Multiscale Modelling for Multilayered Surface Systems
Small Collaborative Project

Final Project Report-
Final Publishable Summary Report

Start date of project: 1.11.2008
Duration: 36 months

Lead contractor: BIM
Participant: All partners

Project co-funded by the European Commission within the Seventh Framework Programme		
Dissemination Level		
PU	Public	**X**
PP	Restricted to other programme participants (including the Commission Services)	
RE	Restricted to a group specified by the consortium (including the Commission Services)	
CO	Confidential, only for members of the consortium (including the Commission Services)	

Table of Contents

1 EXECUTIVE SUMMARY

It is well recognised that the performance of devices, components and equipment of all sizes and shapes relies mainly on their surfaces and more than 90 % of failures in engineering components are related to surface problems, which can be addressed by surface engineering. During past years, a large variety of different multi-layered surface systems (MSSs) with thickness ranging from nanometre to millimetre scales have been developed. The range of possible surface systems has provided more opportunities for application but, due to the lack of reliable surface modelling techniques, the design of MSSs is normally based on experience, empirical formulae, or trial-and-error approaches. These methods are obviously laborious and inefficient, lacking reliability and increasing product development time, energy use and cost. This has slowed down the development, application and adoption of MSSs

Supported by EC, the M3-2S collaborative research project (CP-FP 213600-2 M3-2S) under the EC's Seventh Framework Programme has provided a platform for 12 international partners to address the above urgent scientific, technological and market need for consistently reliable high performance multilayered surface systems, by developing generic, robust multiscale materials modelling techniques.

Over the past three years (1 November 2008 to 31 October 2011), a portfolio of multi-scale modelling techniques and prototype software systems have been successfully developed including molecular dynamics (MD) simulation of PVD deposition process to identify the atomic structure of thin coatings, contact mechanics and load bearing capacity modelling from atomic (nano-scale) through crystal plasticity (micron scale) to continuum mechanics (macro scale). Coupling techniques to bridge the gaps between modelling activities at different scales have been developed. Supported by the multi-scale modelling techniques, a range of novel multi-layer surface systems have been generated and optimised, and a series of specialist techniques and facilities for surface characterisation and validation have been developed to generate materials databases for multi-scale modelling and for the characterisation and validation of the models developed from the project. The modelling techniques and the MSSs have been successfully applied to some industrial components and significantly improved performance and service life have been demonstrated. In conclusion, all the technological targets for the M3-2S project have been achieved based on our effective collaboration.

These advanced techniques will pave the way towards designing optimised surface engineering systems within the shortest possible time and with least cost. Therefore, the above new multi-scale modelling technique developed will facilitate the design and application of advanced multi-layer surface systems in many industrial sectors, thus realising the full potential of surface engineering.

Accordingly, these advances are bound to strengthen science and technology overall, specifically the competitiveness of European surface technology and engineering software industries in the world market. They are expected to produce wide social and environmental benefits including reduced consumption of energy and materials, improved safety and quality of life.

2 SUMMARY DESCRIPTION OF PROJECT CONTEXT AND OBJECTIVES

2.1 The Drivers

A large variety of different surface engineering systems (including coatings and surface modification), with thickness ranging from the nano-meter scale to the millimetre scale, have been developed in past decades to combat surface related degradation such as wear, corrosion, oxidation and fatigue. However, no single surface engineering system or coating can provide a total solution. For example, while thin coatings can provide a surface with significantly improved corrosion, wear and oxidation resistance under low-to-medium loading conditions, they cannot withstand high stresses as encountered in heavily loaded gears and moulds because of their load bearing capacity; on the other hand, deep-hardening (such as carburising and oxygen diffusion) effectively in improving the load bearing capacity of thermo-chemically treated metallic surfaces, but such thermo-chemical treatments cannot change the nature of metallic surfaces and thus cannot notably improve the corrosion, adhesive wear and oxidation of thermo-chemically treated metallic surfaces.

Therefore, significant progress has been made during the past decade in the development of duplex or multilayer multi-functional surface systems to meet the ever-increasing demands for high performance engineering components operating under severe working conditions, for tools for emerging manufacturing techniques (e.g. micro-machining, micro-forming and dry machining) and for the tribological applications of light-weight alloys in the automotive industry. For example: nano-scale multilayer or supper-lattice coatings with high hardness, good oxidation resistance and high wear resistance have been developed for high-speed and/or dry cutting tools to improve cutting efficiency and to address the environmental concerns over the use of lubricants; new self-lubricating coatings with good wear resistance are being developed for micro forming and machining tools which cannot be lubricated by such conventional lubricants as oils and greases; duplex surface systems have been developed by combining oxygen deep-case hardening and low friction, wear resistant multilayer coatings to facilitate the replacement of steel components with titanium for the motor sports and automotive industrials; through the development of deep-case hardening and multilayer self-lubricant (C or MoST) coatings, a wider exploitation of 'light-weight' alloys in automotive engines with low viscosity lubricating oils will provide added fuel efficiencies and CO_2 emission reductions.

The range of possible surface systems has provided more opportunities for application but, due to the lack of reliable surface modelling techniques, the design of multilayered surfaces is normally based on experience, empirical formula or a trial-and-error approach. These methods are obviously laborious and inefficient, lacking reliability and increasing product development time, energy use and cost. To address this, some models have been developed recently to simulate and predict the performance of surface systems. However, no currently available surface modelling technique can deal with multiscale systems from nanometre to millimetre due to the difficulties in bridging the gaps between modelling at different scales – from nano through micro to macro and the limited number of material models for the design and performance prediction of multilayer surface systems under cyclic load conditions at elevated temperatures.

Therefore, it is a timely task from a scientific, technological and market point-of-view to establish integrated, generic, robust multiscale materials modelling techniques for the design and performance prediction of multilayer surface systems, under different working conditions. This is the theme of this focused research project relevant to NMP-2007-2.5-2: Modelling of microstructural evolution under working conditions and in materials processing and NMP-2007-2.1-2: Nanostructured coatings and thin films.

2.2 S&T Aims and Objectives

The overall **aim** of this programme is ***to address an urgent scientific, technological and market need for consistently reliable high performance multilayered surface systems, by developing generic, robust multiscale materials modelling techniques***. These are to cover the range from nano, through micro to macro-scales, for the design, optimisation and performance prediction of multilayered surface systems, for wide ranging engineering applications. The **Specific S&T Objectives (SO)** of M3-2S are:

SO1. To develop molecular dynamics techniques to model atom deposition processes and the atomic structure and layer interfaces of multilayer coatings to identify optimal coating microstructures. This material structural information will be used for multiscale mechanics modelling.

SO2. To develop atomic FE (nano), crystal plasticity FE (micro) and continuum mechanics FE (macro) modelling techniques and software modules for individual length scale modelling for multiscale, multilayered surface systems.

SO3. To create experimental validation techniques to identify the atomic structure of superlattice coatings, to determine nano and crystal behaviour of each layer and to evaluate the macro properties of multilayer surface systems.

SO4. To establish an integrated multiscale modelling approach and a software system to link molecular dynamics (nano) deposition modelling, atomic FE (nano), crystal plasticity FE (micro) and continuum mechanics FE (macro) modelling activities for design and performance prediction of multiscale, multilayered surface systems.

SO5. To develop modelling-based design methodology for optimized multilayered surface systems for high performance components with improved load bearing capacity by **50%**, wear resistance by **75%** and/or fatigue properties by **50%** and reduce market lead time by **60%** for new multilayered surface systems.

In short, this proposed M3-2S project is directed at ***modelling of microstructure*** and properties of multilayer surface systems involving ***nanostructured coatings***. Therefore, this project equally addresses NMP-2007-2.5-2: ***Modelling*** of microstructural evolution under working conditions and in materials processing and NMP-2007-2.1-2: ***Nanostructured coatings*** and thin films.

2.3 Workpackage Structure

The overall structure of M3-2S activities and the interdependencies of the workpackages are shown in Fig. 2-1 and are summarised below:

WP1: Atomic Scale Process & Structure Modelling – Addressing SO1, is to develop novel modelling methods (MD) for the simulation of atomic thermo-chemical deposition processes for coatings.

WP2: Nano- & Micro-Mechanics Modelling – Addressing SO2, is to develop methods, algorithms, numerical procedures and software modules for AFE (nano-mechanics) and CPFE (micro-mechanics) modelling activities for superlattice coatings and for graded layers.

WP3: Continuum Mechanics Modelling - Addressing SO2, is to establish modelling methods and numerical procedures to predict the effects of coatings, deep-hardened case and substrate materials on the macro-performance of surface systems for many engineering applications.

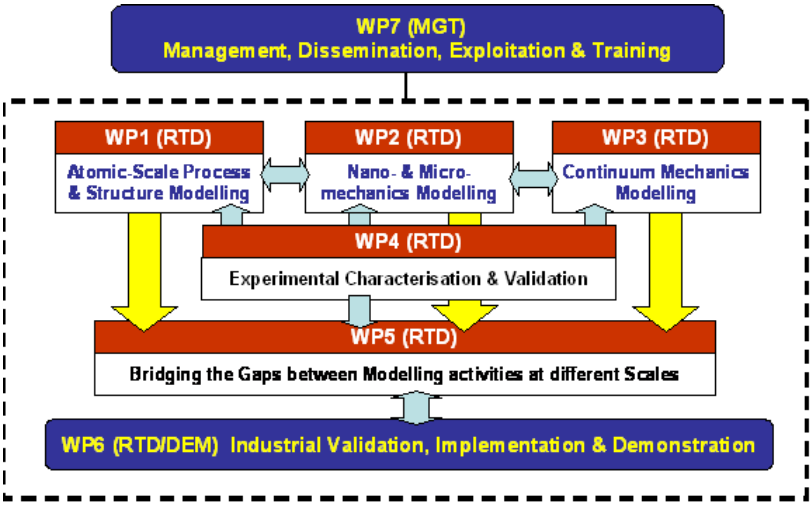


Fig. 2-1: The overall workpackage structure of M3-2S.

WP4: Experimental Characterisation & Validation – Addressing **SO3,** is to create test methodology, programs, database and test standard for validating the multiscale modelling results at individual length-scales, carried out in WPs 1, 2 and 5. The validation has been carried out for a number of selected industrial cases.

WP5: Bridging the Gaps between the Modelling Activities at Different Scales – Addressing **SO4,** is the pivotal WP within the project. Numerical methods, algorithms, procedures and user graphics interface will be developed to link the mechanics modelling activities at different length-scales. The lattice- and micro-structure of coatings obtained from atomic chemical-deposition modelling (WP1) will also be linked to mechanics modelling system (WPs 2 & 3).

WP6: Industrial Validation, Implementation & Demonstration – Addressing **SO5,** is designed; (i) to define industrial requirements for modelling multilayered surface systems; (ii) to carry out studies and design optimisation for the surfaces of selected components; and (iii) to demonstrate the capability of the developed multiscale modelling system.

WP7: Management, Dissemination, Exploitation and Training - contains all the non-RDT related activities, such as those related to innovation, Training and exploitation, dissemination and project management. That is; activities other than "Industrial Validation and Implementation" addressed in WP6).

3 DESCRIPTION OF MAIN S&T RESULTS/FOREGROUND

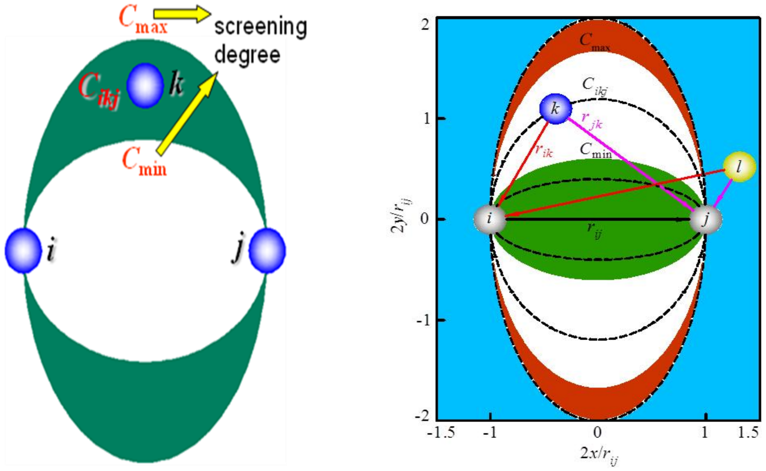
3.1 Atomic scale process & structure modelling

A. Development of reliable Ti-N and Cr-N inter-atomic potential

TiN and CrN are among the most widely used ceramic coatings and the most researched nano multilayer or superlattice coating TiN/CrN consists of alternating layers of TiN and CrN. Therefore, inter-atomic potential of Ti-N and Cr-N is essential for modelling and simulation of nano multilayer superlattice coating based on TiN and CrN at atomic scale (such as MD & AFEM).

However, a literature search and experimental work have revealed that two exiting Ti-N potentials based on the second nearest neighbour (2NN) modified embedded-atom method (MEAM) are not reliable and there is no publically available inter-atomic potential for Cr-N or other industrial coatings. Therefore, efforts have been made to build 2NN MEAM potential for the Ti-N and Cr-N systems in this project.

In order to apply the MD modelling to superlattice coatings, it is essential to describe the atomic potentials of various elements with various crystal structures using the same formalism. The modified embedded-atom method (MEAM) potential is unique in that it can reproduce physical properties of many materials with various crystal structures.



(a) (b)

Fig. 3.1-1: Atomic interaction (a) the first nearest neighbour interactions and (b) the screening of interaction three neighbouring atoms

However, most MEAM only considers the first nearest neighbour interactions (Fig.3.1-1a), which loses good descriptions for some physical properties of bcc and hcp metals. In this study, the effect of the second nearest neighbour interactions was taken into the potential (Fig.3.1-1b) and the second nearest neighbour (2NN) MEAM potential has obtained. This is because an atom between two other atoms is able to screen the interaction between the outer atoms, hence reducing the force.

The reliability of the Ti-N inter-atomic potential has been validated by comparing with experimental and/or first-principles calculated basic properties (such as bulk modulus, elastic constants, surface energy, cohesive energy and thermal liner expansion coefficient) of TiN(B1). For example, the experimentally measured and simulated thermal linear expansion coefficient based on the Ti-N inter-atomic potential is compared in Fig. 3.1-2). The reliability of the Ti-N potential is evidenced by the very good agreement between experiment (9.35×10^{-6} K^{-1}) and simulation (9.31×10^{-6} K^{-1}).

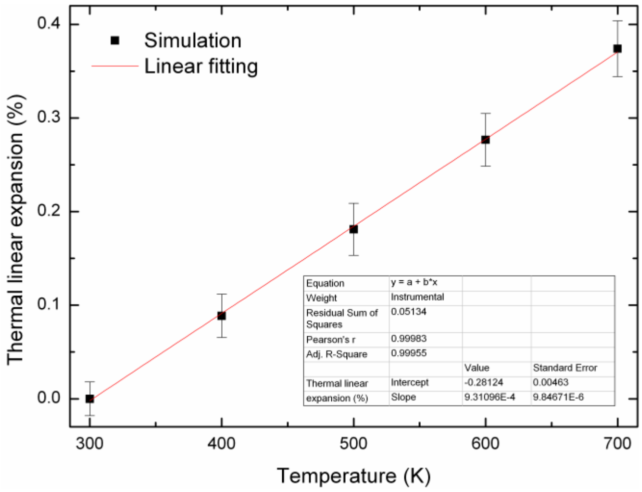


Fig. 3.1-2: **Thermal linear expansion of TiN.**

Using this potential, the atomic insight of TiN film growth on TiN (001) was carried out (see below). The results have been published in *Computational Materials Science*.

B. MD simulation of TiN deposition[1] & absorption[2]

A literature review was carried out, at the beginning of the project, on the modelling techniques for thermo-chemical coating processes. Particular attention was paid to the modelling methods, such as molecular dynamics, for atomic deposition process. The modelling method for atomic deposition process based on the MD model (Fig. 3.1-3) has been developed.

