Tribology International 72 (2014) 13–30

Contents lists available at ScienceDirect

Tribology International

journal homepage: www.elsevier.com/locate/triboint

Computational modelling based wear resistance analysis of thick composite coatings

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ARTICLE INFO

Article history:
Received 22 October 2013
Received in revised form
27 November 2013
Accepted 1 December 2013
Available online 12 December 2013

Keywords:
Modelling
Wear
Composite coatings

ABSTRACT

A computational modelling and simulation approach was developed and applied for wear resistance analysis of composite coatings. Three new numerical finite element models were developed to include microstructural properties of typical thick thermal spray and laser cladded metal matrix coatings. The first was an ideal synthetic defect free material model, the second an advanced synthetic model containing defects and the third an image based real model. A thermal spray WC-CoCr coating and a laser cladded WC-NiCrBSi coating were characterised and the information obtained of their microstructure and properties was used for computational stress and strain simulations. The simulations were carried out for a set of indentation and scratch test contact conditions. Wear related features were validated empirically by abrasive rubber wheel testing and sliding contact pin-on-disk testing in dry conditions. Features like high local curvature, notches, abnormally large particles, thin ligament or throat-like structures of a specific material phase, clusters of interlinked carbides or high local fraction of a specific material phase had a great impact on the resulting stress state and wear resistance of the coating. The composite structures of the coatings offered a 2 to 50 times lower abrasive wear and more than four orders of magnitude lower sliding wear rate compared to the reference steel surface.

1. Introduction

Wear is taking place at the top surface of products, components and tools. The wear resistance requirements are thus focused especially on the surface properties. Advanced surface engineering offers many possibilities to modify the properties of surfaces to become more wear resistant, e.g. by surface treatments, deposition of thin layers or processing of thick surface coatings [1].

Thin coatings, like physical vapour deposition (PVD) and chemical vapour deposition (CVD) coatings, are excellent in many tribological applications and today largely in use. However, they may be vulnerable especially in harsh, high load and high temperature conditions due to both material and structural limitations originating from their tiny thickness, which is typically in the range of 1–3 μm and even less. The use of thick composite coatings is another solution to tailor surface properties of the component. Typical processing methods for thick coatings are thermal spraying and powder cladding, either as welded overlays or laser fused layers. These methods offer a flexible route to produce unique composite-structured, rather thick coatings, in a typical thickness range of 150 μm–3 mm, on a substrate material selected according to other criteria, like price, extent of alloying elements and other additives, mechanical strength and low weight [2–4].

Over the last decades a myriad of hybrid coating materials suitable for thick coatings – mainly mixtures and composites of ceramics, metals and polymers – has been developed. Entirely new possibilities for developing high-performance materials have, however, opened up in the 2000s, with the development of new manufacturing methods, widespread adoption of nanotechnology, and more in-depth understanding through new process diagnostics and higher modelling capacity [5–8]. Particle-reinforced composite materials consisting of a metal matrix and hard dispersed particles offer a potential solution for increased wear resistance demands. An improvement in wear properties is often counterbalanced by the deterioration of other properties, such as impact resistance or corrosion resistance. It is important to tailor and optimise the material for the particular application, taking all the requirements into consideration [8–10].

Computational modelling and simulation of deformations in a material due to surface loading, and calculations of stress and

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0301-679X/$ - see front matter
http://dx.doi.org/10.1016/j.triboint.2013.12.001

strain in loaded contacts is a research approach that is rapidly developing today. Modelling and simulation of a tribocontact helps to understand the mechanisms that result in plastic deformation, surface cracking, wear particle formation and continuous wear. The numerical simulations can be carried out on various dimensional scale levels, from nano size to macro size, by using software representing the material structure from atomic and even sub-atomic to continuum macro and component level [11–14].

The material modelling and simulation approach has been used in contact mechanics [15] and in fracture mechanics of structures [16]. The same FEM-based approach has successfully been used for improved understanding of the wear process of a sliding contact with one of the surfaces coated by a thin surface coating [1,17–24]. Precise measurements of the elastic and the plastic response of the coating and substrate system, and measurements of the contact geometry made it possible to simulate stress and strain conditions, deformations, to calculate fracture behaviour and to evaluate the wear performance of thin, homogenous, coated surfaces and the effect of influencing material and operational parameters.

Thin hard coatings, such as PDV and CVD deposited coatings, can be modelled as a surface layer system, in which both the coating and the substrate material are considered as homogenous and in which the interaction between the coating and the substrate material, as well as the geometrical characteristics, are crucial for the wear behaviour [1,19].

