Modelling of Atomic Structures in Nano-Layers Using the Finite Element Method

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Abstract

Cutting tools for high performance cutting (HPC) processes or for hard-to-cut materials are unthinkable without coatings. For the development of new coatings and for the improvement of known tool coatings the knowledge of the properties of these layers has an immense significance.

The behaviour of the coatings under thermal and mechanical loads can be examined by means of numerical simulation, e.g. using the Finite Element Method (FEM). Thick coatings (measured in microns to millimetres) can be modelled with continuum-mechanical material properties. However, for layers with decreasing layer thickness, the inhomogeneous and anisotropic crystal lattice structures and different material data in the grain boundaries and transition areas play bigger and bigger role.

An increasing importance shows the so-called super-lattice coatings with hundreds of layers each of them having only few nanometres of thickness. Homogeneity or average material properties based on the properties of single layers are not valid in these dimensions any more. Consequently, continuum-mechanical material models cannot be used for modelling the behaviour of nano-layers. Therefore, the interaction potentials between the single atoms must be considered.

A new, so-called Atomic FEM (AFEM) is presented. In the AFEM the inter-atomic bonds are modelled as non-linear spring-and-damper elements. The AFEM is the connection between the molecular dynamics (MD [1]) method and the so-called Crystal Plasticity FEM (CPFEM [2]). The MD simulates the atomic deposition process. The CPFEM considers the behaviour of anisotropic crystals using the continuum-mechanical FEM. The new method can be used to validate in the current

investigations the nano-indenter test results [3]. Using the CPFEM results by means of AFEM the deformation, the crack and dislocation behaviour can be simulated and calculated in the nanometer scale.

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1 Introduction

A large variety of different surface engineering systems (including coatings and surface modifications), with thickness ranging from the nanometer scale to the millimetre scale, have been developed during the last decades to combat surface related degradation such as wear, corrosion, oxidation and fatigue. However, a single coating or surface modification cannot meet the requirements of combined properties such as high resistance to wear and oxidation, low friction values and high bearing load capacity. This has led to the development of duplex or multilayered surface systems by combining hard, stable and/or low friction surface coatings on a deep-case hardened diffusion zone. A graded interlayer is often used to enhance the bonding between the surface coating layers and the diffusion case hardened material beneath. Cutting tools with superlattice layers have also been developed for high-speed and/or dry machining as well as for micro machining [4, 5]. Nano-scale multilayer coatings represent a new class of coating material with high mechanical properties including high hardness (3000-5000HV), higher shear strength and fracture toughness, and hence excellent wear resistance. A typical multilayer surface system for cutting tools is shown in figure 1.

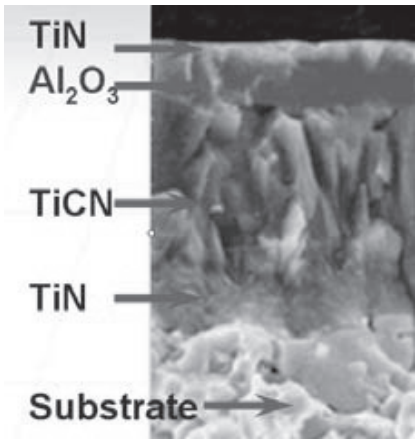

Figure 1: *Typical multilayer surface system of cutting tool coatings [2]*

Although the attempts have been made during the past two decades to design multilayered surface systems based on modelling and simulation, there is no applicable model available today. The aforementioned multilayered surface systems were developed mainly by using empirical methods. The design and optimisation of nano-multilayers require reliable predictive models based on an in-depth understanding of the correlation between material structure and properties from the micro-scale down to the nano-scale.

It is not appropriate to apply a single model to multilayered coatings by simply changing the thickness of individual layers. The potential of multiscale, multilayered surface systems cannot be fully realised until novel multiscale modelling techniques are developed by integrating atomic modelling of surface engineering processes and lattice-/micro-structures, nano-mechanics, micro-mechanics and continuum mechanics modelling (e.g. contact mechanics modelling).

2 State of research (Molecular Dynamics simulations)

Recently, atomic-level computer simulation methods, based on the Molecular Dynamics (MD) techniques have been developed, which makes it possible to simulate the deposition process, the microstructure of thin coatings, the atomic structure and interface of nano-scale multilayers.

Figure 2 shows the result files of MD simulating the Ni-Al deposition on regular Ni-Al atomic substrate layers each consisting of 11x8 Al and Ni atoms.