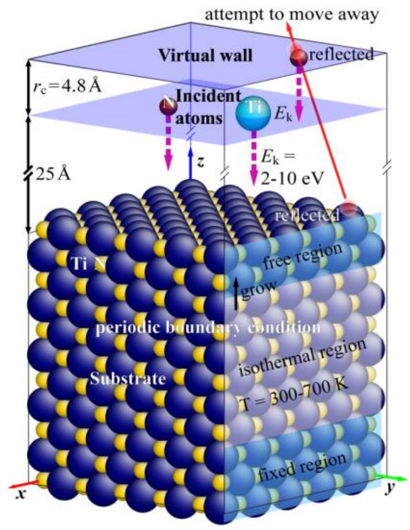


Fig. 3.1-3: MD model of atomic deposition

[1] Z. Xu, Y. Li, D. Shan and B. Guo, Computational *Materials Science*, **20**(2011), 1432-1436.

[2] D. Shan, Z. Xu and Y. Li, the 19th IFHTSE Congress, 20 Oct 2011, Glasgow.

The model was firstly applied to the deposition of copper film with an FCC structure, because of the lack of reliable inter-atomic potential of ceramics at early stage of this project. After building the robust second nearest neighbour (2NN) modified embedded-atom method (MEAM) Ti-N potential, the growth of thin TiN films on the TiN surface during reactive sputtering was simulated by molecular dynamics (MD) with the improved 2NN MEAN Ti-N potential. Fig.3.1-4 shows the film growth process under the condition of T = 600 K and Ek = 6 eV.

The results indicate that TiN_3 is found to be the smallest epitaxial island and the film grows via the layer mode and that vacancy concentration in the deposited films decreases with increasing the substrate temperature and kinetic energy of incident atoms, resulting from the enhancement of the thermal diffusion and kinetic energy assisted athermal diffusion. To get the stoichiometric TiN film, the N:Ti flux ratio should be larger than unity and be increased with higher incident energy due to the weak adsorption of atomic N on TiN(0 0 1).

The adsorption behaviour of atomic Ti and N on TiN surface has also been studied (Fig. 3.1-5). The sticking coefficient of N on TiN surface is predominated by the kinetic energy of adatoms, decreases with increasing the incident energy and do not affected by the substrate temperature. The sticking coefficient of Ti is very close to unity, and the incident energy and temperature have no effect on it.

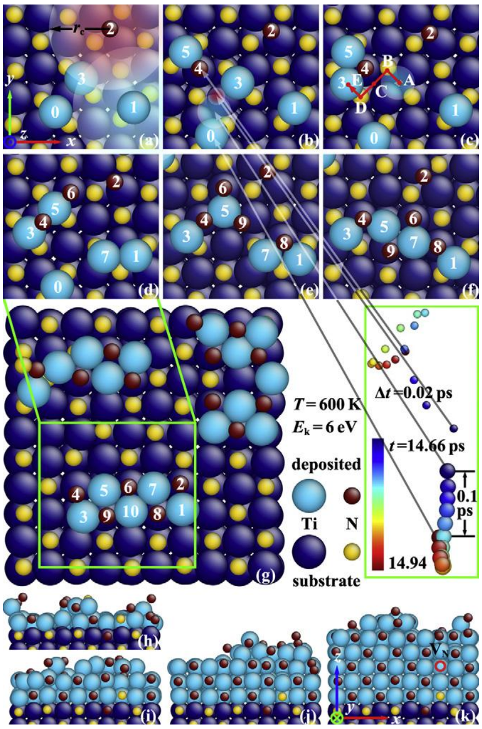


Fig. 3.1-4: Time-resolved process of the TiN film growth under T = 600 K and Ek = 6 eV. *Top view of a section of the TiN film at: (a) 12 ps, the annular shadows with an excircle radius of rc around atoms denote their ranges of the interatomic potentials, (b) 14.94 ps, the circular shadows denote the positions of adatoms 0 and 4 at 14.66 ps, (c) 15.9 ps, (d) 20 ps, (e) 27.55 ps, (f) 27.85 ps and (g)32.87 ps. Side view of the whole TiN film at (h) 100 ps, (i) 200 ps, (j) 300 ps and (k)550 ps. Atoms are coloured by the element types and locations: the light blue and red denote the deposited Ti and N atoms, the dark blue and yellow denote the Ti and N atoms in the substrate. Atoms are sized by the element types: Ti atoms are larger than N atoms. The numbers on atoms denote the deposition turn.*

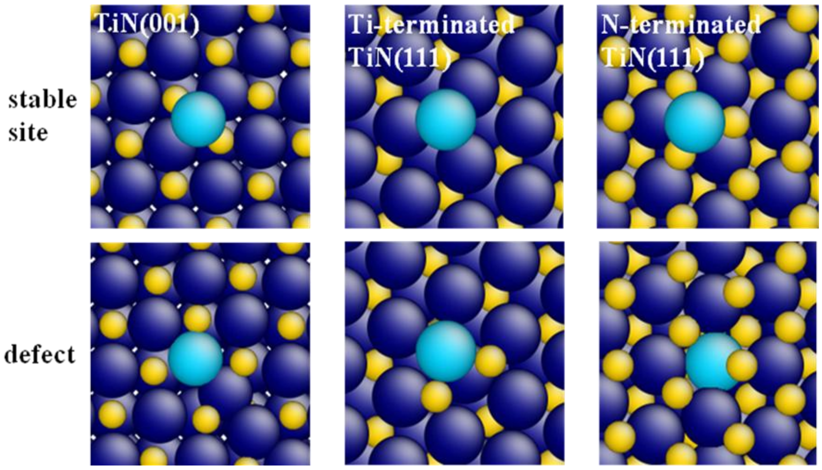


Fig. 3.1-5: Adsorption of Ti on TiN(001) & TiN(111)

C. Quantifying adhesion energy of coatings at atomistic scale[3]

Hard and wear-resistant coatings comprising of carbides or nitrides are increasingly applied in industry in order to protect materials from surface degradation. All of these applications, including their properties and functionalities, rely critically on the specific structure, the local chemistry, and the local adhesive strength at the interface between coatings and their substrate materials. Specifically, the loss of adhesion at interface could result in a premature failure of coatings. However, adhesion or bonding of coatings can be improved greatly by microstructural and/or compositional design, which needs methodology to quantify adhesion at atomic scale.

To this end, a first-principles study of adhesion energy on the TiN coatings (Fig. 3.1-6) was performed and it has been combined with the FEM aimed at calculating initialization process of cracks during nano-indentation and investigating how the residual stress affects adhesion at atomic scale. As shown in Fig. 3.1-6, the Ti and N atoms are located on an individual layer and array alternatively in the (1 1 1) case, while coexisting on each layer in the (0 0 1) case with each atom having two types of neighbours, i.e., on either the same or the neighbouring layer.

In this research, the adhesion energy was TiN coating was studied by the first-principles calculations within the framework of density functional theory. This is also able to provide insight into bonding configuration. The W_{ad} of the intrinsic TiN coatings was estimated, taking into account the residual stress effect and the results indicate that the calculated W_{ad} is small under no residual stress, but increases linearly with the residual compressive stress, whatever the orientation is (1 1 1) or (0 0 1), indicating the critical role of residual stress in influencing adhesion. Several analytic methods are applied to investigate structural change induced by residual stress, and the primary finding is that compressive residual stress shrinks Ti–N bonds and hence strengthens their interactions. Moreover, the initialization process of cracks simulated by combining the first-principles with the FEM agrees well with the experimental observations.

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[3] Yi Qin, Jiling Feng, Zhongchang Wang, Applied Surface Science, 258 (2011), 1451– 1455.

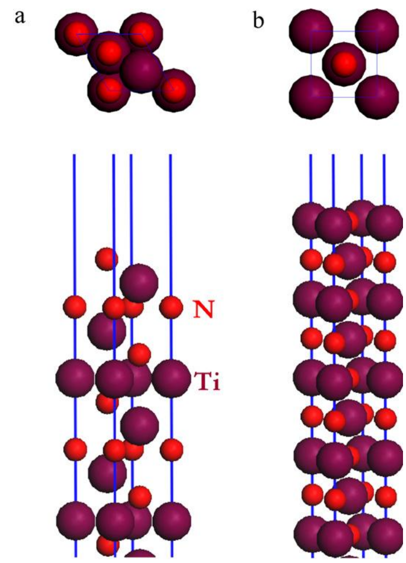


Fig. 3.1-6: Plots of TiN coatings: (a) (1 1 1) and (b) (0 0 1) orientation

To identify bonding character directly and examine effect of residual stress, Figure 3.1-7 show the contour maps of charge density and their differences along (1-10) plane for the surface slabs under the residual stress of 0 and 8 GPa. It can be seen from Figure 3.1-7 that the charge accumulated on N comes predominantly from its adjacent Ti; the electron distribution in between Ti and N is strengthened under residual stress in the (1 1 1) case (marked by dotted circles in a and b), which is due to the more charges transferred from Ti to neighbouring N under stress (c & d). Clearly, the residual stress affects adhesion by means of varying charge distribution in the TiN coatings, in agreement with above analyses on atomic population and bond order.

Further finite elements simulation (FEM) based on calculated adhesion energy reproduces well the initial cracking process observed in nanoindentation experiments, thereby validating the application of this approach in quantifying adhesion energy of surface coating systems.

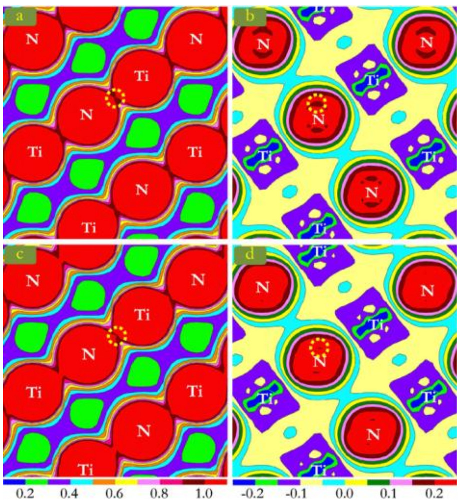


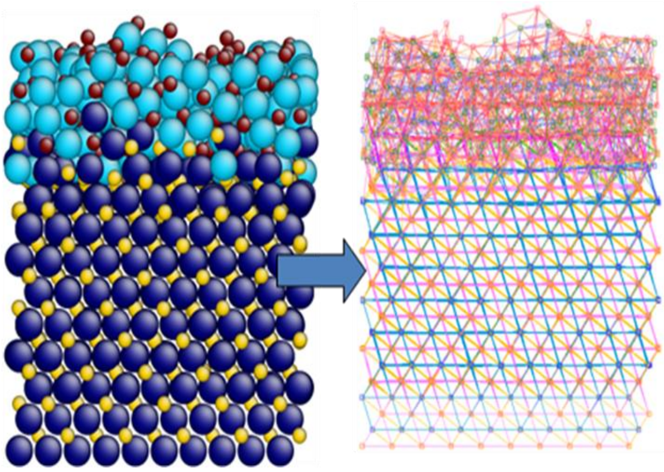
Figure 3.1-7 Contour plots of (a) charge density and (b) its difference without residual stress, and of (c) charge density and (d) charge difference under residual stress of 8 GPa taken along the (1-10) plane for the TiN coatings with (1 1 1) orientation

3.2 Nano- & Micro-Mechanics Modelling

A. Interface programme bridging MD & AFEM [4]

To facilitate AFEM and the related nano-mechanics modelling, an interface between MD and AFEM for Ni-Al and TiN has been defined and successfully used for 3D AFEM models. The interface between MD and AFEM (programme MD2AFEM) for semi-automated model development using the interface has been programmed: MD2AFEM.exe. This programme can automatically generate AFEM meshes on the base of the MD result file.

The program generates a command procedure for MARC. Its execution in MARC builds the required AFEM model. Figure 3.2-1 shows the AFEM model, based on the MD simulation. The resulting AFEM model is a real 3D model with the Angström as the basic length scale. It contains the atoms of the MD simulation as FE nodes and all the inter-atomic bonds as general spring elements (from all inter-atomic bonds, only those with a length not exceeding a predetermined upper bound, are taken into consideration).



(a) (b)

Fig. 3.2-1: Transforming MD lattice (a) into AFEM models (b)

B. Methodology of AFEM for initial failure

The AFEM is used to investigate the initiation of deformation, of nano-cracks and dislocations at an atomic level. This can be done by means of the element deactivation utilities in the used FE programme MSC.MARC/Mentat – a special FORTRAN user subroutine. An AFEM element is deactivated if its length exceeds a-priori defined threshold value (Fig. 3.2-2). The method has been used to simulate the formation nano-cracks under nanoindentation (Fig. 3.2-3) and the delimitation process of atomic layers.

C. A FEM for dislocation and crack modelling

Plastic deformations in form of dislocations in the atomic lattice can be considered as failure of actual atomic bonds. In this project, dislocation and crack were simulated at

[4] R.Neuge-bauer, R.Wertheim, U.Semmler, *Journal of Multiscale Modelling*, **3**(2011), 91-107.

an atomic level using the activation/deactivation utilities in the programme MSC.MARC with the initial mesh of the delamination example (Fig.3.2-3).

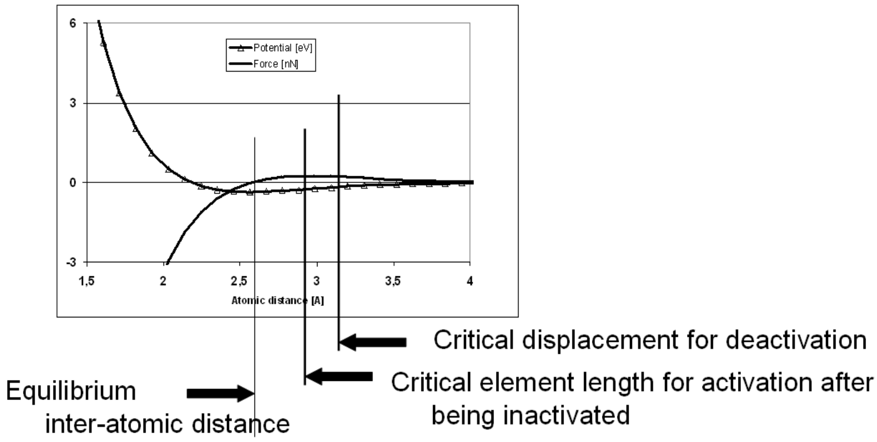


Fig. 3.2-2: **Principle of AFEM element activation/deactivation**

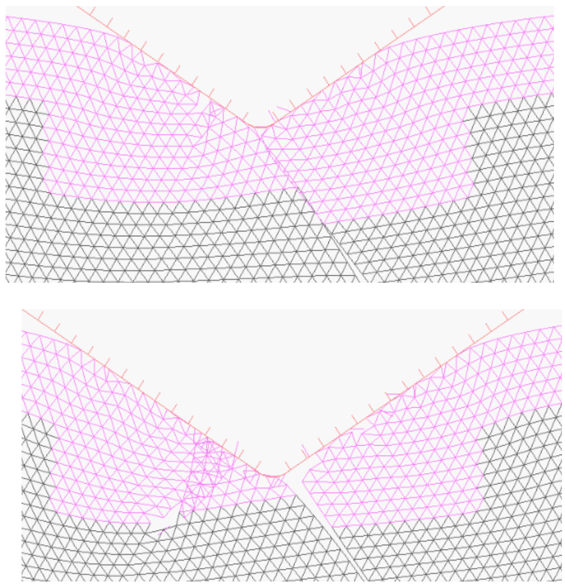


Fig. 3.2-3: Overlapping of crack fronts during the nano-crack simulation

During the deformation process, the atomic bonds are deactivated if the inter-atomic distance exceeds a certain value (see Fig. 3.2-1). The method has been further developed in this period to simulate the delimitation process of atomic layers. Figure 3.2-4 shows the delamination process of atomic layers. The predefined shift of the upper part is divided into 100 sub-steps. After initial element deactivation on both sides of the model the delamination started in step 85 and finished in step 100.

