COMPUTER MODELLING AND SIMULATION APPROACH TO DEVELOPING WEAR RESISTANT MATERIALS

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EXECUTIVE SUMMARY

VTT researchers have been pioneers in international science with their computer modelling and simulation techniques for the development of coated surfaces with superior wear resistance and low friction properties. They have introduced a novel PPSP (Performance-Properties-Structure-Processing) multi-scale concept that is based on linking wear and friction performance by micro-FEM computer models to mechanical surface properties, surface microstructure and coating processing parameters. The modelling methods have been applied on 1–5 μm thick hard coatings, such as TiN, DLC and MoS_2, on steel as well as on about 200 μm thick thermally sprayed WC-CoCr coatings developed through a Process Mapping concept. The novel approach offers completely new possibilities of systematic and focused material development of wear resistant and low friction coated surfaces with the aim to control and prolong the lifetime of machine components and industrial tools.

INTRODUCTION

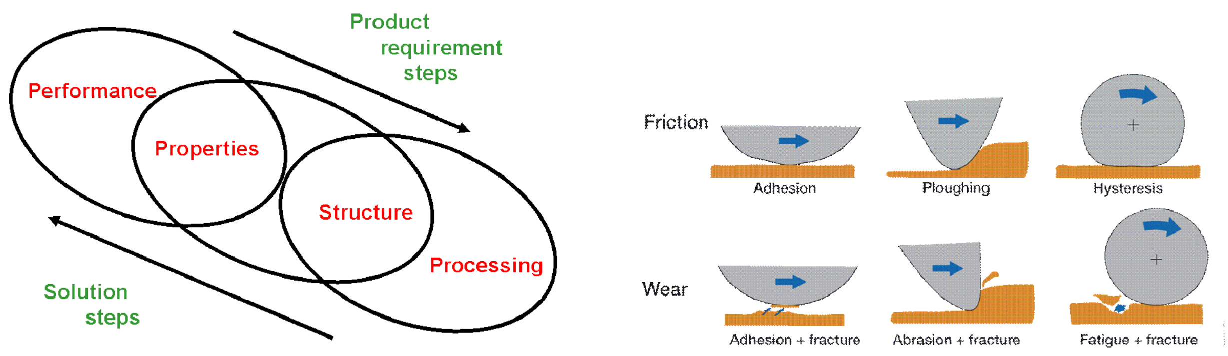
Wear is a major issue in our modern society since about 30–50% of the industrial production in industrialised countries is used to replace worn out products. Wear of products and components results in high maintenances costs, interruption in production, unpredicted break down that may cause human safety risks, high energy consumption and environmental pollution. Very commonly people are used to wear – it has always been there – and if a product is worn out it is just replaced without thinking that there are possibilities to influence wear. The rapid recent technological and scientific development has brought many new tools and techniques that make it possible to develop new materials and new constructions that can radically reduce and sometimes even eliminate wear.

Wear is defined as the process of continuous material removal from a surface due to the loading from a contacting moving substance or substances. Wear is a part of the field of science and technology named tribology, which includes topics related to wear, friction and lubrication. It has been difficult to study the wear process because it occurs at the interface between interacting bodies and is thus usually hidden from investigators by the wearing components. It becomes visible in malfunctions and on the damaged surfaces of worn parts when they are replaced. Traditionally, the wear processes have been investigated mainly experimentally by a large variety of wear testing devices and with a trial-and-error approach. There is typically a large scatter in wear test results reported today due to the large number of influencing parameters, including material, design, input energy and environmental parameters, and also due to the difficulty to control the testing conditions well. The results may be conflicting and are often difficult to analyse and interpret.

A NOVEL PPSP METHOD

VTT has taken a pioneering role in developing a novel concept for the development of wear resistant materials. The novel PPSP method (Performance-Properties-Structure-Processing) is a systematic approach starting from product lifetime and reliability requirements, transferred to requirements in terms of wear performance. The wear rate of the defined contact system is directly influenced by the material properties of the surfaces which are determined by the microstructure of the materials. The microstructure again is a result of the material processing which includes a large variety of influencing parameters (Figure 1a).

