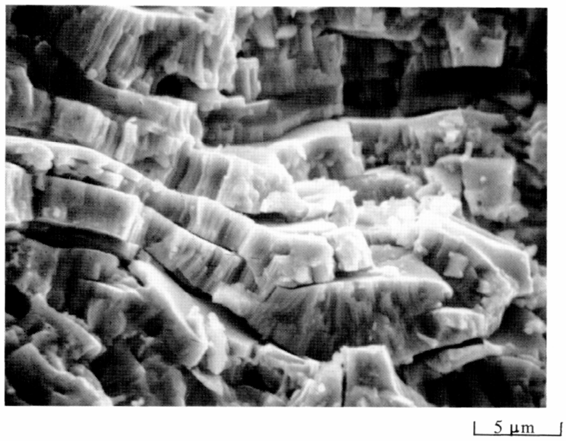

Fig. 3 Example of thermal barrier coating lamellar microstructure

In the fabrication process powder particles are melted and accelerated in a plasma jet and projected against the surface to be coated. A coating with a typical lamellar microstructure is built-up by splashing and solidification of molten particles (Fig. 4). The microstructure, by nature and distribution of the porosity, controls both the average material properties relevant to the application (i.e. thermal conductivity, Young's modulus) and the material behaviour such as crack growth and spalling resistance.

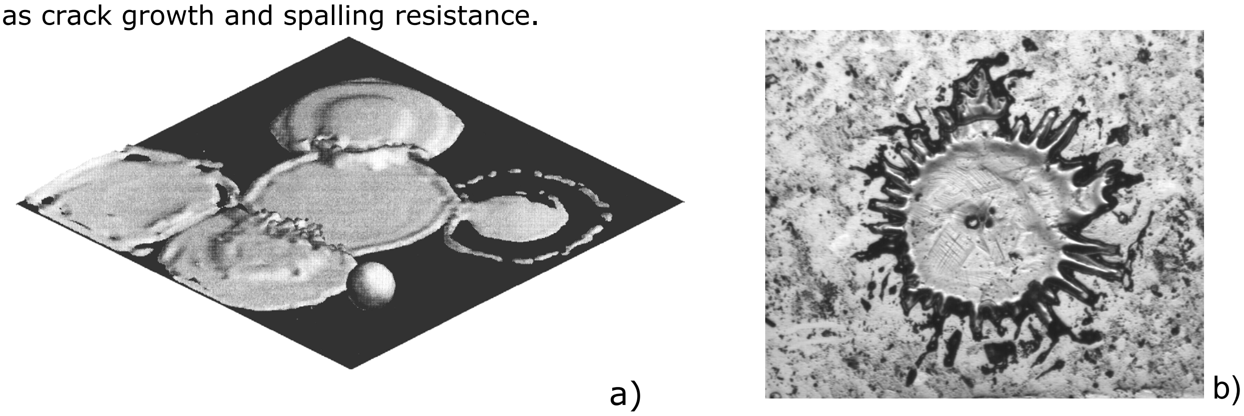

Fig. 4 Splash of plasma sprayed particles: a) simulation; b) experimental

The design of better performing coatings requires a predictive understanding of how the microstructure depends on the manufacturing process. In this case the timescale for a particle to splash and cool (about 10ms) is about a tenth of the mean time between the arrivals of particles at a given point, so that it is possible to study the coating built up through sigle splashing events. Studies of splashing have been carried out experimentally and theoretically as a function of droplet speed and temperature. These information coupled with information from experiments and theory on how the parameters of the plasma torch affect droplet behaviour, allow to define rules for splashing and coating build-up. This approach correlates coating microstructure to the spray process. About coating properties, prediction one option is an extended effective medium theory which provides averaged properties using statistics of the porosity distribution. A second possibility is based on direct simulation of the microstructure evolution under load, by using finite element methods and thus obtaining a distribution of possible behaviours, intended as propensity to fracture. In any case the appropriate scales are set by droplet size and arrival time. Given these scales, simulations result in microstructures and they control properties. With this approach a data base of simulations could be obtained and the process could also be inverted: on the basis of required coating properties, plasma spraying parameters can be defined. This approach has already been demonstrated in principle, by a genetic algorithm acting as a search engine. The case is a good example of what can be realized with mesoscale modelling (Fig.5).