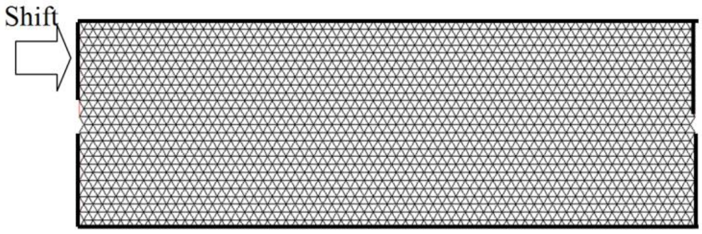
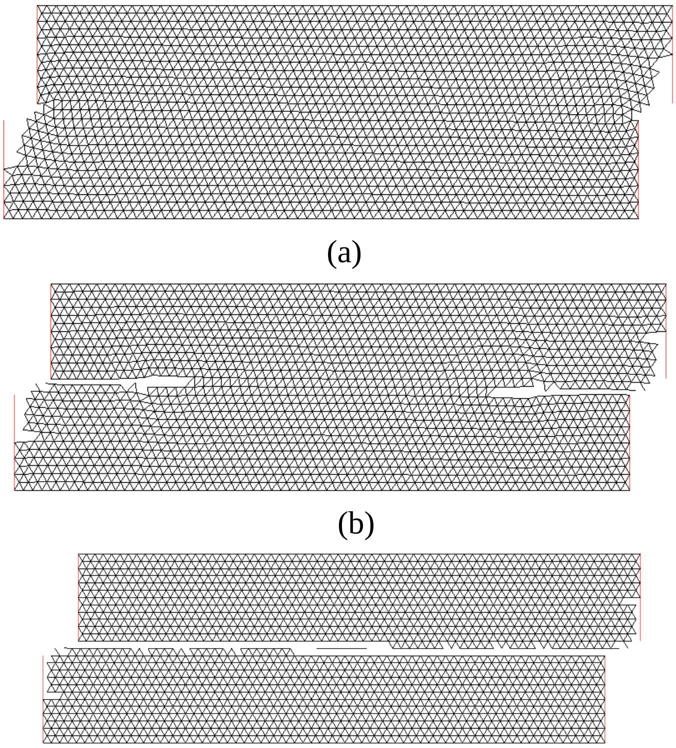


Fig. 3.2-4: Model for horizontal nano-crack simulation



(a)

(b)

(c)

Figure 3.2-5*: AFEM simulation of atomic layer delamination*
(a) Step 85, (b) Step 95 and (c) Step 100

D. CPFEM for multilayer coatings

To facilitate CPFE, a software system, Virtual grain structure generation (VGRAIN) has been developed to implement all types of virtual grain generation schemes, to build materials models for CPFE simulations, and to analyse properties of produced grain structures. Figure 3.2-6 shows the multi-zone VGRAIN model for CPFE simulation. CPFEM was implemented for the deformation of graded microstructures for a multilayer surface system (Figure 3.2-7).

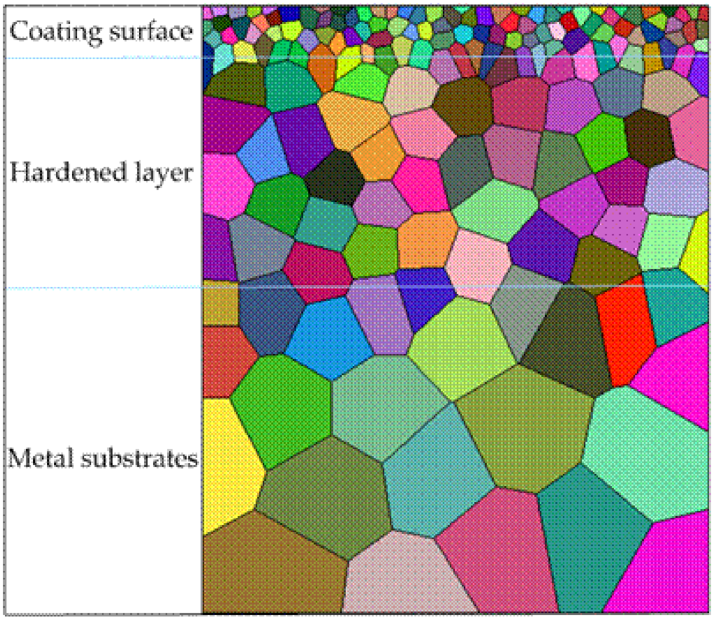


Fig. 3.2-6: Multi-zone VGRAIN model for CPFE simulation

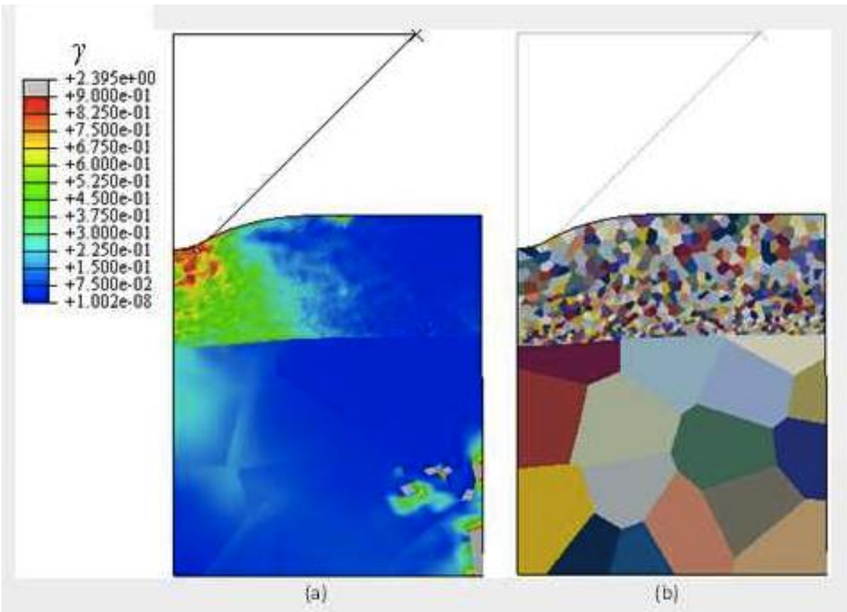


Fig. 3.2-7: CPFEM simulation of deformation of graded coating microstructure

E. Coupling of CPFEM to AFEM

Submodelling approach has been used as the primary solution for integrating the length scales, rather than a direct coupling and concurrent solution approach. The submodelling approach allows for communication of relevant information, passed from one scale down to the next, starting at the macro-scale, facilitated by a unifying web-based software interface for the overall problem which allows different software packages to be used for the modelling at the different length scales.

Two submodelling technique has been identified: (i) Node-based submodelling, which uses a nodal results field (including displacement, temperature, etc.) to interpolate global model results to the submodel nodes. (ii) A surface-based technique, which uses the stress field to interpolate global model results onto the submodel integration points on the driven element-based surface facets. Figs. 3.2-8 (a-e) show the integration of different scales from MCFE to AFEM by submodelling and parameter information techniques in Load Bearing Test (LBT) simulations for M3-2S project. The driving nodes linking the submodel and global model are shown as blue dots (Fig.3.2-8b). In this flowchart, MCFE and LCFE are used to identify the maximum load for the coating system, CPFEM and AFEM are used to investigate the features of crack initiation and its propagations.

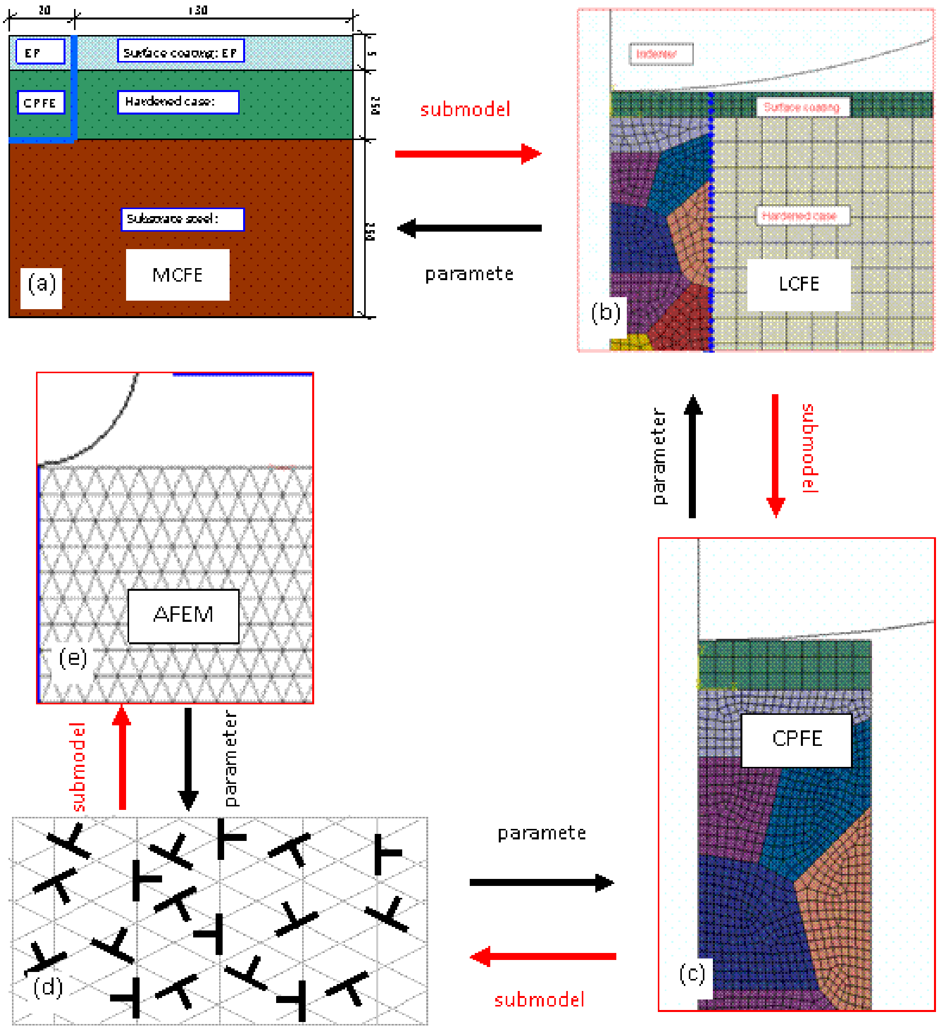


Figure 3.2-7: The integration of different scales from MCFE to AFEM by submodel (top to bottom) and parameter information (bottom to top) with load bearing test.

3.3 Continuum Mechanics Modelling

A. Methodology for Continuum Mechanics Modelling

Continuum Mechanics Modelling techniques are developed with a view to completing a system for design and optimisation of multi-layered systems, based on which some case studies were carried out. The modelling strategy and analysis procedure used is shown in Fig.3.3-1.

A generic continuum mechanics FE model of the multi-layered system has been developed, of which the modules and parameters for multi-layered coating, hardened case and substrate, are defined. The parameterised modelling – a strategy used in this model, allows for parameterised programming of a variety of variables including: geometry of modules/layers; meshing schemes & control; element and node generation; module assembly; definition of hardened case; definition of residual stresses; definition of tool/indenter; definition of material properties (averaged from mm modelling); definition of initial temperature; definition of interfacial condition (friction, heat transfer); definition of cohesive zone model; sub-modelling definition; definition of constraints; output definition and definition of analysis procedure.

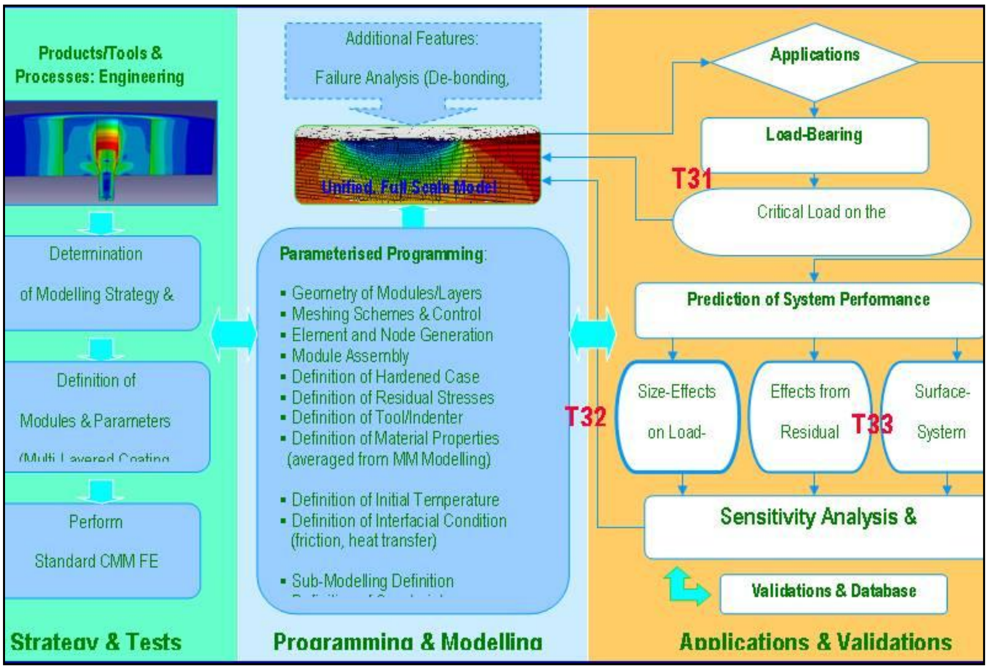


Fig. 3.3-1; **Methodology for the development of Continuum Mechanics Modelling techniques and applications**

Geometry, meshing schemes, element and node were defined and constructed for a multilayer surface system (Fig.3.3-2). This multi-layered system is indented by a spherical indenter. Based on the assumption of an axisymmetric problem, only half of this model is presented. The axisymmetric model is made up of five blocks including central and outer coating, central and outer hardened case and the substrate, where the W1 and W2 indicate the widths of central and outer parts, respectively, and T1, T2 and T3 indicate the thickness of coating, hardened case and substrate, respectively. The meshing scheme is controlled by the parameters of density of elements and the dimensions of model. The function of yield strength of the hardened case against the depth is given by a curve fitting procedure on the experimental data.

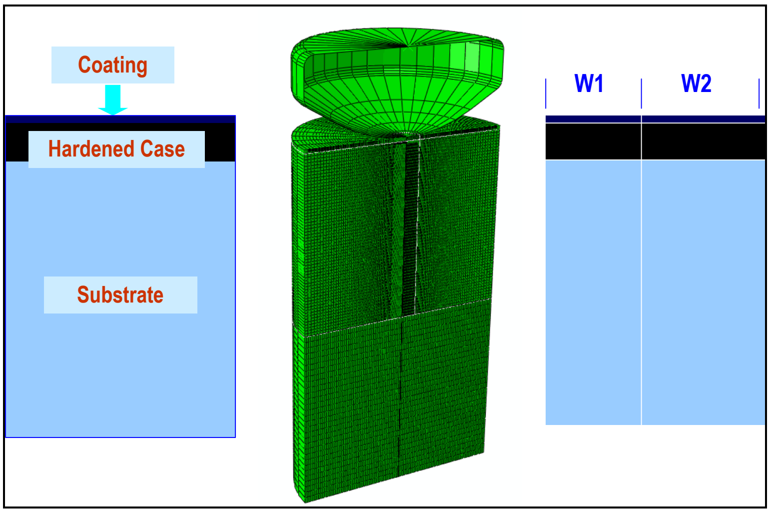


Fig. 3.3-2: An FE model considering real dimensions of coatings, deep hardened layers and substrate materials

A sub-modelling technique is incorporated into this model to link macroscopic continuum FE (cm-mm), lower continuum FE, refinement (mm-μm) and crystal plasticity FE refinement (μm-nm). The submodelling technique is used to: study a local part of a model with a refined mesh based on interpolation of the solution from an initial (undeformed), relatively coarse, global model; to obtain an accurate, detailed solution in a local region (the detailed modelling of that local region has negligible effect on the overall solution); and drive a local part of the model by nodal results, such as displacements or by the element stress results from the global mesh. Both node-based sub-modelling and surface- based sub-modelling techniques are used in this model, as exemplified in Figure 3.3-3.