A better understanding of the links from material processing to surface microstructure, from microstructure to surface properties and from the properties to wear performance opens completely new possibilities to optimised surface design and to tailor surfaces for specific low wear applications. Each tailored product surface is related to the estimated prevailing wearing conditions that might include adhesive, abrasive, fatigue and chemical wear or a combination of these (Figure 1b).



a) b)

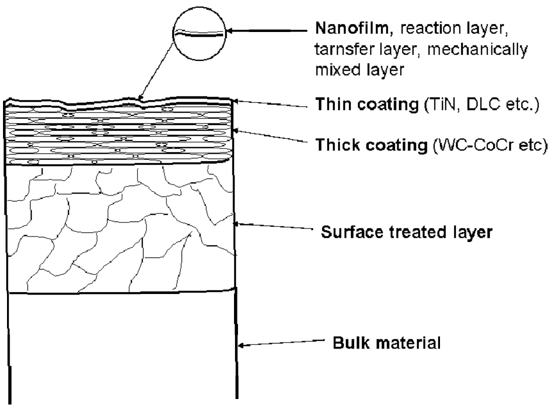
Figure 1. The required lifetime defines the required wear performance, the material properties, the microstructure at the surface and the surface processing methods that are linked to each other by interactions to be modelled (a). A tribological contact analysis defines the dominating wear and friction mechanisms for the chosen application (b).

The choice of different surface designs may include bulk surfaces with optimised microstructure, thick lamellar coatings, thin surface films with, e.g., nanocomposite, multilayer, gradient or lattice structures (Figure 2a).

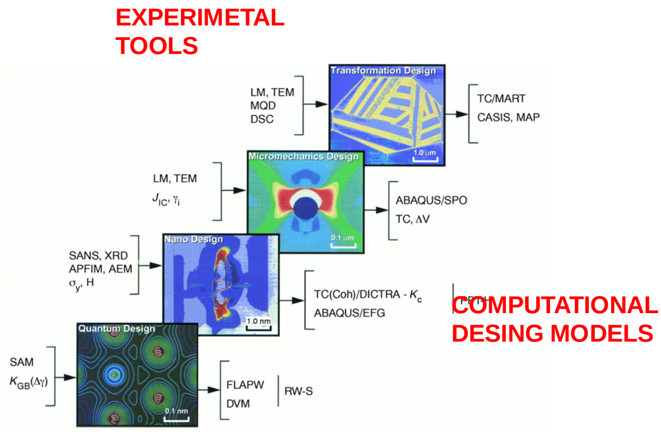
COMPUTER SIMULATION ASSISTED DEVELOPMENT

Wear testing is today not the only way to increase our knowledge of prevailing wear mechanisms. The rapidly increasing computer capacity, the new material modelling tools and the improved micro- and nanolevel characterisation techniques makes it possible to perform computer simulations where the stresses, strains and deformations are calculated for a defined contact with defined surface properties. The calculated loading conditions can then be compared with the strength of the material and the risk for deformation, cracking, fracture and wear can be estimated. The simulations show the interaction between the different influencing parameters and help to find the dominating parameters to be optimised.

Depending on the studied contact conditions the modelling and simulation may be relevant to perform either on macro-, micro- or nanolevel (Figure 2b, Olsson, 1997; Holmberg et al., 2007). The advantage with the holistic modelling and simulation approach is that it supports a logical fundamental understanding of the influencing parameters and the effect of different parameters can be precisely calculated without any problem of scatter and repeatability.



a)



b)

Figure 2. A variety of different surface modification techniques are available for the optimal tailored surface solution that may be a simple or a more complicated surface design including various material structures (a). Computational surface design models are developed at different scale levels and verified by experimental tools (b).

The computer modelling and simulation approach is believed to be the future route to better understand and control the wear process. It is supported by the rapid development of the last few decades, which has brought about several new techniques and possibilities, such as:

- the continuous increase in computer capacity makes it possible to run very complex material models and simulations and get results out in a reasonable time frame,
- new computer modelling and simulation tools have been developed that make it possible to model the surface material response to loading in a wear situation and to simulate the generated stresses, strains and deformations that form the conditions for crack initiation and crack growth with wear particle detachment as result; such tools are:

1) continuum methods (1 μm - 1m): FEM (Finite Element Method),
2) meso-, damage and fracture mechanics (1 - 100 μm): FEM, EFG (Element Free Methods), X-FEM (Extended FEM),
3) dislocation dynamics (100 nm-100 μm): FEM, DDD (Discrete Dislocation Dynamics), and CDD (Continuum Dislocation Dynamics),
4) molecular dynamics (0.1nm - 1 μm): MDS (Moleculra Dynamic Simulation), and

5) first principles methods (0.1 - 10 nm): DFT(Density Functional Theory),

- there is an increasing understanding of the fundamental wear mechanisms that result in material removal from the surface and the interactions related to the macrolevel as well as microlevel, and now also to some extent, the nanolevel, and
- new material characterisation techniques give the possibility to characterise the surface properties and their changes at the surface and very close under the surface with great precision; such techniques are, e.g., SEM and TEM (Scanning and Transmission Electron Microscopy), Raman Spectroscopy, SIMS (Secondary Ion Mass Spectrometry), AES (Auger Electron Spectroscopy), AFM (Atomic Force Microscopy), nanoindentation, etc.