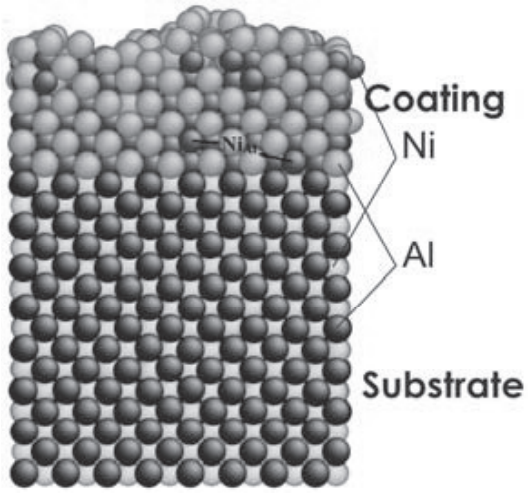

Figure 2: *Ni-Al Molecular Dynamics simulation*

Although attempts have been made to predict the elastic modulus of a thin coating, predictive models for hardness and elastic modulus, based on molecular dynamic simulation methods, are required. The current MD configurations are generally based on ideal microstructures. For real engineering problems, different material lattice structures, crystal orientations, defects, including dislocations, need to be considered in modelling activities. In addition, it is difficult to measure the mechanical properties of nano-scale multilayered coatings.

The basic assumptions of MD are different from that of FE, which makes it difficult to integrate with other lengthscale FE analyses. Currently, there is no FE-based nano-mechanics modelling software available. Consequently one objective of the current work is to develop an atomic FE method (AFEM).

3 The Atomic Finite Element Method (AFEM)

3.1 The basic idea of the AFEM

The basic idea of the AFEM is the following:

- The single atoms in the simulated atomic structure using MD are considered as nodes of the AFEM model.
- The atomic lattice is in equilibrium because of the inter-atomic potentials acting as repulsive-attracting forces between the atoms.
- In the new AFEM method these inter-atomic bonds are modelled as string elements having non-linear force-displacement behaviour.

An interface program **md2afem** is able to transform the simulated by MD atomic structure into an AFEM model. In this interface program all atomic distances, which do not exceed a predefined threshold value, are considered as AFEM elements. For small threshold values only first order inter-atomic bonds are defined in the interface, while for bigger values the model includes also the second order bonds.

The Ni-Al MD simulation example (figure 2) leads to the AFEM model shown in figure 3 (only the upper part of the model is shown, different colours indicate inter-atomic bonds of different types). The modelling was done using the general purpose FE software MSC.MARC® in its 2008 version. In the terminology of MSC.MARC the non-linear string-and-damper elements are called CBUSH elements.