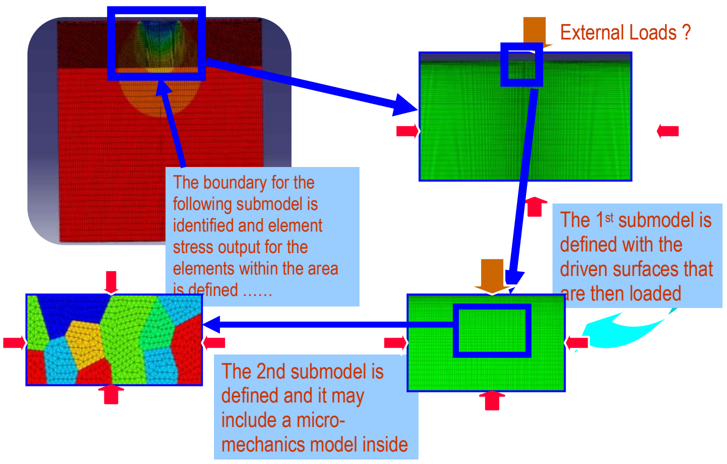


Fig. 3.3-3: Illustration of the sub-modelling technique for the analysis of multi-layered systems and the link of different length-scale modelling

B. Method for Simulation of Surface/Interface Damage/Debonding

Fracture in a hard coating is complex and controlled by many factors. Delamination between layers may be attributed to the dissimilarity of material properties between layers. Perpendicular cracks in a coating are a common form of failure in multi-layered systems observed in the indentation experiments. Under the pressure of an indenter, circumferential cracks might initiate from the coating surface or from the coating side of the interface and might grow into a through-thickness crack. Failure in the multi-layered system, regardless of delamination, or crack, can be modelled by means of a cohesive zone model. One of approaches to simulate coating failure is by placing the cohesive elements in between all continuum elements in the coating, by which crack initiation and propagation is investigated using the traction-separation law.

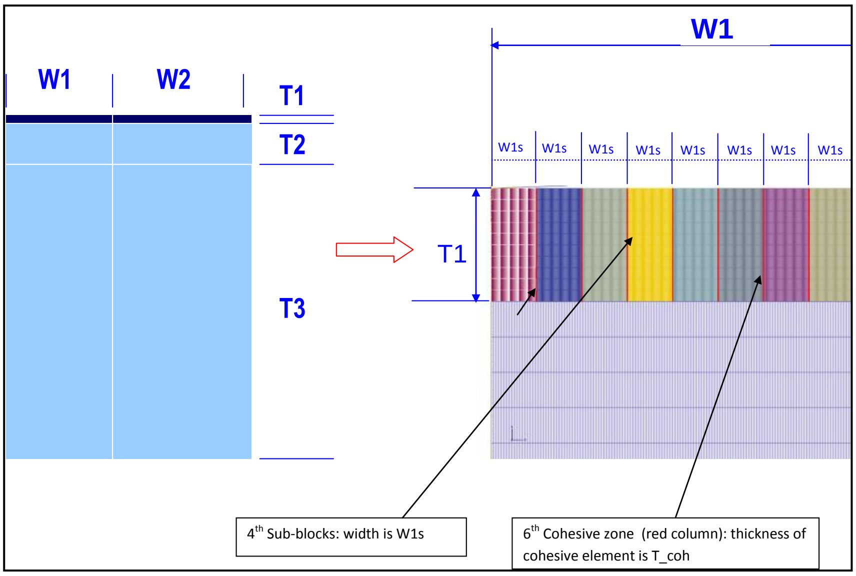


Fig. 3.3-4: Implementation of the cohesive zone model into the continuum mechanics FE model

A typical traction-separation response with a failure mechanism, bilinear cohesive zone model is used to simulate surface damage and interface debonding. The methodology is based mainly on an elastic constitutive matrix, interpretation of material properties, damage modelling, damage initiation, and damage evolution. The cohesive zone model has been applied to multi-layered surface systems (Fig. 3.3-4). The blocks of multi-layered systems are split into sub-blocks, between which the cohesive zone is inserted. Here, it is assumed that crack occurs in the block of the central coating. To simplify the problem, the columns of cohesive elements are arranged evenly in the horizontal direction in the central coating layer. The meshing scheme for sub-block and cohesive is also controlled by the density of elements and the dimensions of model. All the elements and nodes were generated using the key words command in ABAQUS.

C. Simulation of Indentation of Multilayered Systems

As agreed during the project meetings, indentation method will be used to test the load bearing capacity of multi-layered surface systems under point-contact conditions (such as cutting tip). Therefore, simulation of indentation of ball indenters have been conducted using the Continuum Mechanics Modelling technique developed during this period.

The surface systems considered included a 2μm TiN coating on heat treated bulk H11 steel (single coating coded as PNU) and on plasma nitrided H11 steel (duplex treated coded as PN1 or PN2). Two types of indenters were used for simulation: (1) WC balls with diameters of 1, 2.5 and 5mm and (2) Rockwell indenter with a tip radius of 200 micron (0.2mm). Figure 3.3-5 shows the model created and the simulation results for the 5mm ball indenter. The predicted critical load increases with the diameter of the ball indenters used: 0.6-0.8 for 1mm ball, 4-5 for 2.5mm ball and 13-15 for 5mm ball.

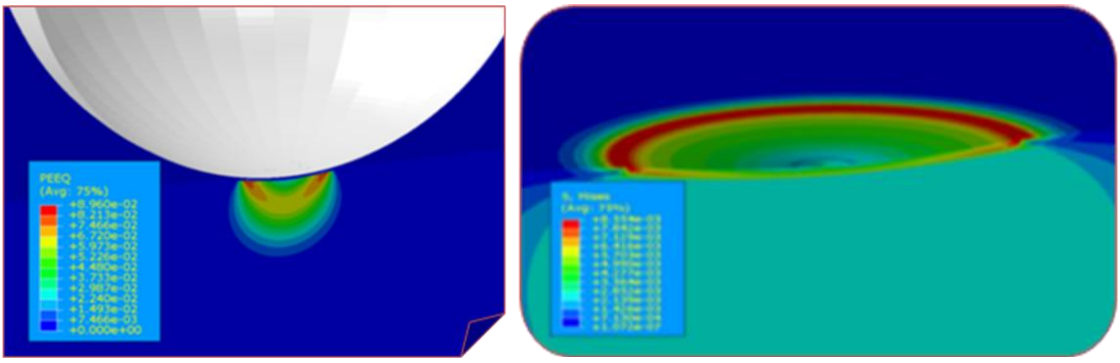


Fig. 3.3-5: Simulation results of a PNU sample indented by a 5mm ball

The initiation of the cracks around the edge of the concave impression was predicted. For example, Figure 3.3-6 clearly demonstrates that circular cracks will start to form for single TiN coating on H11 (PNU) when the applied load exceeded about 20N, which is the load bearing capacity (LBC) of the single coating system. Once the applied load is higher than the LBC, plastic deformation occurred in the substrate and the coating collapsed due to the lack of support - ‘thin-ice effect’.

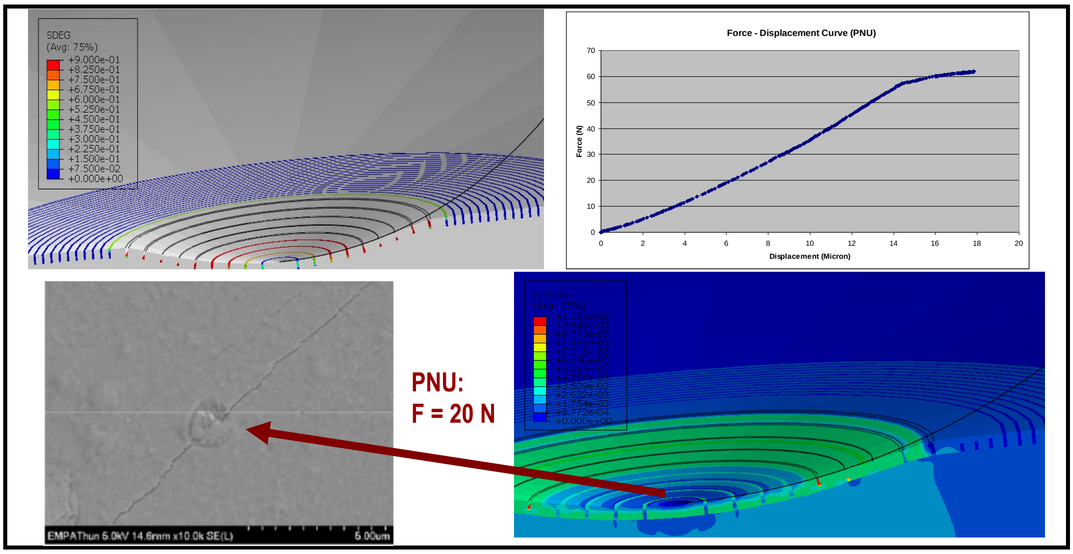


Fig. 3.3-6: Simulation of crack development (PNU, 200 microns indenter)

The corresponding simulation results for the duplex system, TiN on plasma nitrided H11is shown in Fig. 3.3-7. It seems that the critical load predicted for the PN1 is between 30 and 40N.

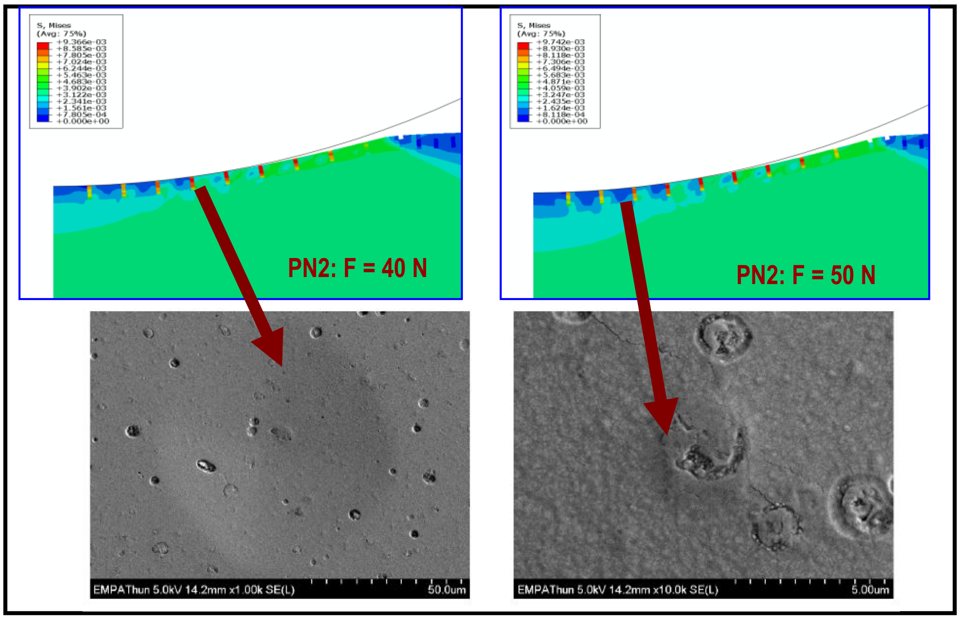
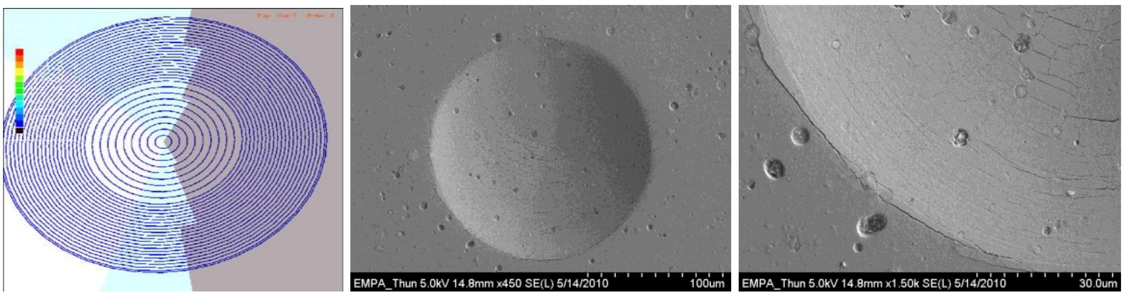


Fig.3.3-7: A **three-layer system (coating, hardened-case and substrate) loaded to 40 & 50N**

The predicted circular cracks (Fig. 3.3-8a) were validated by micro-indentation tests. As shown in Figs. 3.3-8b & c, many circular cracks were formed during the micro-indentation tests. The load bearing capacity values predicted using the Continuum Mechanics Modelling technique developed from the project for PNU and PN2 are about 10 and 30N, which are in good agreement with the directly measured values, ≤20N for PNU and ≤40N for PN2, using a Rockwell indenter with a tip radius of 200 micron indenter. In summary, the model has been validated by the fact that the predicted load bearing capacity values and the crack geometry are in good agreement with the experimental results.



(a) (b) (c)

Fig. 3.3-8: Circular cracks: (a) predicted, (b) and (c) observed in PUN

D. Prediction of residual stress in TiN/VN and TiN/CrN multi-layered coatings[5]

Local residual stress fields often influence and even govern some of the mechanical properties of multi-layered coatings at nanoscale. An approach is developed for the evaluation of the local residual stress with a representative volume element (RVE) (Fig. 3.3-9) of TiN/VN and TiN/CrN multi-layered coatings and the concept of lattice mismatch between neighbouring layers, incorporating high-precision density–functional-theory calculations.

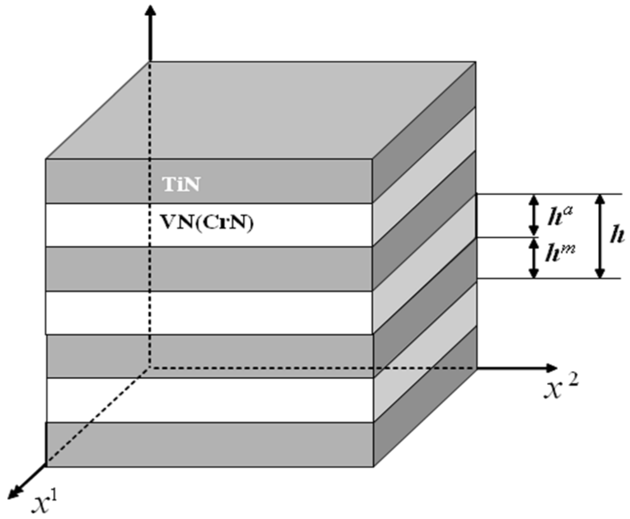


Fig. 3.3-9: RVE of the coating

The calculated results are in good agreement with experimental reports, even if each individual host constituent is assumed linearly elastic, demonstrating the validity of the proposed approach in the evaluation of the residual stress. In addition, it is found that lattice mismatch is a reasonable key-factor to account for the extremely large residual stress in multi-layered transitional metal-nitride coatings (Fig. 3.3-10).

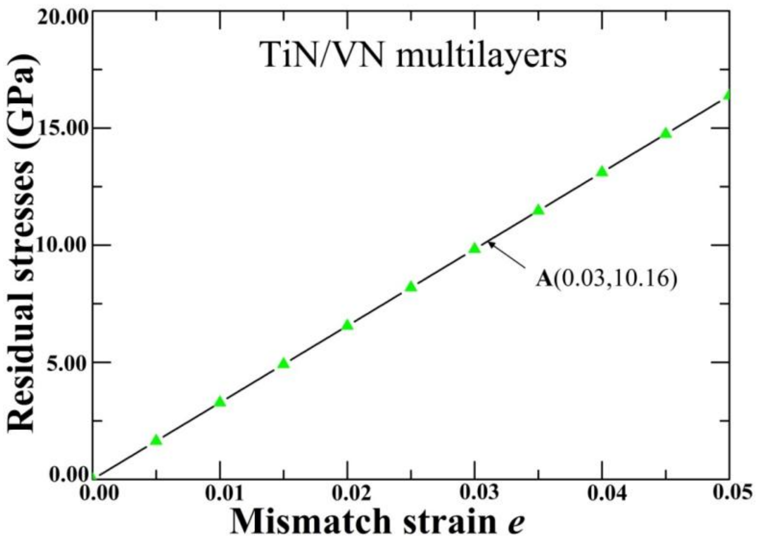


Fig. 3.3-10: Residual stresses v. lattice mismatch strain

5 D. Yin, X. Peng,Y Qin,and Z. Wang, Journal of Multiscale Modelling, 3(2011), 65-78.

3.4 Experimental Characterisation & Validation

A. Development of advanced surface engineering systems[6]

In this project, a series of advanced surface engineering systems were produced for generating a materials property database as inputs for modelling work and for validating modelling results.

