New concepts for micro-structural simulations of coating-substrate-systems

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Abstract

The stability of coating-substrate-systems influence the chip formation and also the surface integrity of the new generated workpiece surface. Using FE simulation, deformations, strains and stresses in coated tools caused by external and internal loads can be computed on a microscopic scale. Since both, the whole macroscopic tool (in mm scale) and the microscopic coating layers (in µm scale) must be included in the same geometrical simulation model, graded high-resolution FE meshes must be used. Nevertheless, the number of nodes in the 3-D computational FE grid reaches some millions, leading to large computational time and storage requirements. For this reason, multi-processor hardware and parallel working software have been developed and used for the computation.

Four levels of length scales considered in the proposed multiscale modelling approach for multilayered surface systems will be discussed and the first set results of simulations for coating-substrate-systems will be presented.

1. INTRODUCTION

Coating technology gains growing importance in industrial applications [1]. Besides the well-established monolayer coatings, multilayer and gradient coatings are increasingly applied. Over the years, manufacturers of coated cutting inserts have gained a lot of experience and knowledge about coating technology and well-suited material combinations for specific industrial applications. However, they do not yet integrate simulation methods for investigating the mechanical properties of their coatings [2]. Coating optimisation is still mostly achieved by means of "more or less inspired" trial and error approaches. The development of new coating systems, especially for new advanced machining technologies, requires a series of expensive experiments, in which the suitability of the coated cutting insert for the technological process, its resistance against mechanical and thermal loads and the adhesion between the different materials must be investigated. To achieve further progress in the development of new coating-substrate systems, it is desirable to combine this experimental dominated developing process with numerical simulations.

The stability of coating systems at various substrate surfaces under operating conditions crucially depends on the adhesion forces and on the stress distribution in a surrounding of the material interfaces. The stress distribution, determined by the macroscopic mechanical loads, the clamping boundary conditions and the thermal influences, can be analysed by FE simulations with a microscopic spatial resolution. Stresses inside the coating layers and in a surrounding of the material interfaces become available this way. Thus, this approach can support developing engineers in the design of new coating-substrate systems for industrial applications and in adopting newly developed layer systems for niche applications.

Since the coatings' thickness, typically a few µm, is very small compared to the measure of the mm-sized cutting inserts, these computations must be performed on highly graded meshes, to capture the whole insert's geometry and the boundary conditions, acting in this scale, as well as of the microscopic coatings and it's material properties [3]. Three dimensional models must be used for these simulations for a proper reflection of boundary conditions and of the cutting insert's shape. Even when the mesh density is nearly optimal adapted to the mentioned items and to the accuracy requirements, the number of nodes in the 3D finite element mesh and therefore the computational effort and the storage requirements are extremely large. This demands for advanced storage technologies for the FE matrices and vectors as well as for powerful solvers for the FE equation systems. To solve the high computational expense and the large storage requirements of those computations, a parallel operating FEM software is used, which is suitable for parallel computer systems with an arbitrary number of processors, and multiprocessor hardware, since on parallel computers the runtime may be considerably reduced and the available storage is substantially enlarged. A variety of coating-substrate systems were analysed with this software on our LINUX-PC cluster, consisting of 8 processors [4,5].

On the other hand, crystal plasticity theories have been developed and used for predicting the mechanical response of crystal materials and for modelling micro-forming processes. The identification of physical and mechanical properties of nano- and micro- coatings is based on the use of instrumented-indentation loading and unloading curves. To enable the mechanical properties of a coating to be uniquely determined, multi indentation loading and unloading curves, obtained from the indenters with different included angles, are used. All these techniques are based on the continuum mechanics theory, which is not suitable for individual and multilayer coatings. For micro-coatings, if the ratio of coating thickness to grain size is small (say <7), then it is necessary to use crystal plasticity theory. For the same case, if the indentation area does not cover a sufficient number of grains, the continuum-mechanics theory also breaks down. For micro coatings, this is always the case as research evidence also shows that grain boundaries have different mechanical properties from grains. Furthermore, limited research has been carried out to identify mechanical properties of the interface of coating layers, either with sharp or blurred interfaces. As the thickness of coatings reduces to the nanometer scale, molecular dynamics theory is needed to determine the mechanical properties of coatings and interfaces accurately.