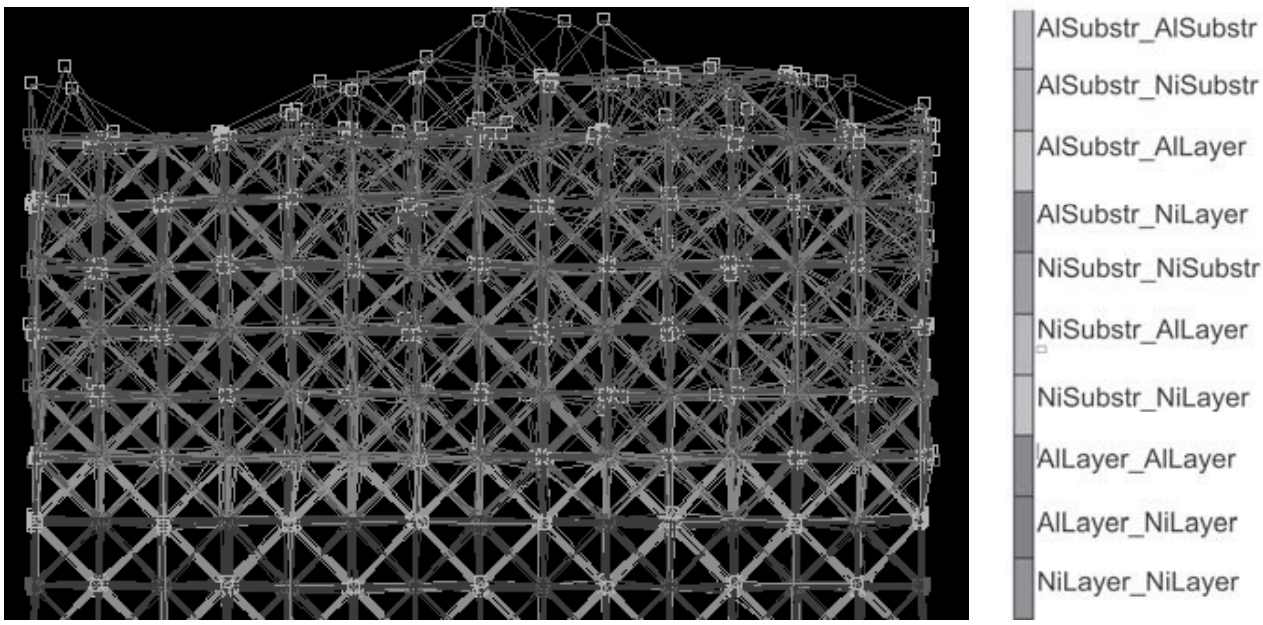

Figure 3: *AFEM model of Ni-Al deposition on Ni-Al substrate*

3.2 Inter-atomic potentials

For the definition of the non-linear behaviour of the AFEM elements the inter-atomic potentials are needed.

A pair of neutral atoms or molecules is subject to two distinct forces within the limit of large and small separation: an attractive force at long ranges (van-der-Waals force) and a repulsive force at smaller distances (the result of overlapping electron orbitals, referred to as Pauli repulsion according to the Pauli exclusion principle). A simple mathematical model that represents this behaviour is the Lennard-Jones (LJ) potential

$$V(r) = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$

(r – distance between the atoms, σ - distance at which the potential is zero, ε - depth of the potential swell). Many other representations of the inter-atomic potentials are known, for instance the Modified embedded-atom method (MEAM) potentials [6], or the inter-atomic potentials which are represented as experimental curves. In all cases the non-linear displacement-force characteristic as the first derivative of potentials must be defined (in the AFEM method realized by means of the programme ***potentials2table***). Figure 4 shows the Al-Ni inter-atomic potential

as a function of the atomic distance and the derived from the potential non-linear displacement-force function (dotted curves show schematically how a linear string behaviour looks like).

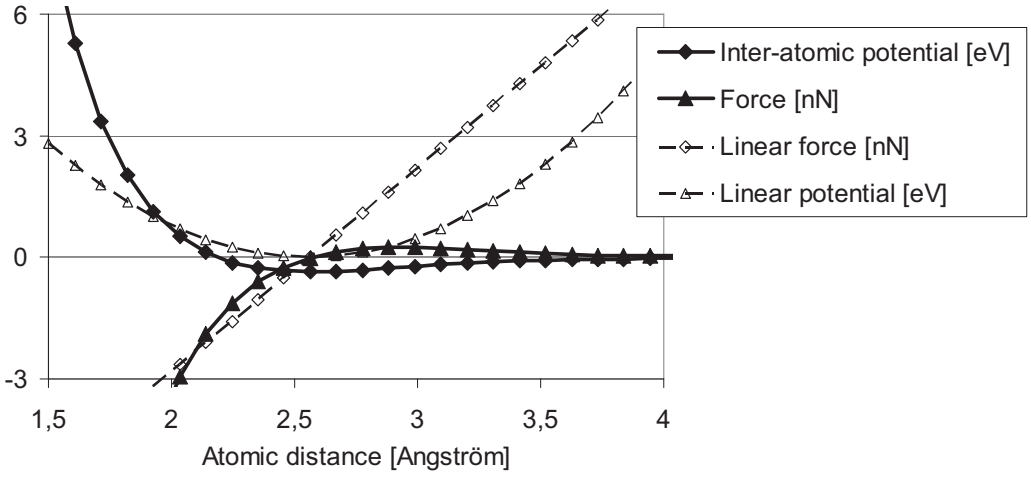

Figure 4: *Inter-atomic potential of Al-Ni and derived non-linear inter-atomic forces (linear behaviour as comparison)*

In the simulated Ni-Al lattice the inter-atomic potentials are taken from [7].

3.3 2D AFEM method with ideal atomic structure

During the first step of the current investigations simplified 2D AFEM models have been developed. If considering only the ideal and regular structure in the substrate part of the lattice, the 3D atomic structure can be projected into a 2D model with a regular tri- or rectangular mesh. In this case the inter-atomic bonds parallel to the projection direction will not be considered, and the other ones which are not parallel to the considered 2D area must be scaled and projected in this area.