Substrate materials

Six types of substrate materials were used as the substrates because they are representative materials for many industrial applications and for M3-2S demonstrators in particular: 42CrMo4 for general engineering components (e.g. gears); AISI H11for hot work tools (e, g, dies & moulds); X153CrMoV12 for cold working tools (e.g. rollers); AISI M2 for cutting tools (e.g. drills); WC-(6%) Co cermet for cutting tool inserts and Si_3N_4 ceramic for cutting tool inserts.

PVD coatings

Two major groups of PVD coatings were designed and produced from the M3-2S project: (i) Monolayer coatings - TiN, CrN, TiAlSiN and CrAlSiN and (ii) Nano multilayer coatings - nTiN/CrN, nTiAlSiN and nCrAlSiN with different bilayer thickness (5-10nm). Fig.3.4-1a shows XSEM of nCrAlSiN and Fig.3.4-1b shows an example of supper-lattice diffractions from the nTiAlSiN.

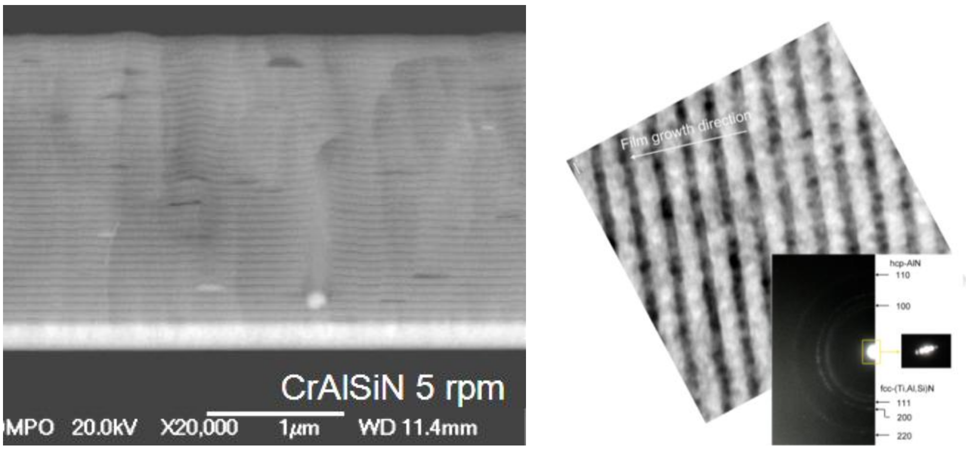


Fig. 3-4-1: Nano-multilayer structure of CrAlSiN (a) and TiAlSiN (b)

Active-screen plasma nitriding

A new environmentally friendly, energy efficient and low carbon footprint plasma nitriding technology, active screen plasma technology was employed to harden the surface case of selected steel substrate. The typical cross-sectional microstructures of active-screen plasma nitrided steels samples are shown in Fig.3.4-2. The thickness and surface hardness of the hardened case is 100-600 microns and 900-1300HV, respectively.

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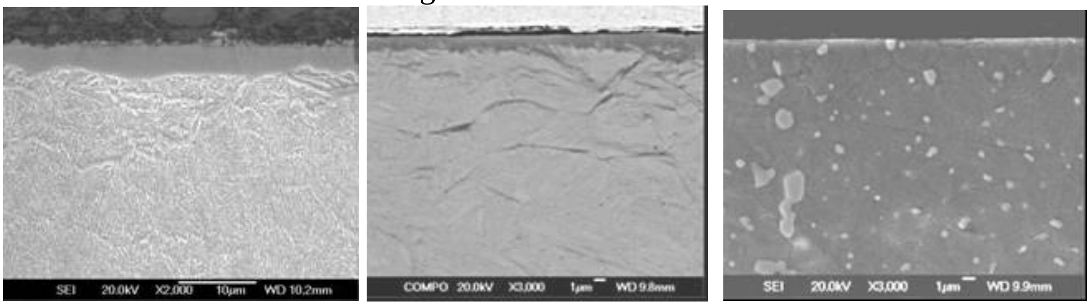
[6] R. Ji, R.H.U. Khan, E. Almandoz, G.G. Fuentes, X. Li, H. Dong, the 19th IFHTSE Congress, 20 Oct 2011, Glasgow.

Duplex surface engineering

Duplex treatments combining plasma nitriding with ceramic coatings (such as TiN), were successfully used to form multi-layered surface systems in order to enhance the load bearing capacity (LBC) and fatigue properties of engineering components. For example, load bearing capacity tests using the Vickers indenter, indicated that the single TiN coated H11 cracked under a load of 200g whilst the duplex treated (PN+TiN) withstood a maximum load of 1000g.



(a) (b) (c)

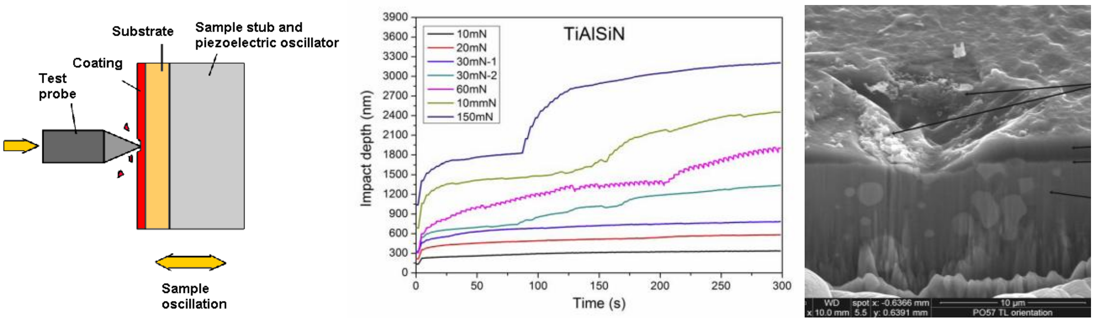
Fig. 3.4-2 XSEM micrographs of plasma nitrided (a) 42CrMo4, (b) H11 and (c) M2

B. Advanced surface characterisation techniques for multilayer surfaces

A portfolio of advanced surface characterisation techniques have been developed to generate a database for modelling deposition processes, for determining mechanical properties of surface materials and for validating modelling methods developed. In particular, the following five special techniques have been developed and used for this M3-2S project: (1) environmental nanoindentation at different temperatures in different mediums; (2) In-situ SEM indentation; (3) in-situ SEM four point bending; (4) nano-impact and (5) FIB/SEM bonding study. By way of example, the power of these novel surface analysis techniques is demonstrated in the following examples.

- Nano-impact /FIB characterisation of M3-2S coatings[7]

The nano-impact tests were carried out in a multiple impulse impact mode (Fig. 3.4-3). A solenoid connected to a timed relay was used to produce the repetitive probe impacts on the surface. A blunt cube corer diamond probe was accelerated from a set distance (~12μm) above the surface to produce impact at different. A hold period (2s) was given to record the depth variation. Then the probe was retracted to the set distance and stayed for another 2s. Then these steps repeated at the same area for 75 times which was controlled by the computer program and the final depth was recorded (Fig. 3.4-3b).



(a) (b) (c)

Fig. 3.4-3: Nano-impact (a), crater depth v. impact number (b) and FIB/SEM crater (c).

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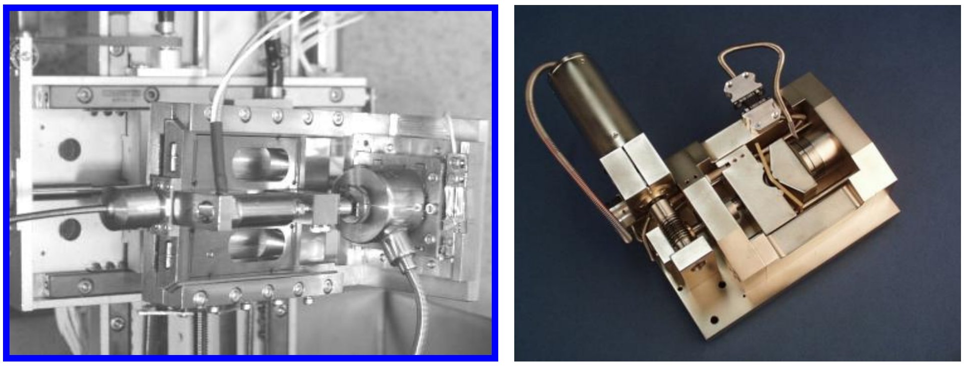
[7] J Chen, R Ji, R Khan, X Li, H Dong, *Surface & Coatings Technology*, **206**(2011), 522–529.

Following the nano impact tests, detailed study of the impact craters was conducted using SEM combined with FIB. It is clear from Fig. 3.4-3c that the bonding between the surface coatings and the M2 substrate is fairly good as no cracks could be identified from the SEM/FIB images. Clearly, the nTiAlSiN coating shows better toughness than the TiN coating.

- In-situ SEM micro-indentation & 4-point bending testing[8]

In order to investigate the deformation and cracking behaviour of the multi-layer coatings, in-situ SEM indentation and bending method and equipment were developed for nano multi-layer coatings.



(a) (b)

Fig. 3.4-4: *In-situ* SEM equipment for indentation (a) and in-situ bending (b)

During *in-situ* SEM micro-indentation, movies can be recorded throughout the indentation process. Indentations to a maximum load of 150 mN were recorded, and the residual impressions are compiled in Fig. 3.4-5. It can be seen that the nano multilayer TiN/CrN coating (d) outperformed individual monolayer TiN (a) or CrN (c) in terms of improved toughness.

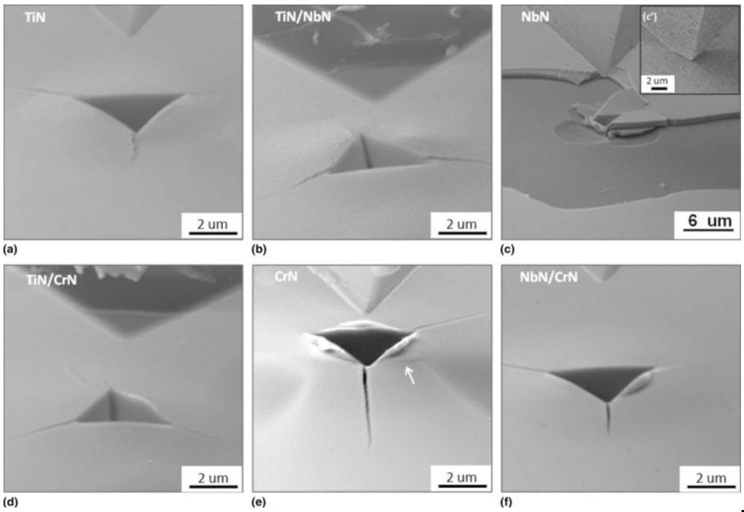


Fig.3.4-5: **In situ SEM nanoindentation images**

Fig.3.4-6: **Zigzag cracking**

In order to in-situ observe the formation and propagation of cracks, a new in-situ four-point bending testing method has been developed. The experiment was carried out in a

[8] K.A. Rzepiejewska-Malyska et al., *Journal of Materials Research*, **24**(2009), 1208-1221.

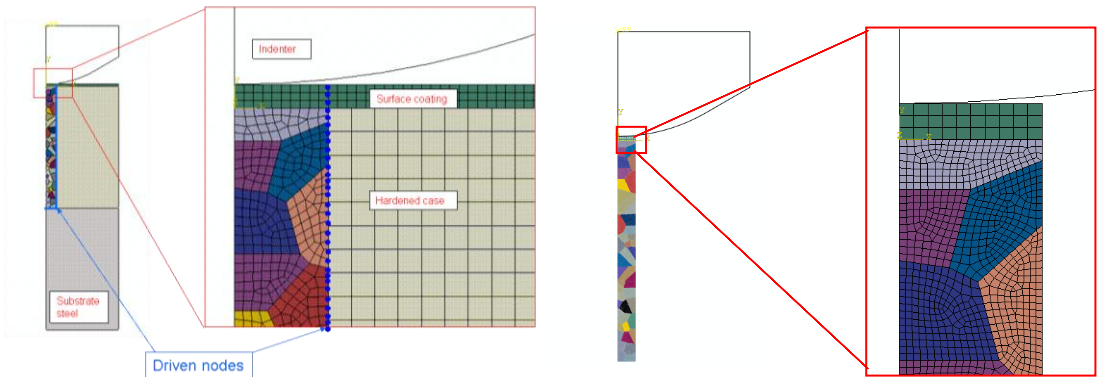
bending device inside a SEM chamber (Fig. 3.4-4b). The cross section of the sample was observed during the test. The deflection rate was 2 μm/sec and the load/strain at first crack was recorded in order to define the fracture strength, and the crack distance was evaluated as the strain increased. It has been found that whilst straight cracks were observed for monolayer CrN coating, slight zigzag cracks were observed for nano-multilayer CrAlSiN coating (Fig. 3.4-6). This indicates that the nano-multilayer CrAlSiN coating possesses a higher resistance to crack propagation.

3.5 Coupling for Multi-Scale Modelling & Software System Design

A. Fundamentals of Integration

Two approaches were initially suggested for bridging the gaps between the various length scales in the project: (1) submodelling with data passing and a web-based software interface and (2) direct coupling leading to a concurrent, single-software calculation. This is because the submodelling approach allows for communication of relevant information, passed from one scale down to the next, starting at the macro-scale, facilitated by a unifying web-based software interface for the overall problem, which allows different software packages to be used for the modelling at the different length scales (end user flexibility).

Based on the extensive literature survey and examination of these two methods, a submodelling approach has been identified as the primary solution for integrating the length scales, rather than a direct coupling and concurrent solution approach. Two submodelling techniques are available: (i) Node-based submodelling and (ii) A surface-based technique. Figs 3.5-1 shows an example of both the global and submodel for a coating problem of the M3-2S project. The driving nodes linking the submodel and global model are shown as blue dots.



(a) (b)

Fig. 3.5-1: FE analysis for a multi-layered surfaces with (a) global and (b) submodel.

The simulation of the Load Bearing Test (LBT) has been implemented with the above general framework of multi-scale modelling techniques, where submodelling was carried out in the direction of decreasing scale, starting with the macro-scale and finishing with the nano-scale. All parameters are to be calibrated from the bottom level with communication to higher levels. A schematic of the linkage for the load bearing test is shown in Figure 3.5-2.

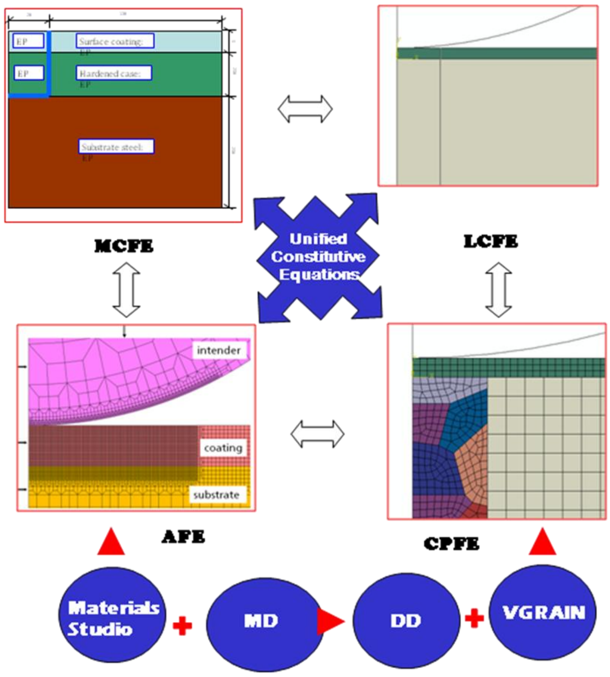


Fig. 3.5-2 Flow diagram for the functioning of the integrated software system

B. Virtual gradient microstructure generation [9]

In micromechanics simulation plasticity is defined based on the presented grain structure. Therefore it is essential for grain-level finite element (FE) simulations such as CPFE (Crystal Plasticity FE) to model polycrystalline grain structure. Gradient grain structures are common in, e.g., a coating system. Hence, representation of a gradient virtual grain structure in agreement with micromechanics simulation requirements is critical to study the materials property. In this period, a multi-zone CPVT model has been developed based on a Controlled Poisson Voronoi Tessellation (CPVT) model to generate (i) gradient mean grain size control across adjacent regions and (ii) grain size distribution control for individual sub-regions.