2. PRELIMINARY INVESTIGATIONS

Coated cutting inserts under operating conditions are stressed by external forces and thermal loads, and the layer system's stability is additionally influenced by other features like residual stresses or cracks. The process forces acting on the coated insert's surface and the clamping principle are included in the model as boundary conditions for the mechanical field problem.

2.1 Technical problem

The main goal of new coatings for cutting inserts is to increase the lifetime of the cutting tool. Using new self lubricant final coating structures (MOST), the tool life for dry manufacturing can be increased. For the cutting tests turning and milling operations are used. The turning conditions are: Workpiece material: 34CrNiMo6 (21-25HRC); v_c=250/min; f=0,315mm/rev, a_p=2,5mm; Standard cutting inserts SNMA120408 (TiN-TiCN-Al_2O_3-ZrCN) and SNUN150412 (TiN-TiCN-TiN) and 6° negative rake angle. For the face milling operations the following conditions has been used: Workpiece material: GGG-60; v_c=145m/min; f_z=630mm/min, a_p=4mm; Standard cutting inserts TN5515 for finish milling and TN5520 for rough milling. The wear tests give the following results [6].

The chemical and material properties of the self lubricating hard coatings (MoS_2/metal composite coating) are given in [7]. The following different coatings have been compared for their advantages and disadvantages:

TiN, TiCN, Cr - less efficient wear protection due to high friction coefficient.

DLC - low application due to problems with hardness and brittle and low adhesion levelness.

Me-CH (Me= Ti, W, Cr …) – less hard, less brittle, low friction (μ=0,15) – but no self lubrication

MOST – self lubricant; very low friction coefficient (0,04<μ<0,12); higher hardness > low wear rate.

Using these coatings, the total cutting length was increased up to 11.700 m - 130 days manufacturing with the same cutting inserts [8].

2.2 Simulation of Chip Formation

To investigate the external loading at the cutting edge – the chip formation process was cal-

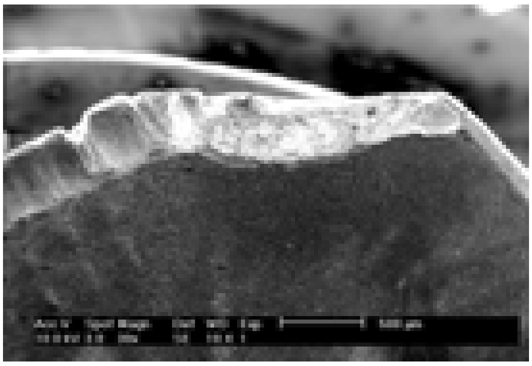


Fig. 1a: Without a MoST coating at the top

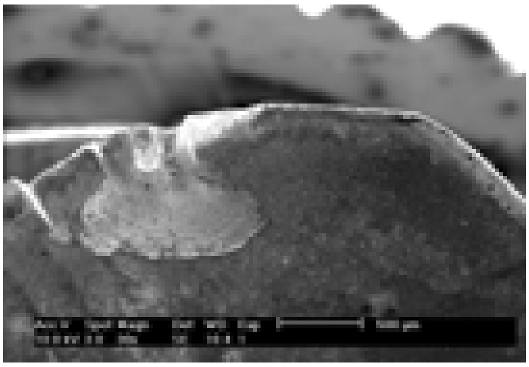


Fig. 1b: With a low MoST coating at the top

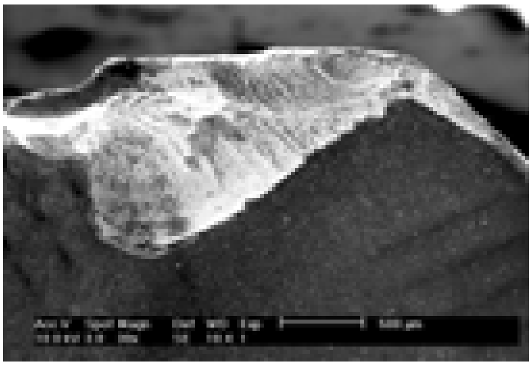


Fig. 1c: With a high MoST coating at the top

Fig. 1: Comparison of worn surfaces of milling inserts dependent on the MoST coating.

Fig. 2: Milling tool

culated by a Finite Element Program [9]. Based on the experimental investigation, dry cutting simulations are carried out, the process parameters are fitted to the same and the influence of different coatings are investigated. The chip formation process is non-stationary, as presented with Figure 3.