Thick composite coatings, such as the thermal spray and laser cladded coatings, need to be modelled in terms of their complex composite microstructure, including grains, pores, cracks and various phases in the matrix, in order to achieve representative stress and deformation simulations that correlate with the real situations. Composite surface structures of materials such as cast iron, WC-Ni alloys, metal matrix composites and PVD nano-composites have been modelled mainly with the two-dimensional (2D) finite element method (FEM) and with analytical models [25–29]. Microstructural models are more precise representations of the material microstructure and they have been developed based on three-dimensional (3D) FEM modelling for e.g. polycrystalline, SiC–Al alloy and Ti6Al4V alloy surfaces [30–34].

Microstructural models developed for representing real materials have been generated by numerical techniques based on image analysis of cross section images obtained by scanning electron microscopy (SEM) or light optical microscopy (LOM) [35,36,13]. A 3D microstructural representation can be generated in a similar way, but by taking microscopy images of several layers below the surface. Wiederkehr et al. [37] took LOM images from 15 parallel cross sections below the surface, exposed by polishing, with an average inter-distance of 4 μm, and they used an FEM based image morphing method for producing a 3D microstructural material model of a thermal spray surface with pores and cracks.

The modelling of the wear process, in which material is detached from the contact surfaces and interacts in the dynamic triboprocess between the two moving surfaces, needs other kinds of modelling techniques, such as the movable cellular automata (MCA) methods used by Österle et al. [38]. Additionally finite elements can be applied by considering cracking mechanisms like in the work by Mohd Tobi et al. [39] when applied to thick coatings, or by considering material abrasion, like in the work by Anwar et al. [40]. Discrete methods overall provide several advantages for the modelling of material failure and removal processes, as has been demonstrated in the peridynamics approach by Seleson et al. [41].

Both 2D and 3D microstructure modelling and simulation methods have been demonstrated for characterising the mechanical properties of alumina, metallic FeCrBSi and TiC/Cu coatings with pores and cracks [37,42,43]. Based on empirical experience, it is known that size, shape and spatial arrangement and orientation of pores and cracks have a strong influence on the material properties of thermal spray coatings [2,4]. Since the pores can add material flexibility and stop crack growth, the porosity is not always detrimental. Other microstructural material parameters that need to be optimised in a composite coating for a favourable tribological surface behaviour, in addition to the pore-related parameters, are the size, shape, density and spacing of the reinforced particles, the interfacial bond strength and the binder mechanical properties [27,29,33].

Modelling the response of thick composite coatings and their behaviour, including explicitly their microstructure, falls within the scope of mesoscopic analysis methods. In the current context, the most stringent additional requirement set to the modelling methods is the need to treat the weak and strong discontinuities of the coating microstructure, which can be performed by incorporating suitable tailored finite elements and extended finite element methods. Finite element methods with properly developed meshing strategies can be applied for microstructure modelling, but strong discontinuities and their evolution within the microstructure commonly require a more refined approach, such as extended finite element methods.

The aim with this article is to present how computational FEM models can be developed for the purpose of estimating wear resistance of composite thick coatings. The developed models are used for stress and strain simulations of thermal spray WC-CoCr and laser cladding WC-NiCrBSi coatings. The wear resistance analysis is based on microlevel finite element modelling as well as empirical indentation testing, scratch testing, rubber wheel abrasion testing and pin-on-disk tribotesting for model validation.

2. Methodology

In this computational modelling and simulation study we use the so called PSPP (processing–structure–properties–performance) approach modified after Olsson [11] and illustrated in Fig. 1. The following three links need to be modelled to achieve a holistic model for the wear performance of a surface:

(1) the interaction between the wear process and the material properties of the surface,
(2) the interactions between the material properties and the microstructure, and
(3) the interactions between and the microstructure and the surface manufacturing process.

It is often too complex to build a computational model covering the whole PSPP range with today's knowledge. Thus is it more adequate to use a step by step modelling strategy. We have previously demonstrated how the properties can be linked by FEM modelling to wear performance for tribological contacts with

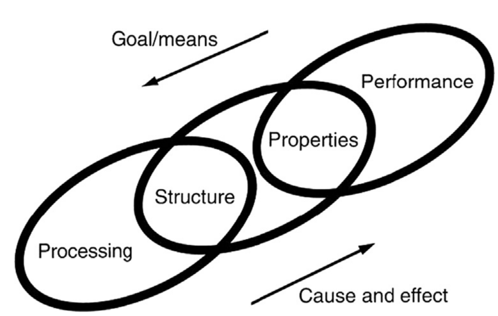

Fig. 1. The PSPP approach links tribological design performance criteria to surface properties, microstructure and coating processing.