In practice, there are general two types of multi-zone grain structure: 1) distinct multi-zone grain structure features and 2) continuous multi-zone grain structure. Applying the proposed multi-zone CPVT model to generate distinct discrete zones is straightforward. That is, input the work-piece related parameters and the regularity related parameters for each individual zone. While, for the continuous multi-zone type of grain structure generation, it can be realised by sub-divided the continuous region and linearised to multiple individual zones. Having discretised the continuous region, the multi-zone features can be produced by means the multi-zone CPVT model. Some coating structures have been generated using this technique, and Figure 3.5-3 shows a single layer coating structure with hardened case and substrate.

[9] P. Zhang, D. Balint, J. Lin: 'Virtual graded microstructure generation for crystal plasticity analysis', 19th IFHTSE Congress, 17-20 October 2011, Glasgow, Scotland.

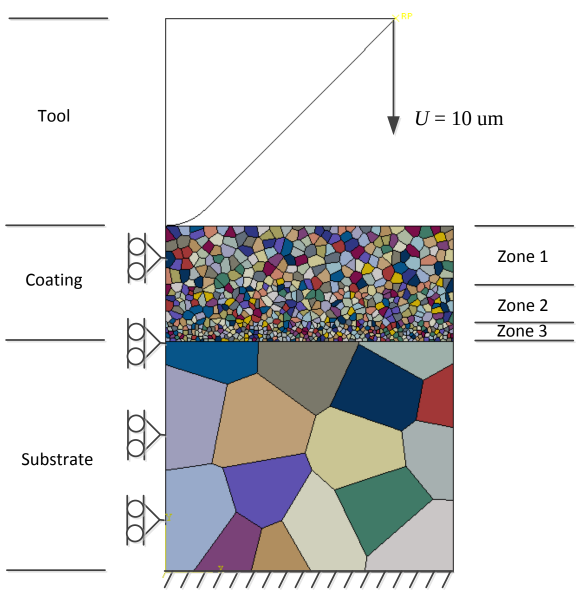


Fig. 3.5-3 Multi-zone model for CPFE simulation

C. Coupling CPFE to DD

Concurrent multiscale frameworks have only very recently been used for the coupling of dislocation dynamics and crystal plasticity formulations. The present model is the first attempt using submodelling and a CPFE description implemented in a commercial finite element package, which should greatly increase the usability of the model. Two dimensional- plane discrete dislocation (DD) simulations are applied in this study (Fig. 3.5-4). Plasticity occurs from the motion of edge dislocations that can nucleate, glide and interact in materials. The rectangular plate under plane strain tension is used to investigate the feasibility and accuracy of the coupling methodology proposed between DD and CPFE.

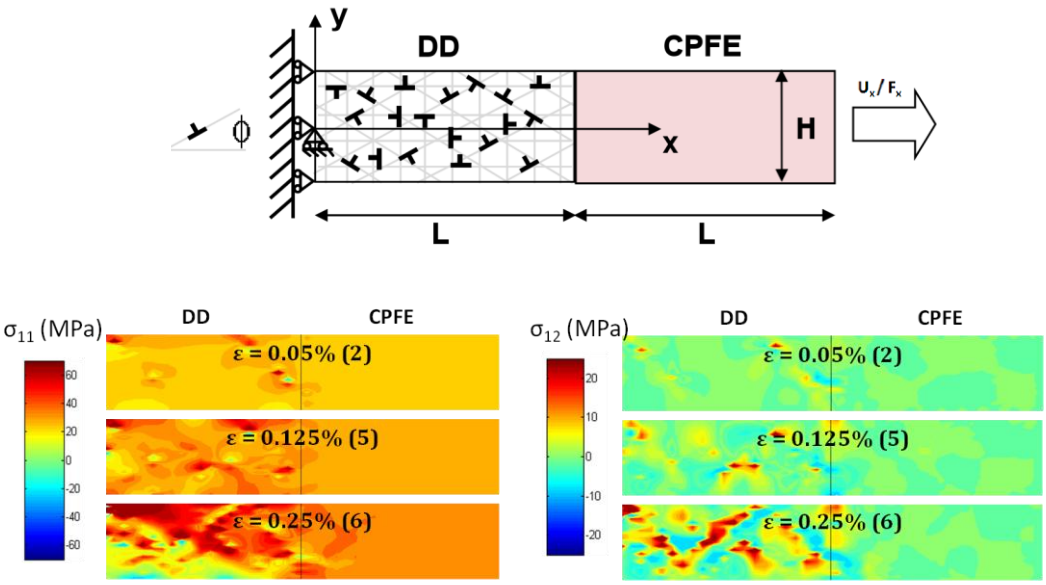


Fig. 3.5-4: Stress contours for coupled systems at step 6, ε=0.25%.

Two stress contour plots at step 6 with maximum strain of 0.25% are shown in Fig. 3.5-4. One can notice that the boundary is well-convergent. The methodology implemented in this study produces an approximate matching at the interface between the two domains due to the fact that discrete dislocations produce singularities and local stress concentration induced by the presence of dislocation cores near the boundaries that cannot be transferred to the crystal plasticity region without causing unphysical behaviour. Furthermore, discrete dislocations are characterised by incompatible deformation gradients while the crystal plasticity formulation is continuous.

D. CPFE coupling to atomic FE

An integrated coupling strategy from MCFE to AFEM has been designed, as shown in Fig. 3.5-5. AFEM can be coupled directly to Discrete Dislocation (DD), (Figs.3.5-5 c & d) then DD to CPFE (Figs.3.5-5b). Finally, CPFE to lower- and macro-level FE (Fig.5a) can be achieved. Hence, the entire system can be simulated with a single FE calculation without approximations. Both the AFEM mesh and the transition area can be easily embedded into DD and an arbitrary CPFEM mesh. The meshing can be done by means of MARC procedures or by using the Python scripts of MARC (or similar API commands in the other FE programs, for instance DEFORM).

An example of simple coating system under nano-indentation is shown in Fig. 3.5-6, where an AFEM region can be easily embedded into DD, then CPFEM region with available FE software. Because there is no principal problem to transform the FE models and the simulation results into other FE programs the presented AFEM can be easily connected to other commercial Finite Elements programs like DEFORM.

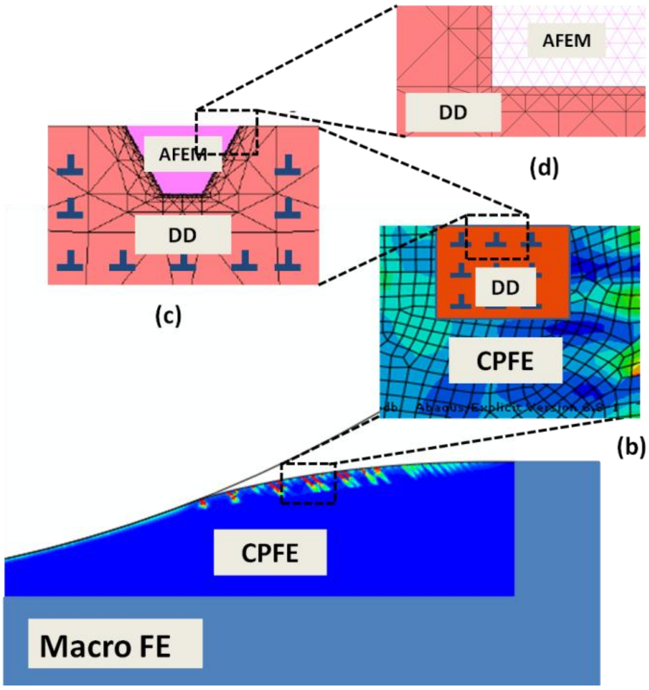


Fig.3.5-5 Integrated simulation strategy

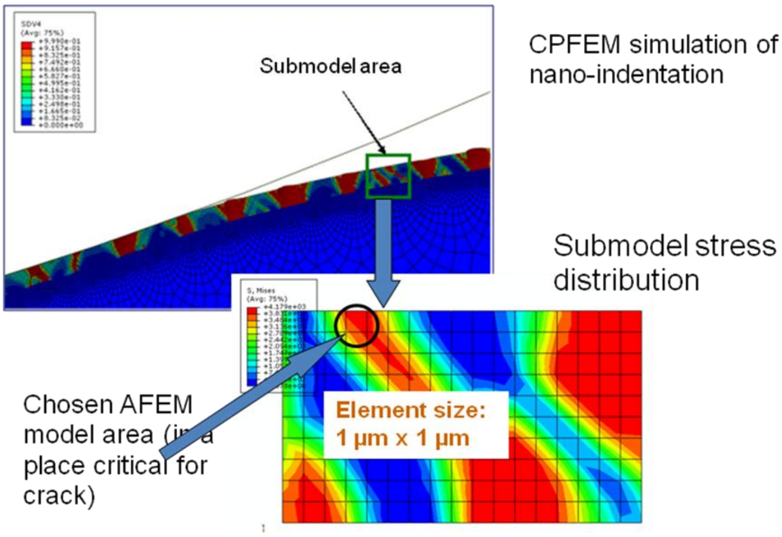
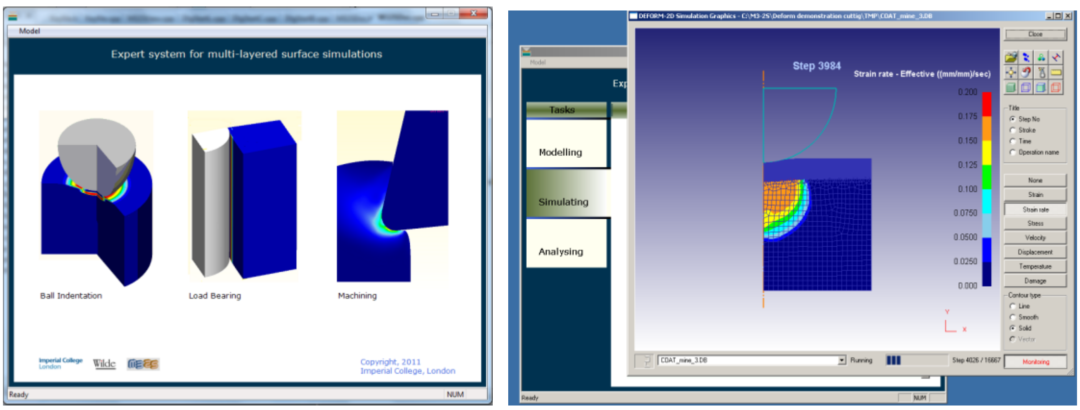


Fig.3.5-6 An example of CPFE coupling to AFE

E. Expert system for multi-layer surface modelling –'Virtual test'

The ESMSM software provides integrated and robust (multiscale) materials modelling for the design and performance prediction of multi-layered surface systems, under different loading (working) conditions including: point contact (e.g., load bearing), line contact (e.g., spur gear contact) and Machining/cutting. The ESMSM is a fully automatic and easy-hands-on system for simulating multilayer surface system performances, under different working conditions. The user-friendly graphical user interface provides easy data preparation and analysis so that engineers and researchers can focus on their design and improvement without learning complex simulation skills and finite element (FE) procedures. Three types of models are currently available: point contact (axial symmetric), line contact (plane strain, e.g., gear contact) and machining/cutting. Each type of simulation can be activated by clicking the corresponding picture/box under the picture (Fig. 3.5-7a).



(a) (b)

Fig. 3.5-7: Model definition window (left) and run-time simulation graph (right)

For a selected model, user can see three main procedures: modelling, simulating and results. Modelling is used for pre-processing, i.e., creating, assembling, and modifying the information required before simulation. Simulating acts as an engine to perform the solution calculation. Results is post-processing that is used for displaying the simulation results. The damage information can be accessed during run time (Fig. 3.5-7b). The initiation of damage is recorded (after appearance). The current damage contour is shown as well. It helps users to monitor the failure of the coating systems.

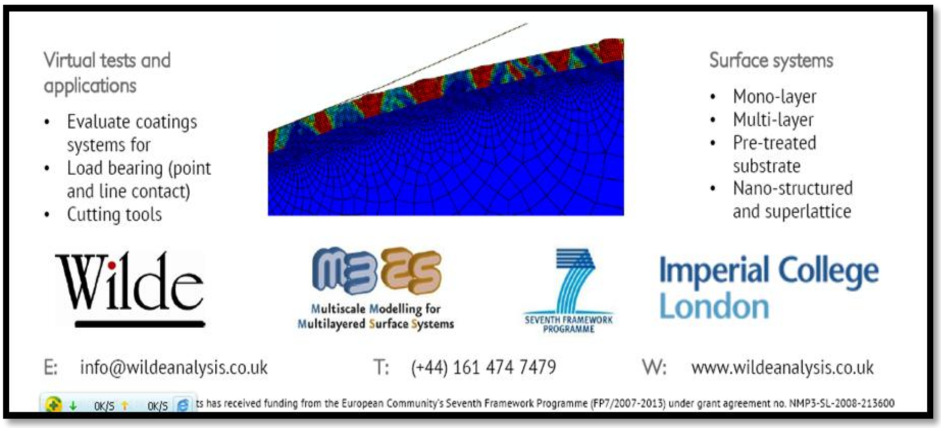


Fig. 3.5-8 Flyer for M3-2S virtual test software

The multi-scale modelling software system developed from the M3-2S project have been demonstrated a wide range of audience including surface engineering society and modelling and simulation society at international conferences, exhibition and many workshops. A flyer promoting the software has been circulated to potential users (see Fig. 3.5-8).

3.6 Validation & demonstration

A. Validation of LBC for engineered surfaces

The macro FEM (MFEM) methodology and software developed from the project have been used predict the load bearing capacity of surface engineered components under point-contact and line-contact conditions.

The validation of MFEM for point-contact (such as in ball bearings) using indentation method has been discussed in Section 3.3. Two surface systems: (1) PNU – TiN coating on H11 and (2) PN2 TiN (2μm) on plasma nitrided (120μm) H11 and the results can be summarised in Table 3.6-1.

Table 3.6-1 Validation resulsts

Surface systems	PNU	PN2
LBC predicted	10N	30N
LBC measured	10-15N	30-35N

The developed MFEM model for line-contact was also used to predict the load bearing capacity (LBC) of two rollers (Fig. 3.6-1). The simulation and experimental results are compared in Figure 3.6-2. It can be seen that the predicted LBC by the MFEM developed from the M3-2S project is in good agreement with the experimentally measured value. In addition, it is also clear that duplex treatment (coating on plasma nitrided) outperforms single coated and that nano-multilayer TiN/CrN coating is better than monolayer CrN coating.

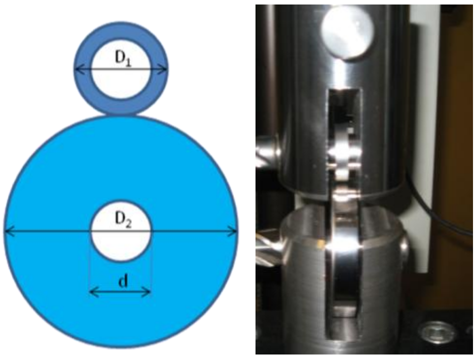


Fig.3.6-1: Roller-on-roller contact

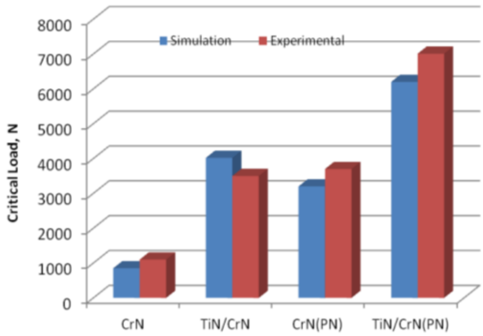


Fig.3.6-2: Validation of line-contact model

B. Industrial validation

Following the successful validation of the multi-scale modelling tool for multi-layer surface engineered 42CrMo4 steel under controlled laboratory conditions, the advanced multi-layer surface systems have also been applied to real industrial components – gears. The gear geometry of the tested gears is based in the FZG type C spur gear (Fig.3.6-3). The gears were manufactured in T-condition 42CrMo4 steel (350HV).

The multi-layer surface systems were optimally designed according to multi-scale modelling and laboratory validation results: (i) Single coating system (SCS): nano multilayer TiN/CrN coating deposited over T-condition 42CrMo4 steel; (ii) Duplex surface system (DSSa): nano multilayer TiN/CrN coating deposited over plasma nitrided 42CrMo4 steel and (iii) Duplex surface system (DSSb): nano multilayer WC/C coating deposited over plasma nitrided 42CrMo4 steel.