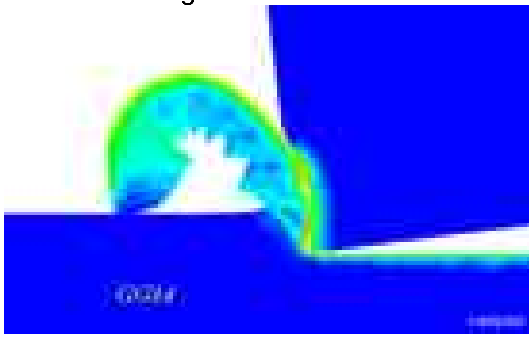


Fig. 3: Non-stationary chip formation

The computational results are compared with the High-Speed Camera investigation carried out in IWF [10] shown in Fig. 4.

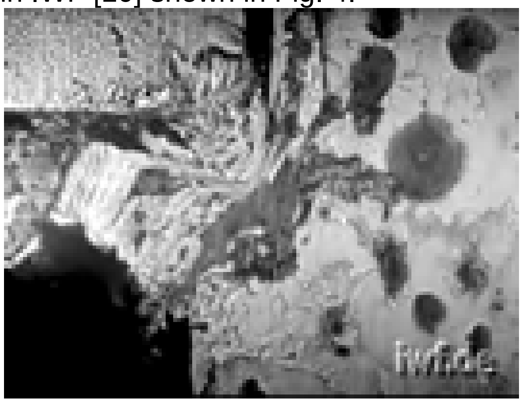


Fig. 4: High-Speed-Camera image for GGG-60

The forces acting at the cutting tool and its coating are also non stationary.

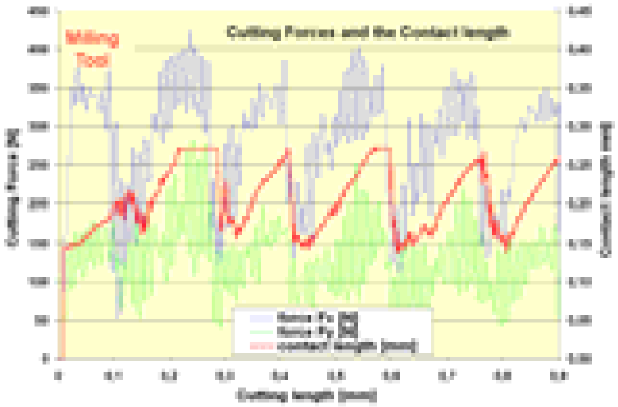


Fig. 5: Cutting forces and contact length

2.3 Determination of Coating Properties

Besides the Poisson´s ration, the Young's modulus is, the basic parameter for the description of the elastic behavior of isotropic materials and therefore is very important for modeling. But the result of indentation experiments often differs from modulus values measured by other methods. Therefore in the recent draft of an international measuring standard [11] the term indentation modulus is used. It should be pointed out that there is no physical reason in contact mechanics that may explain why it should not be possible to obtain correct values for the Young's modulus from indentation experiments. For layered materials the situation is more complicated. The measurable effective modulus is always influenced by the elastic properties of the substrate. Moreover, a one tenth-rule as in the case of hardness (the indentation depth should be less than one 10^{th} of the film thickness to measure pure film properties) is difficult to apply for modulus measurements. Some evaluations of this effect are given in [12]. The modulus result for the compound depends on the film to substrate modulus ratio and the ratio of contact radius to film thickness. An example of a standard investigation is given in Fig. 6.

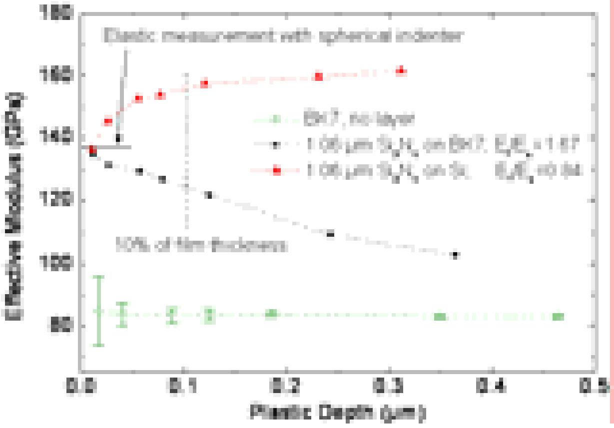


Fig.: 6: Depth dependent effective modulus of 1.06 µm thick Si_3N_4 coatings on BK7 glass and Si, measured with a Berkovich indenter [13]