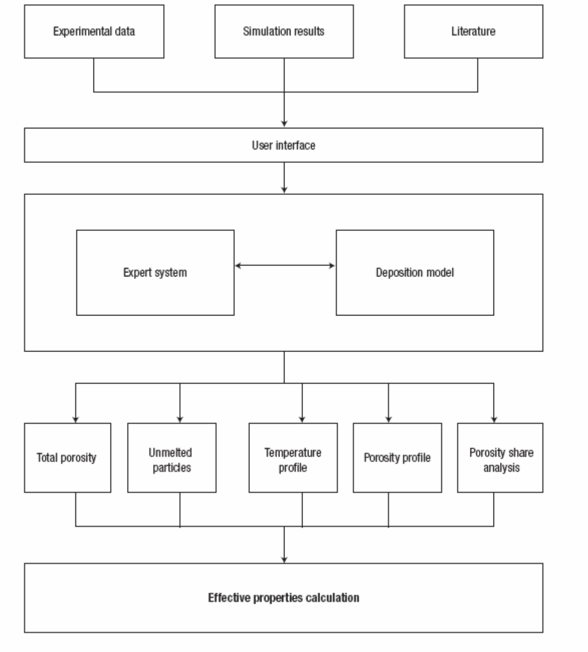

Fig. 5 Plasma-sprayed coatings properties prediction by an expert system

Another example of multiscale feature of a thermal spray process is related to HVOF. The importance of this technololgy is increasing for the aero sector, being also proposed for hard chrome replacement. A schematic representation of multiscale features involved in HVOF coating development is given in Fig. 6: also in this case modelling a proper selection of the length scale to achieve suitable responses for process/materials development and optimization is required due to the multiple involved aspects.

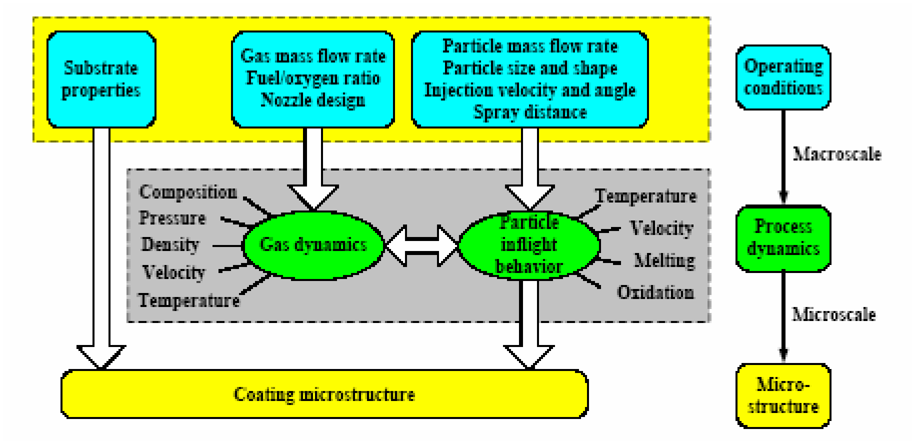

Fig. 6 Multiscale features of an HVOF process

Thus for many properties materials behaviour is controlled by mesostructure: the same applies to surface engineered components and coatings. Simulative and predictive approaches are getting increasing importance, but correct strategies have to be selected to obtain useful information for research and development, guaranteeing proper efficiency and reliability. At the present stage and for practical purposes, the top down approach seems to be the more reliable: a correct choice of the length scale for the various phenomena involved from the process side to the material side is thus essential.

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