Gear type	C	
	Pinion	Wheel
Number of teeth	16	24
Module [mm]	4.5	
Centre distance [mm]	91.5	
Pressure angle [°]	20	
Face width [mm]	20	
Addendum modification	+0.1759	+0.1772
Addendum diameter [mm]	82.405	118.417
Flank roughness [μm]	0.30	
Tip relief (C_a)	$50 \pm 5 \mu m$	
Crowning (C_b)	$30 \pm 3 \mu m$	

Fig. 3.6-3: Geometry of the FZG test gear Type C.

Two different tests were designed: a micropitting test and an FZG load stage test. The critical load for initiation of the crack in three types of multi-layer surfaces for gear system was predicted and the results are compared with the experimental value in Fig.3.6-4 and fairly good agreement has been achieved.

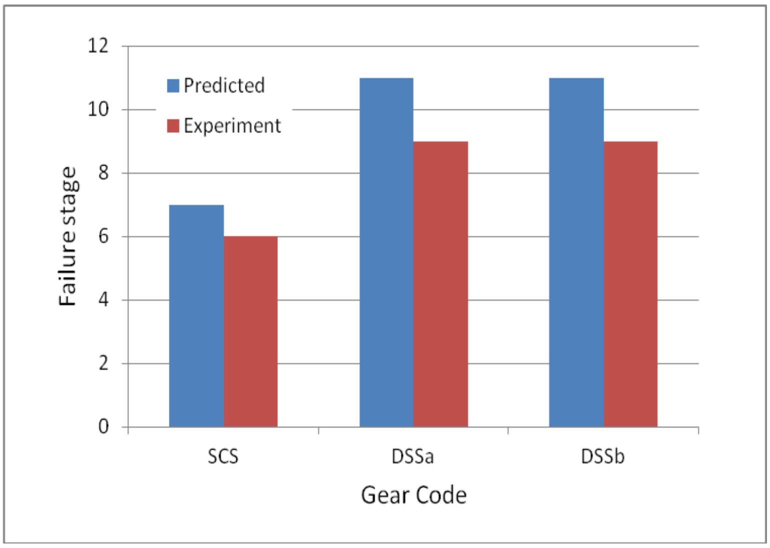


Figure 3.6-4: Numerically predicted and experimentally measured failure stages for gears

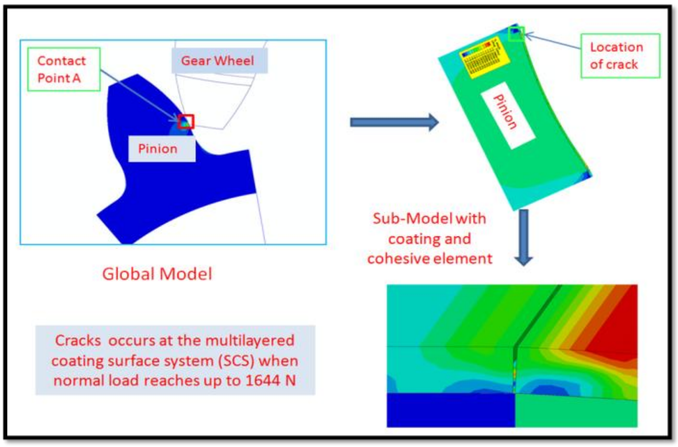
C. Contact analysis

Three possible failure locations of gear system have been investigated through the two steps analysis: global model and sub-model developed from the M3-2S project. Contact mechanical mechanics and failure mechanisms in the points A (where tooth of pinion starts to mesh with gear, Fig.3.6-5a) and C2 (where the load is only supported by one pair of teeth, Fig.3.6-5b) of pinion were investigated.

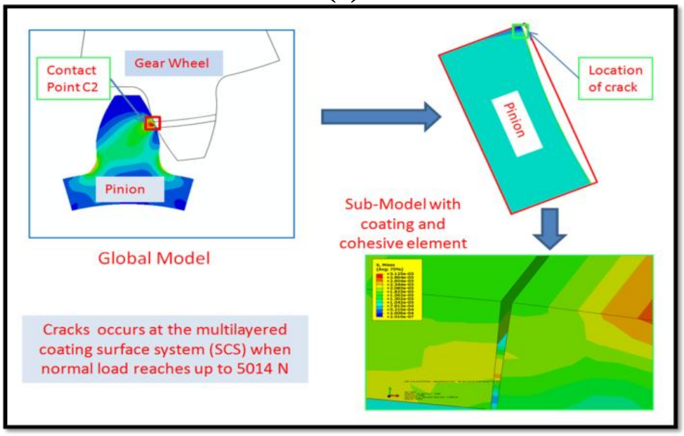
Based on the modelling work, the critical load (Table 3.6-2) for initiation of the crack in three types of surface systems for gears: (1) simple nano multilayer TiN/CrN coating on steel (SCS): (2) nano multilayer TiN/CrN on plasma nitrided steel (DDSa) and (3) nano carbon based composite coating on plasma nitrided steel (DDSb).

Table 3.6-2: Calculated critical load for initiation of cracks

	SCS		DDSa		DDSb	
	Point A	Point C	Point A	Point C	Point A	Point C
maximum pressure (MPa)	1438.04	1533.84	3767.7	3244.84	3633.73	3239.49
Average pressure (MPa)	1320.95	1278.84	3331.1	2917.98	3283.63	2930.65
Normal force (N)	1644.19	5013.72	4882.8	10588.1	4742.88	9693.41
Torque (Nm)		169.62		358.21		327.94
Loading stage	K7		K11		K11	



(a)



(b)

Figure 3.6-5: Contact analysis of surface engineered gears (a) at initial meshing point and (b) at pitch line

D. Industrial validation/demonstration

The impact and potential of the novel multi-layer surface systems designed and optimised using the multi-scale modelling tool have been demonstrated using three industrial demonstrators: (i) WC cutting tool inserts for machining gray cast iron bars and cast steel brakes for railways, cold rolling rollers for rolling Al alloy sheets for jewels, biomedical and food applications and (iii) transmission gears for many industrial sectors (such as transportation).

- Rollers

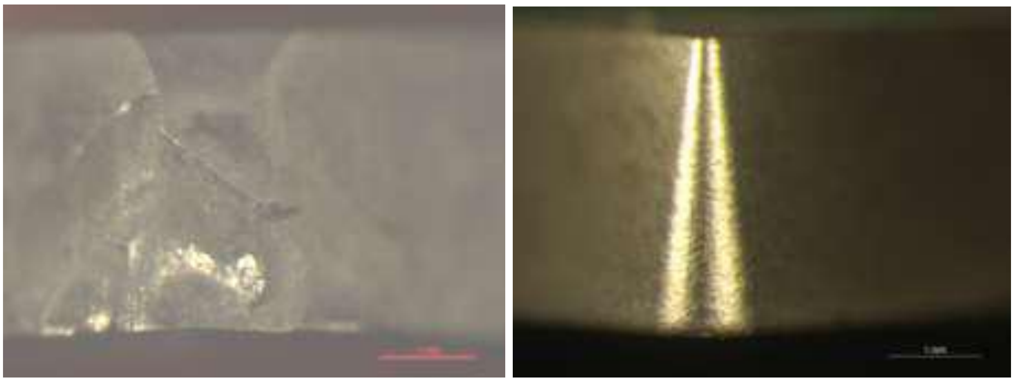
The industrial problem to be addressed is wear and material transfer during rolling Al alloy sheets for jewels, biomedical and food applications. This is a typical problem in rolling thin sheets of Al alloys due to the precipitation of such hard and sharp intermetallics embedded in Al alloys is the main cause for severe damages to the roller surface (Fig. 3.6-6a). The substrate material used is AISI D2 cold working steel, which was heat treated to 58 HRC. Prior to PVD TiN coating, a so-called flash plasma nitriding was applied so as to produce a 50 µm hard diffusion layer without any white layer. Thin slabs of Al alloys reinforced with hard B4Cparticles were used for rolling trials. The main output of the rolling trials was a comparison between the predicted load bearing capacity and the actual resistance of the roller surface in rolling. The visual inspection of the roller surface revealed that as predicted by the M3-2S multi-scale modelling tool, no cracks or grooves were introduced on the surface of the multi-layer surface modified roller (see Fig. 3.6-6b).

(a) (b)

Fig. 3.6-5: Rolling mill (a) and damaged roller (b)

- Cutting tools

The impact of the advanced surface systems has also been demonstrated by surface engineered inserts for cutting tools for machining gray cast iron bars and cast steel brakes for railways. The substrate material was out sourced WC-Co inserts. Based on the modelling work, these inserts were coated by TiN, CrN and nano-multilayer TiN/CrN. The effectiveness of the surface coating systems is evaluated by the wear of cutting tool after the turning tests in terms of cutting force and land wear width. Although it is also cutting condition dependent, in general the wear resistance of WC inserts can be improved by these coatings in the order of TiN, TiN/CrN and CrN. The internal turning of cast steel brakes also demonstrated that while all uncoated inserts failed after machining less than 20 pieces the surface coated WC inserts with TiN and TiN/CrN survived after machining 20 pieces (Fig. 3.6-7).



(a) Uncoated insert (b) TiN/CrN coated inserts

Figure 3.6-7: Damage of cutting edges after machining 20 pieces

3.7 Summary and Conclusions

All the work planned in the original work programme has been performed, converging the following three broad themes according to the type of the activities: (1) Multi-scale modelling; (2) Characterisation, validation and demonstration and (3) Dissemination, training & management. It can be concluded from investigation during this stage. The main scientific and technological achievements can be summarised as follows:

- A portfolio of multi-scale modelling techniques and prototype software systems have been successfully developed including molecular dynamics (MD) simulation of PVD deposition process to identify the atomic structure of thin coatings, contact mechanics and load bearing capacity modelling from atomic (nano-scale) through crystal plasticity (micron scale) to continuum mechanics (macro scale). Coupling techniques to bridge the gaps between modelling activities at different scales have been developed.

- Supported by the multi-scale modelling techniques, a range of novel multi-layer surface systems have been generated and optimised, and a series of specialist techniques and facilities for surface characterisation and validation have been developed to generate materials databases for multi-scale modelling and for the characterisation and validation of the models developed from the project.

- The modelling techniques and the advanced multi-layer surface systems have been successfully applied to some industrial components and significantly improved performance and service life have been demonstrated.

The above advanced techniques will pave the way towards designing optimised surface engineering systems within the shortest possible time and with least cost. Therefore, the above new multi-scale modelling technique developed will facilitate the design and application of advanced multi-layer surface systems in many industrial sectors, thus realising the full potential of surface engineering.

Accordingly, these advances are bound to strengthen science and technology overall, specifically the competitiveness of European surface technology and engineering software industries in the world market. They are expected to produce wide social and environmental benefits including reduced consumption of energy and materials, improved safety and quality of life.

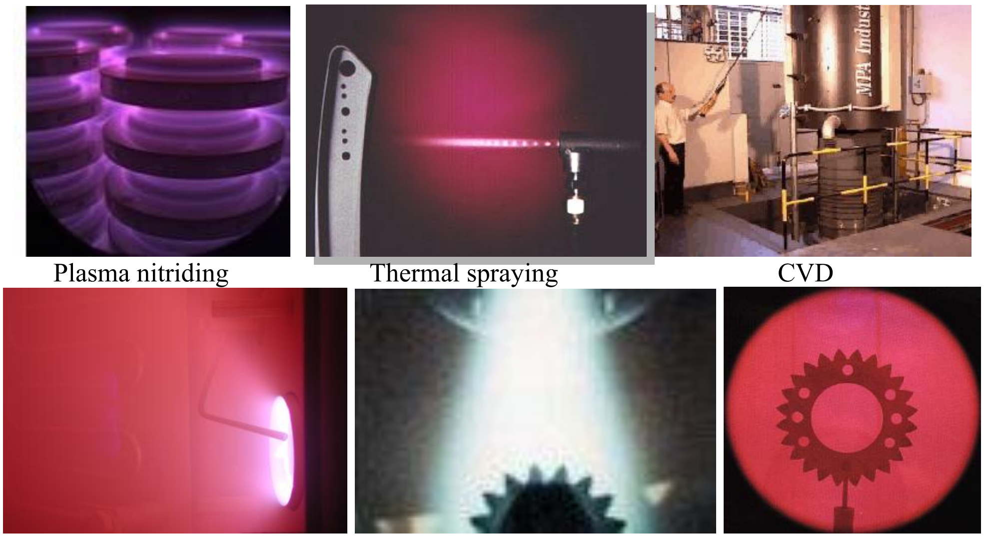
In conclusion, all the scientific and technological targets for the M3-2S project have been achieved based on our effective collaboration.

4 POTENTIAL IMPACT, MAIN DISSEMINATION AND EXPLOITATION

4.1 Potential Impact

4.1.1 Background

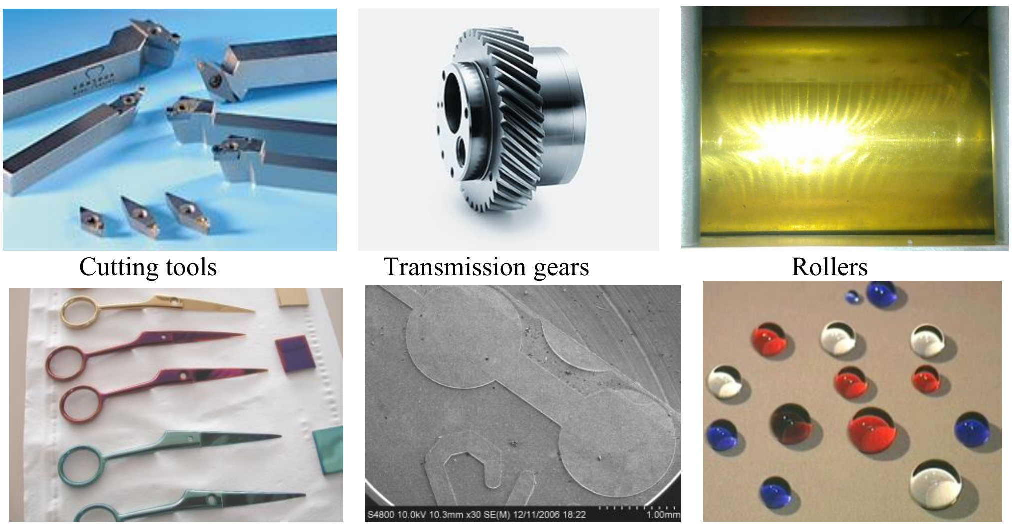
Surface engineering involves the use of traditional and innovative technologies (Fig. 4.1-1) for the design of a surface and substrate together to form a functionally graded multilayered system. It is well-recognised that surface engineering is an ***enabling technology***, applicable to all classes of materials and capable of greatly enhancing a range of properties: chemical, physical (magnetic, optical, thermal, electronic, optoelectronic), mechanical and tribological. As a consequence, it has found wide applications throughout the whole spectrum of industry including aerospace, automotive, power generation, manufacturing (metal forming, machining and fabrication), processing (chemical, food, petro-chemical etc), off-shore, biomedical engineering and general engineering (gears and bearings)(Fig.4.1-1).



Plasma nitriding | Thermal spraying | CVD

PVD | Ion Implantation | PI3

Fig. 4.1-1: Industrially important surface engineering techniques



Cutting tools | Transmission gears | Rollers

PVC coloured scissors | Patterned surfaces | Functionalised textile

Fig. 4.1-2: Typical examples of surface engineered end products

The range of possible surface systems has provided more opportunities for application but, due to the lack of reliable surface modelling techniques, the design of multilayered surfaces is normally based on experience, empirical formula or a trial-and-error approach. These methods are obviously laborious and inefficient, lacking reliability and increasing product development time, energy use and cost.

Supported by EC, the M3-2S collaborative research project (CP-FP 213600-2 M3-2S) under the EC's Seventh Framework Programme has provided a platform for 12 international partners to address the above urgent scientific, technological and market need for consistently reliable high performance multilayered surface systems, by developing generic, robust multiscale materials modelling techniques.