A 1.06 µm thick Si_3N_4 film was deposited with a PACVD process on silicon and BK7 borosilicate glass as substrates. The measurements were carried out with a conventional Berkovich indenter in the load range between 0.3 mN and 50 mN. The Young´s modulus was determined according to [11] but using a radial displacement correction and a variable ε-factor as additional corrections. Young's modulus and Poisson's ratio of the BK7 are 82 GPa and 0.21, respectively. For a single crystal an average of Young´s modulus over the different crystal orientations has to be used for indentation experiments. The corresponding values were E = 163 GPa and ν = 0.223 for our single crystal silicon substrates. In the case of hard coatings the film modulus is often 100 % higher than that of the substrate, which would give a rise to a much sharper modulus change. Therefore it is nearly impossible to measure the correct modulus of films with a thickness less than 1µm with a Berkovich indenter via plastic indentations.

Wholly elastic measurements with a spherical indenter can overcome this limit because they allow a complete separation of the film modulus from the substrate. The principle was already explained in [12]. Measurements were carried out on the same samples with a spherical indenter of about 50 µm radius and a maximum load of 50 mN. Loading and unloading curves agree better than 1 nm and can not be distinguished. In the next step the film modulus is determined by a fit with the help of the software package Elastica [14], assuming a Hertzian pressure distribution on a coated halfspace. The accuracy of the modulus determination is better if the modulus difference between film and substrate is larger and the indenter radius is smaller. In the case of hard carbon coatings on Si the measuring of the Young's modulus of very thin films with a thickness between 110 nm and 25 nm using a 4 µm radius indenter was successful.

The yield strength is the main parameter for the characterization of plastic behavior. It determines the load carrying capacity of materials. For massive samples it can be obtained from tensile tests but for thin films a standard measurement method does not exist and it is very difficult to obtain accurate values. A new method developed by [14] is illustrated in fig. 5 with a 2.1µm thick DLC coating on M2 tool steel as an example. Using the UMIS 2000 nanoindenter the deviation of the two curves can be detected with an accuracy of about 1 nm. Plastic deformation during indentation was theoretically analyzed using the von Mises comparison stress.

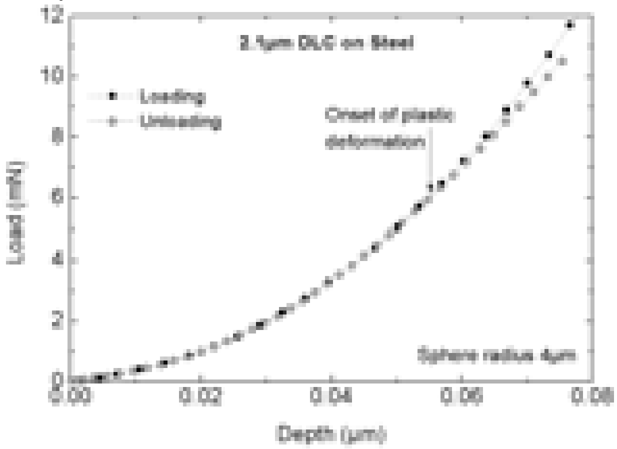


Fig. 7: Cyclic load-unload curve for a 2.1 µm thick DLC coating on steel

By means of the von Mises stress a complicated multiaxial stress state can be can be related to the uniaxial tensile test.

Using the method of image loads mentioned in [15] all stress components and from them the von Mises stress can be calculated in three dimensions within films and substrate. For the analysis of spherical indentation experiments, however, knowledge of the von Mises stress along the axis of symmetry is usually sufficient. In Fig. 8 this is shown for film and substrate of Fig. 5 for that particular indentation state where plastic deformation starts, i. e. for a load of 19 mN.