Figure 1a shows that the following three links are needed to be modelled for a holistic modelling of the wear performance of a surface:

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

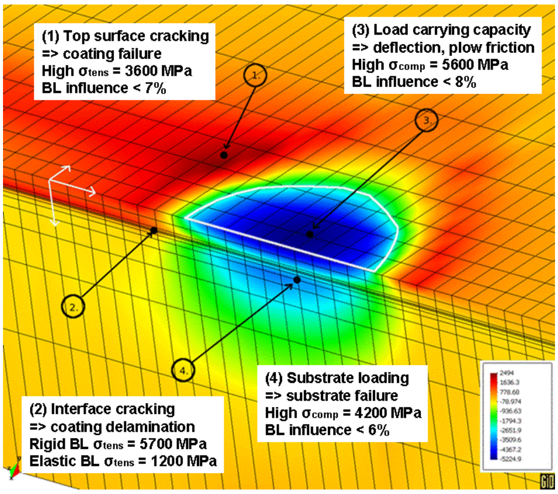
The modelling and simulation approach has been used in contact mechanics (Wriggers, 2002) and in fracture mechanics of structures (Andersson, 2004). The same FEM-based approach has successfully been used for improved understanding of the wear process of a sliding contact with one of the surfaces coated by a thin surface coating (Gong and Komvopoulos, 2004a,b; Holmberg et al., 2003, 2007; Holmberg and Mathews, 1994, 2009). Precise measurements of the elastic (elastic modulus), plastic (yield strength) properties at and close under the surface and the contact geometry made it possible to simulate stress and strain conditions, deformations and calculate fracture behavior and evaluate the wear performance of the coated surface and the effect of influencing parameters.

The modelling approach is fairly laborious and requires a good fundamental understanding but when a good model has been developed the information is very generic and can be used for different applications. A requirement is always that the validity of the model must be tested by comparing the results with some suitable empirical test.

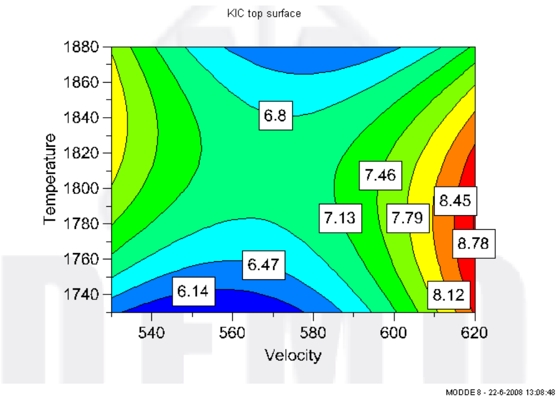
RESULTS

This approach has successfully been used by VTT researchers that have modelled the link from surface material mechanical properties to the surface fracture and wear performance for steel surfaces covered by a thin, 1-5 μm thick, hard ceramic titanium nitride coating (TiN), diamond-like carbon coating (DLC) and molybdenum disulphide coating (MoS_2). In experimental studies these coatings have excellent wear resistance and low friction properties. The stresses, strains and deformations in a loaded contact were simulated. The crack initiation effects and the crack growth mechanisms were studied and the fracture toughness of the surfaces was calculated. The influence of coating hardness, coating elasticity, coating thickness, bond layer thickness and Youngs modulus between coating and substrate, as well as residual stresses have been reported (Holmber et al., 2003, 2007). Figure 3 shows the dominating effects of bond layer parameters on surface first principal stresses in a 2 μm thick coating on a steel surface with a rigid 500 nm thick bond layer between the coating and the substrate.

VTT researchers have developed a Process Mapping concept (Turunen, 2005; Turunen et al., 2005, 2006) that links the processing parameters to surface microstructure and residual stress and further to material properties in thermal sprayed coatings. With this systematic approach a complex multi-variable thermal spray process has been simplified and logical cause and effect interactions demonstrated. This is an important step for introduction of the thermal spray process into the PPSP-method.



a)



b)

Figure 3. First principal stresses resulting in cracking and wear initiation on top surface and at a depth section in the symmetry plane of sliding when a diamond ball is sliding on a 2 μm thick TiN coating on steel with a 500 nm thick rigid bond layer. The major failure mechanisms and the influencing parameters are indicated (a). Variation in fracture toughness of a WC-CoCr coating in the T-v plot obtained from thermal spraying Process Mapping (b).

CONCLUSIONS

The new PPSP (Performance - Properties - Structure - Processing) method is a holistic and systematic approach to developing wear resistant and low friction materials. It opens possibilities to find new material solutions for energy efficient and well controlled machinesproduction tools and consumer products. VTT has successfully used this technique for optimising the surface properties of very thin and hard TiN, DLC and MoS_2 coatings and somewhat thicker WC-CoCr thermally sprayed coated surfaces.

ACKNOWLEDGEMENTS

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