4.1.2 Main Scientific/Technological Outputs

Over the past three years (1 November 2008 to 31 October 2011), a portfolio of multi-scale modelling techniques and software systems have been successfully establish, a range of novel multi-layer surface systems have been produced and a series of specialist surface characterisation and validation techniques and facilities have been developed. Most of these technologies are close to applications.

(I) A portfolio of multi-scale modelling techniques and software systems:

1) MD model of TiN deposition process, adatom distribution and nanoindentation of thin films.
2) Interface programme to bridge MD & AFEM for TiN and AFEM model for dislocation and crack formation.
3) VGRAM module for CPFE modelling for graded multilayer surface systems.
4) Macro and lower FE for the prediction of load bearing capacity under point-contact (e.g. bearings & cutting tools), line-contact (e.g. rollers & sliding bearings) and complicated (e.g. gears) conditions.
5) Coupling of models for different scales: direct coupling of DD/CPFE and coupling via submodelling for DD/AFE, CPFE/AFE and lower FE/CPFE
6) Integrated software system designed and all features implemented

(II) Advanced multi-layer surface systems & characterisation techniques and facilities:

1) Nano-multilayer or supper-lattice coatings: nTiN/CrN, nTiAlSiN and CrAlSiN for general engineering components, cutting tools and hot working dies
2) Advanced duplex surface systems combining surface coatings with deep-case hardening for many demanding components
3) Techniques and equipment for environmental nanoindentation, nano impact and FIB/SEM.
4) Techniques and facilities for *in situ* SEM nano-indentation, 4-point bending and micro compression
5) Methodology facilities for laboratory validation under controlled conditions and industrial in industrial environment.
6) Three industrial demonstrators: WC inserts for machining cast iron bars and cast steel brakes, rollers for cold rolling of non-ferrous thin sheet materials and steel gears for transmission

These advanced techniques will pave the way towards designing optimised surface engineering systems within the shortest possible time and with least cost. Therefore, the above new multi-scale modelling technique developed from the M3-2S project will facilitate the design and application of advanced multi-layer surface systems in many industrial sectors, thus realising the full potential of surface engineering. It is expected that the new technologies developed from the M3-2S project will produce huge scientific and technological impact, as well as economic, social and environmental impact, thus maintaining European competitiveness in the world surface engineering market.

4.1.3 Scientific and technological impact

In the M3-2S project, a novel, integrated multiscale modelling technology has been established through a bottom-up approach based on molecular dynamics (MD) modelling and top-down approach based on four lengthscale FE mechanics modelling. Finite element simulation theories have been adapted and used for all four lengthscale mechanics analysis. Theses predictive models are essential for the design and performance prediction of surface engineering systems covering nano-scale multilayer (i.e. superlattice), micro-scale monolithic layer or graded interlayer and mm-scale deep hardened surface cases.

Scientifically, the M3-2S project has provided new insights into the atomic-level structure of the individual layers and interfaces in nano-scale multilayered or superlattice coatings through MD simulation of PVD deposition and the formation of the layer structures. The reliable 2NN MEAM inter-atomic potential for Ti-N and Cr-N can provide essential scientific database for future atomic level modelling (such MD and AFEM).

The MD modelling for nano-indentation, AFEM modelling of and crack initiation, DD modelling of dislocation, first-principle modelling of interface adhesion energy and macro FEM failure analysis of tested gears have greatly advanced scientific understanding of hardening, toughening, deformation and failure mechanisms involved in multi-layer surface systems. In addition, M3-2S has certainly advanced the state of knowledge and ensure the international leading position of EC research in modelling activities and coupling techniques for modelling at different scales in particular.

Technologically, the M3-2S project will enable surface engineering designers to optimise efficiently their existing multiscale multilayered surface systems and to develop new applications. This will underpin the technological development in virtually all industrial sectors; in particular, this will pave the way for the future development of new tools and thus technologies for high-speed dry machining, micro-forming and micro-machining, pressure-die casting of non-ferrous alloys, application of high-performance components for transportation and cost-effective high speed hot forming.

In addition, efficient modelling procedures have been established for the complex modelling problems encountered in multiscale and multilayered surface systems on different substrates across a wide range of applications. Furthermore, the advanced techniques developed from the project for surface characterisation and property evaluation at nano- and micro-scales (such as environmental nanoindentation, nano impact and *in situ* SEM nano-indentation, 4-point bending and micro compression) will provide an important technical basis for the development of procedures and standards for R&D and quality control for emerging nano and micro-manufacturing.

4.1.4 Economic, social and environmental impact

As discussed in last section, the predictive models for the processing, structure and properties of multiscale layered surfaces developed and validated from this project will allow the performance of surface engineered components to be successfully predicted and, conversely, specific performance characteristics to be achieved, quickly and efficiently. This will significantly **enhance the competitiveness** of European coating specialists, tool and engineering component manufacturers in the ever-competitive global market, thus producing important economic, social and environmental impact:

(A) Increased service life and reduced down-time
The validation and demonstration work in project has clearly demonstrated that the advanced multi-layer surfaces systems can increase effectively increase the wear resistance, the load bearing capacity and life of the industrial demonstrators. For example, the modelling tool developed from the project has enabled the design of optimal duplex system combining nano multilayer TiN/CrN coating with active screen plasma nitrided hard case can increase the load bearing capacity and wear resistance by more than 3 and 1000 times respectively compared currently used monolayer TiN or CrN coating on hardened steel. In addition, the high temperature wear resistance of new nano-multilayer CrAiSiN coating is much better than the currently widely researched nano-multilayer TiAiSiN coating.

The significantly improved load bearing capacity and wear resistance conferred by the advanced nano-multilayer coatings or multi-layer duplex systems can prolong the lifespan of many manufacturing equipment and products such as cutting tools, forming tools and general engineering components. Longer component life can reduce the need for replacing failed cutting tools, hot working dies and engine and transmission components, thus reducing the machine down-time and improving productivity; the early failure of tools can lead to the waste of valuable components, especially in high-speed automatic production; and long service life of surface engineered tools and components can reduce the need for new production of the same item, thus reducing the consumption of raw materials, energy and natural resources and contributing to sustainable development.

(B) Saving on lubricant oil use – metal forming & metal shaping
The use of high hardness and oxidation resistant nano-multilayer CrAiSiN coating also enables dry machining, thereby impacting environmental concerns relating to the use of, and disposal of, liquid cutting coolants. In addition, novel dies coated with a multilayered coating with self-lubricating layers will make sheet metal forming possible without using lubricating oil.

(C) Improved fuel efficiency and reduced CO_2 emission
Light alloys, such as titanium and aluminium alloys, are attractive for transportation applications because of their high strength-to-weight ratio and thus weight saving potential. However, their poor tribological behaviour has restricted, to date, the very large-scale uptake of light alloys, especially under dynamically loaded conditions. This is mainly because these light alloys are soft and cannot be deep hardened by conventional surface treatment methods; furthermore thin ceramic coatings failed quickly because of the lack of mechanical support from the substrate (i.e. poor load-bearing capacity).

Therefore, the duplex surface systems and the methodology of modelling-based design and optimisation could be applied to dynamically loaded light alloy components by combining oxygen diffusion or energy beam surface alloying with the nano multilayer coatings developed from the project. It is estimated that the application of surface engineered light alloys in engines, valve trains and driving trains can lead to the reduction of fuel consumption by 3%. Currently there are a total of about 170 million cars used in Europe and if an average family car uses 1500 litres per year, the total fuel savings in Europe can be calculated to be: 1500 (litres) x 170,000,000 (cars) x 3% = **7.65 billion litres /year**.

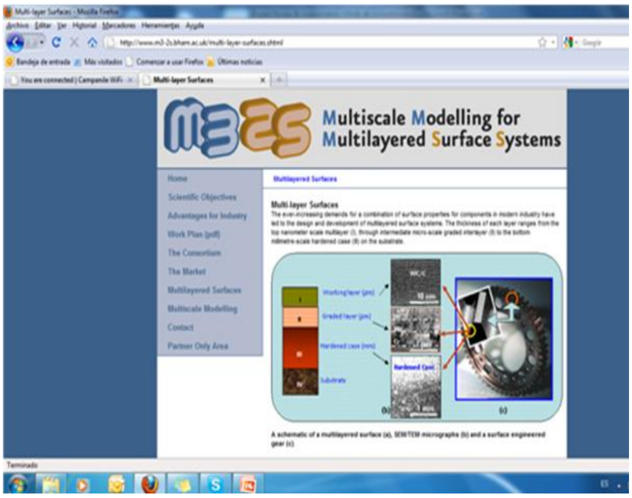
(D) Safety, health and quality of life
The proposed ***predictive*** modelling tools will significantly improve ***performance and reliability*** of multilayered surface systems, and result in better safety factors in manufacturing industry and with the components subjected to better-designed multiscale multilayer surface treatments. The innovations resulting from the proposed research may positively affect the health of the population, no less due to the reduction in CO_2 emissions following reduced fuel consumption. Moreover, potential applications of the high performance multilayered surface systems to such medical devices as joint prostheses and other body implants can improve the health and quality of life of the aging population.

4.2 Main Dissemination Activities

A portfolio of dissemination activities have been conducted during the course of the M3-2S project to implement the Dissemination Plan defined in the Section 3.2 of Annex I. The main dissemination activities undertaken by the M3-2S consortium can be summarised as follows.

A. Website & webpage
The project website (Fig. 4.2-1a) has been set up at the home address of the Coordinator's institution (The University of Birmingham) www.m3-2s.bham.ac.uk and updated periodically to serve as a communication platform with in the consortium and promote dissemination and new collaborations outside the consortium. Following the satisfactory interim assessment outcomes, the M3-2S project has been selected by CORDIS Technology Marketplace to disseminate our research achievement via a dedicated web page (Fig. 4.2-1b).

B. Special sessions in major international conferences
In addition to many presentations by individual partners, the M3-2S consortium have been successfully set up M3-2S special sessions in two major international conferences: (1) **Multiscale 2010 International Conference** (Sept. 2010, Paris) – the unique international conference in multi-scale modelling to address modelling specialists from all over the world. Seven talks were present to the Conference in two special sessions; (2) **The 19th Congress of International Federation for Heat Treatment and Surface Engineering, IFHTSE** (Oct. 2011, Glasgow, Fig.15) – official Congress of IFHTSE (Fig. 4.2-2a). Ten presentations were delivered by the M3-2S consortium (Fig. 4.2-2b) to disseminate M3-2S project results to top surface engineering specialists from about 30 countries.



(a)

(b)

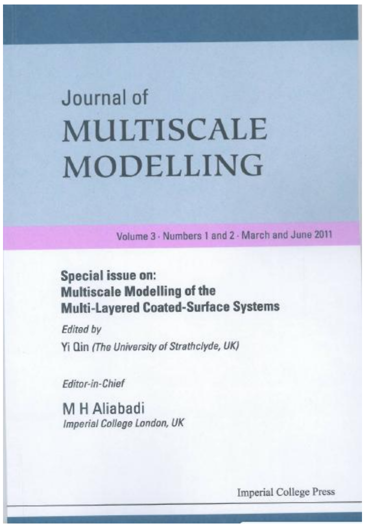
Fig. 4.2-1: M3-2S **project website (a) and CORDIS webpage (b)**

(a) (b)

Fig. 4.2-2: 19th IFHTSE Congress (a) and M3-2S special session (b)

C. Special issue of Journal of Multi-Scale Modelling

Seven peer reviewed papers on multi-scale modelling of multi-layer surface systems have been published in international journal dedicated to multi-scale modelling, *Journal of Multi-scale Modelling* (Fig.4.2-3)



Volume: 3, Issues: 1-2 (March & June 2011)

PARAMETERIZED FINITE ELEMENT MODELING OF THE SURFACE SYSTEMS WITH COATINGS WHICH CONSIDERS THE CRACKING OF THE COATINGS AND INFLUENCES OF THE CASE-HARDENING OF THE SUBSTRATE
J. FENG, Y. QIN, Q. ZENG, E. ALMANDOZ, G. FUENTE, H. DONG, R. RAGHAVAN and J. MICHLER
DOI No: 10.1142/S1756973711000315
Page: 1-22

MOLECULAR DYNAMICS STUDY OF THE INTERFACE-STRUCTURE FORMATION OF A COPPER/SILVER BILAYER
Z. H. XU, L. YUAN, D. B. SHAN, B. GUO, H. S. DONG and X. Y. LI
DOI No: 10.1142/S1756973711000327
Page: 23-38

THE ATOMIC FINITE ELEMENT METHOD AS A BRIDGE BETWEEN MOLECULAR DYNAMICS AND CONTINUUM MECHANICS
R. NEUGEBAUER, R. WERTHEIM and U. SEMMLER
DOI No: 10.1142/S1756973711000339
Page: 39-47

MODELING OF FAILURE FEATURES FOR TiN COATINGS WITH DIFFERENT SUBSTRATE MATERIALS
S. WANG, J. LIN and D. BALINT
DOI No: 10.1142/S1756973711000340
Page: 49-64

PREDICTION OF RESIDUAL STRESS IN MULTILAYERED COATINGS WITH A LINEARLY ELASTIC MODEL INCORPORATING DENSITY FUNCTIONAL THEORY CALCULATIONS
DEQIANG YIN, XIANGHE PENG, YI QIN and ZHONGCHANG WANG
DOI No: 10.1142/S1756973711000352
Page: 65-78

AUTOMATED CALIBRATION OF A VOID CLOSURE MODEL FOR HIGH-TEMPERATURE DEFORMATION
S. AFSHAN, D. BALINT, J LIN and D FARRUGIA
DOI No: 10.1142/S1756973711000364
Page: 79-90

AN ADVANCED ADAPTIVE FINITE ELEMENT CODE APPLIED FOR COATING-SUBSTRATE SIMULATION
JÜRGEN LEOPOLD, KATRIN HELLER, ARNDT MEYER and REINER WOHLGEMUTH
DOI No: 10.1142/S1756973711000376

Fig. 4.2-2: Special issue of *Journal of Multi-Scale Modelling* on M3-2S

D. General publications

Based on the outcomes of this project, scientific publications in the form of journal papers and conference presentations have been generated from the project. Peer reviewed papers have been published in more than 10 international leading journals. As can be seen from Table 4.2-1, the publication target for the M3-2S project has been fully achieved.

Table 3-1: M3-2S scientific publications

Type of Publications	Planned	Achieved To-date
Conference presentations	9-12	25
Journal papers	6-9	20

4.3 Exploitation

The main exploitable outcomes from the M3-2S project is summarised in Table 4.3-1. Some exploitation activities have started towards the end of this project as indicated by the start from 2011 in Table 4.3-1and the timing for the other exploitable outcomes is also indicated.

Table 4.3-1: Main exploitable outcomes from the M3-2S project

Outcome/Results:	Expected Impact/ Targeted User Groups:	Timing (Y)
Software System & GUI design & development	Design engineers in manufacturing and software companies	2012-2017
New Advanced Adaptive Finite Element Code (AAFEC)	This code can be used to simulate cutting and damage of cutting tools. Users: cutting tool companies and software companies	2011-2012
Modelling-based design methodology and software systems for the design and process prediction of multilayered surfaces at atomic level	Development of design methodologies Design engineers in the manufacturing industries	2012-2018
Continuum Mechanics Modelling Techniques for Multilayered Surfaces	Improving efficiency and accuracy in the design and analysis of coated engineering-surface systems. The targeted user-groups include: Surface Engineering; Manufacturing and Software Suppliers.	2012-2016
Techniques and Models for Macro-Mechanics Modelling of Multi-layered Engineering Surface-Systems	Enabling methods, procedures and computational techniques for more efficient design and analysis and manufacturing planning of the multi-layered engineering-surface systems. This will have impact to the coating industry and engineering designers.	2012-2015
Database of load bearing capacity and residual stresses of mono and multilayer coatings	Future MSC Engineers	2011-2014
Mechanical properties database of mono and multilayer coatings	Future MSC Engineers	2012-2014
New multi-layered duplex surface engineering systems	Multi-functional surfaces important for surface engineering subcontractors and engineering & medical device designers	2011-2014
Design of surface modified roller to be used for cold rolling operations on metallic alloys with hard particles	Producers of small to medium rolling mills	2011-2013
Environmental nano-indentation technique of nano multi-layer coatings	Unique mechanical property measurement technique for multilayer surfaces. Users: surface characterisation facility manufacturers	2012-2016