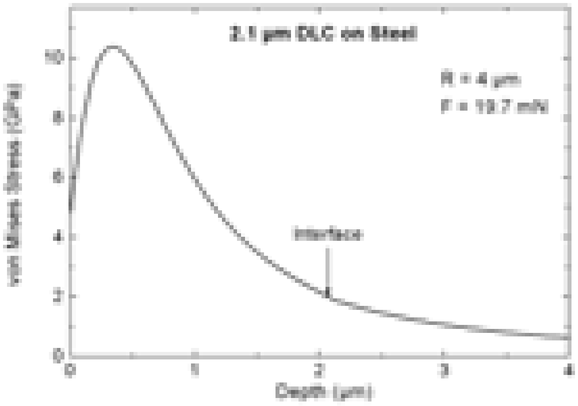


Fig. 8: Von Mises comparison stress along the depth axis for the sample of fig. 5.

The maximum von Mises stress in the substrate is located directly at the interface and it is lower than the known yield stress of 3.2 GPa of the steel substrate.

We can finalize, that at this moment most of the investigation are using homogeneous and isotropic material, which is not in conformity with the coating structure.

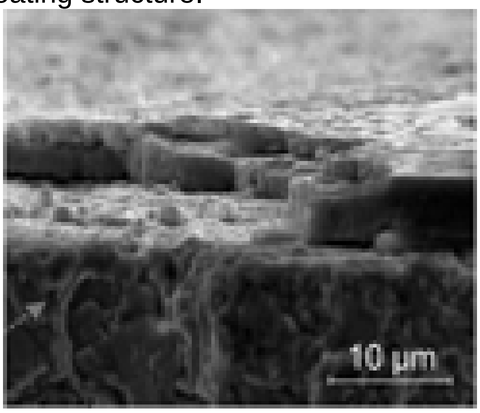


Fig. 9: (Ti,Al)N-VN - Superlattice-Coating [16]

3. CRACK INITIATION IN COATINGS

Fracture in materials and several components of high technology engineering displays one of the central problems in modern strength analyzes. Today, fracture mechanics forms an autonomous research area of solid mechanics in order to explain phenomena of fracture, fatigue, and strength of materials for development of materials which are better failure-

Fig. 10: Interfacial structure of multilayer coatings [17]

resistant than the conventional materials and to develop design methods that are better failure-safe than the conventional ones. Although, the entire fracture mechanics approaches cannot altogether be ascribed to crack type problems, the consideration and examination of the essential conditions leading to crack propagation, crack detection and crack arrest is of highly practical and theoretical interests. Generally, analytical solutions for most of these crack problems in finite body domains are not attainable. Thus, numerical techniques for strength analysis of cracked structures subjected to various kinds of loads have been developed.

Three well known numerical methods having the ability to solve crack propagation boundary value problems for finite body domains can be mentioned:

- the Finite Element Method,
- the Boundary Element Method,
- the Meshless Galerkin Method

The Finite Element Method (FEM) is used to solve crack and crack propagation problems for over 30 years. On the one hand, one can find nowadays a big number of publications concerning even dynamic crack growth as can be seen from a lot of papers [18] and the references therein as well as from the reviews [19]. An overview to the advantages and disadvantages of these methods are given in [20]. In this paper, the authors focused on efficient solution techniques for the numerical simulation of crack propagation in 2D linear elastic formulations based on FEM together with the conjugate gradient method (PCGM) solving the corresponding linear equation systems. Thus, one gets the possibility to simulate crack advance in a very effective numerical manner including adaptive mesh refinement and mesh coarsening.

One test example (Figure 11) represents the crack propagation simulation of a symmetrically loaded tension specimen (KIc=450MPa $\sqrt{mm}$, scale =2:5mm, E=2 10^5MPa, $\nu = 0.3$).

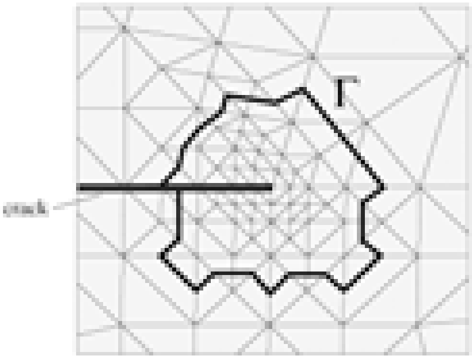


Fig. 11: Crack simulation with PCGM [20]

The given load induces the crack propagation immediately and the crack propagates continuously up to its arrest. The results are comparable with crack initiation [21] due to indentation (Fig. 12).