Taking into account only one type of atoms in the Ni-Al deposition example the 2D atomic structure has a regular triangular form, shown in figure 5 with a nano-indenter before being in contact.

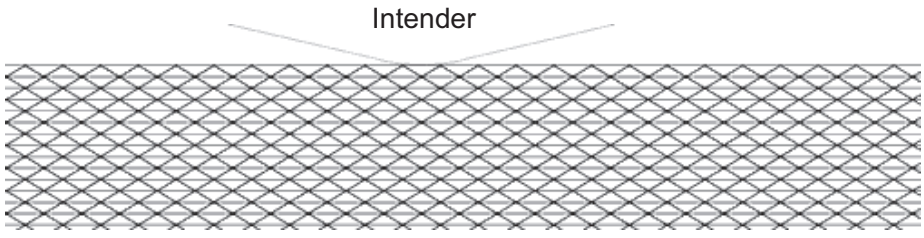

Figure 5: *Regular 2D AFEM mesh with nano-indenter tip*

3.4 Using the AFEM for nano-crack and dislocation modelling

The described AFEM is used to investigate the initiation of deformation, of nano-cracks and dislocations in the atomic level. This could be done by means of the element deactivation utilities in the FE programme. Atomic bonds are deactivated if the inter-atomic distance exceeds a certain value. Figures 6 and 7 show different nano-crack results. In figure 6 the crack initiation is initiated by a nano-indenter tip, and figure 7 represents a delamination of atomic layers in a nano-layer.

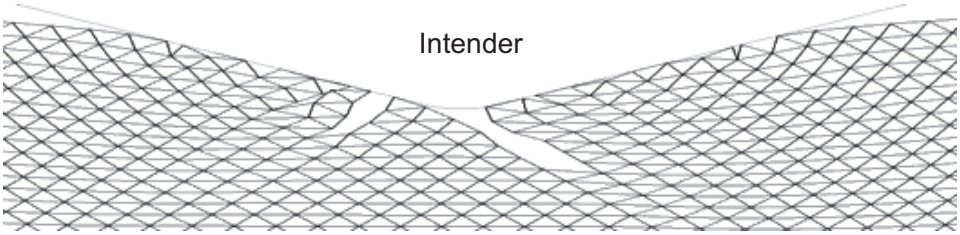

Figure 6: *Nano-crack initiation simulated by deactivation of inter-atomic bonds*

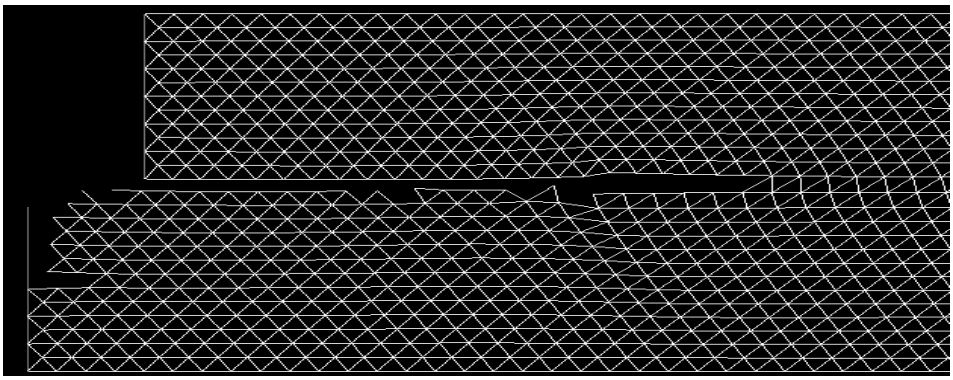

Figure 7: *Atomic layer delamination simulated by deactivation of inter-atomic bonds*

4 Outlook

The applicability of the developed AFEM including the evaluation of nano-crack and deposition initiation has been demonstrated for regular Ni-Al atomic deposition structures. During the next step of the current investigation it will be applied for TiN nano-layers which are frequently used as layers on cutting tools. The MD simulation results are available as well as the inter-atomic potentials of the Ti-Ti, Ti-N and N-N atomic bonds. The AFEM models are created using the available interface programs ***md2afem*** and ***potentials2table***. Actual nano-indenter experiments provide the required values to be implemented in the various models. CPFEM

simulations of these experiments will deliver the necessary boundary conditions for the AFEM. The results of the AFEM simulation will be presented in a continuation of this paper.

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