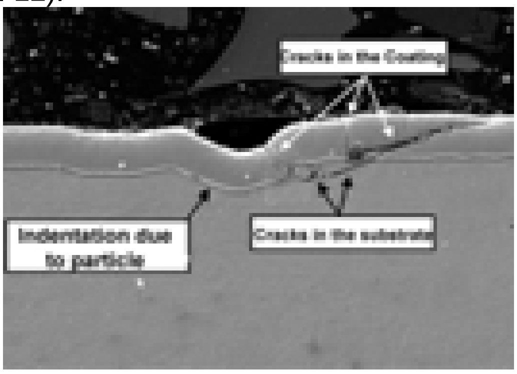


Fig. 12: Cracks in an coating-substrate-system

3.1 Theoretical Models for Indentation

To investigate the material behaviour of coatings, different methods can be used. From the experimental point of view, nanoindentation [22] is the most commonly used method. In addition, there are a lot of theoretical papers dealing with the principles of indentation in thin films [23-25]. Schwarzer developed an analytical model – but in some cases the surfaces of the coating-substrate-systems are not plane, so numerical methods are most commonly used.
With conventional FE - simulation methods, the stress-strain-state in the coating up to the substrate can be calculated [26].

3.2 Numerical Models of Coating-Substrate-Systems

Normally in cutting tool simulation, the boundary conditions for the fixing points of the cutting insert are far away from the mechanical-thermal loading at the rake face. So, from the mathematical point of view this is a big dimensional problem. To realize a fine grading mesh in the coating and coursing up to the boundary conditions – the total amount of elements are rising up to few milling.
To get enough computing power, a parallel software tool for coating-substrate-simulation is

Fig. 13: Indentation – Principle (Brinell)

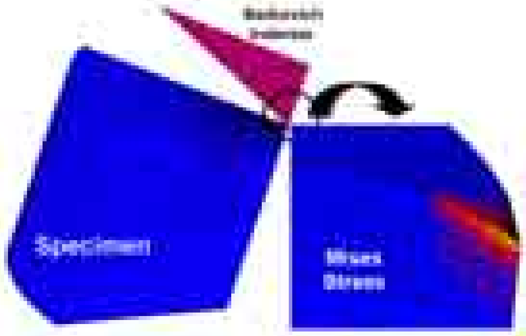


Fig. 14: FE model for Berkovich Indentation

developed and applied on different systems [4]. The computational time can be decreased theoretically up to 4 times by using 8 processors compared with a single one (Fig. 15)

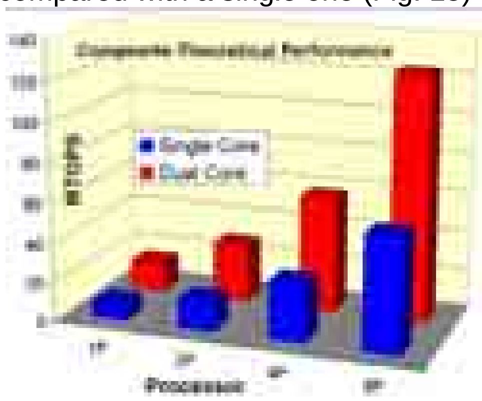


Fig. 15: AMD Opteron™ x86-64 Server Benchmarks [27]

The coating-substrate simulation is a typical two - scales problem with a geometrical model measured in millimetres and boundary conditions applied in this scale, and with material properties changing in a µm- or nm-scale and a corresponding spatial resolution of the computational results. Two geometrical models of cutting inserts shown in Fig. 16 had been selected to be subject of the performed simulation computations. Since the main interest of the stress analysis is aimed at the stress distributions within the coating layers, the stresses σ_{xx}, σ_{yy}, σ_{zz} are calculated over intersecting planes z=constant in a surrounding of the contact area.

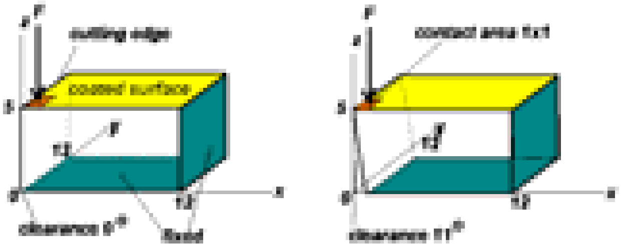
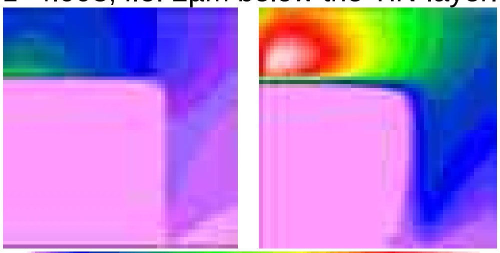


Fig. 16: Typically cutting insert

These planes were placed in the middle of each material layer and in the substrate at z=4.998, i.e. 2µm below the TiN-layer.



0 1890 MPa

Fig. 17: σ_{yy} below the contact area

The different coating-substrate-structures investigated within this research are given in Figure 18. Compared with the cutting tests (discussed in1.1), the L5 structure was selected. The structure of the calculated stress-strain field near the tool tip of the cutting insert is comparable with the wear tests.

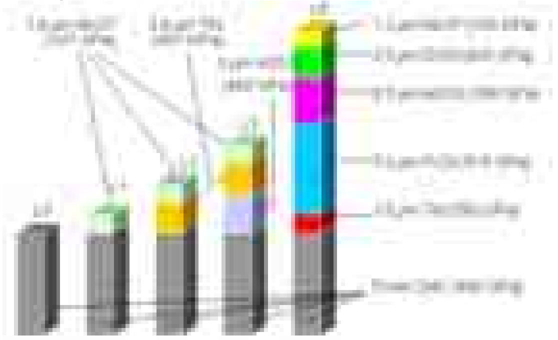


Fig. 18: Five different coating-substrates

Coating optimisation for specific applications can be performed by computing and analysing the stress situation with varying layer thickness and/or layer sequences to find out the best stress situation.

4 FUTURE TRENDS

Looking in to the coating-substrate-structure (Fig.:19), so homogeneous and isotropic material behavior can not be used further more for detailed investigations. There are some new trends to investigate such systems based on a multi-scale approach. A typically 4 stages multilayer coating -substrate-system is in an

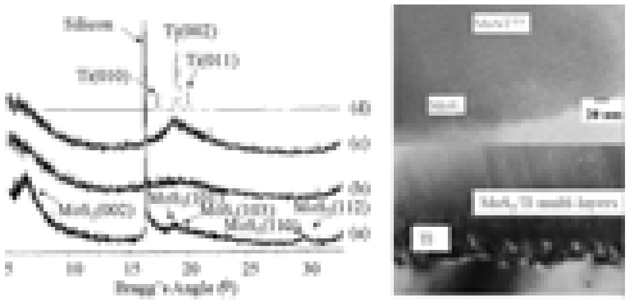


Fig. 19: X-ray diffraction pattern (a:pure MoS_2, b:pure MoST, c:MoS2 + titanium multilayer, d: pure titanium) [28]

ongoing investigation right now .

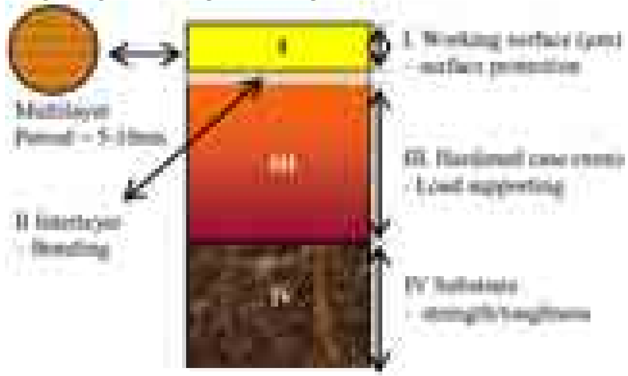


Fig. 20: A typically multilayered surface system

The presentation will used to discuss in detail the comparable methods: micro structured fe-method, molecular dynamics, ab-inito-simulation and methods to close the gap between this four layers.

SUMMARY

The ever-increasing demands for a combination of surface properties for components in modern machinery have further led to the development of multilayered surface systems. Analytical and numerical methods can be applied for homogeneous, isotropic coatings. The challenge lies extending the modeling capability to predict the behaviour of nanoscale multilayered coating. The gap between macroscopically scale and atomistic scale will be closed with current investigations.

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