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MODELLING AND SIMULATION OF COATING-SUBSTRATE-SYSTEMS
STATE-OF-THE-ART AND FUTURE TRENDS

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Outline

- State-of-the-art
- Why do we need Multiscale Modeling?
- Bridging the Gaps Between the Modelling Activities at Different Scales (M3-2S Project)
- Summery

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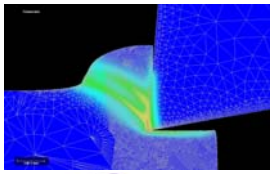
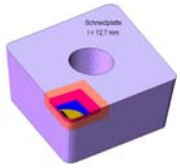
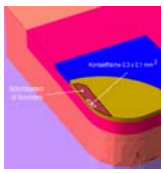
State-of-the-art

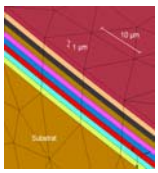


From the mathematical point of view: Big dimensional problem

2.6 Mio DOF







Source: Oosterling; van den Berg; Renevier, Meisel; Leopold: **ICMCTF 2002**

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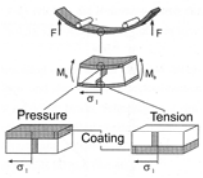
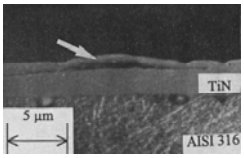
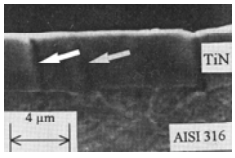
State-of-the-art



Damage	Stress criterion	Energy criterion
Tension stress cracks $\sigma_{\perp}$	$\sigma_{\perp,L} \geq \sigma_{R,tension}$	$K_{Iceb} \geq K_{IC,Iceb}$
Shear stress cracks $\tau_{\parallel}$	$\tau_{\parallel_L} \geq \tau_{R_b}$	$K_{IIceb} \geq K_{IC,IIceb}$
Buckling	$-\sigma_{\perp,L} > \sigma_{kl}$	$K_{IIceb} \geq K_{IC,IIceb}$





Source: Th. Bertram; PhD ThesisTU Freiberg 2001

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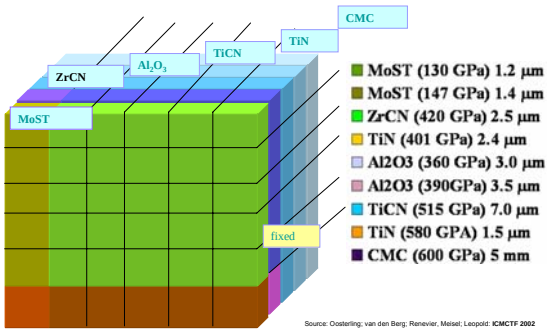
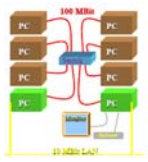
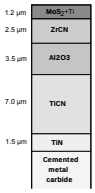
State-of-the-art



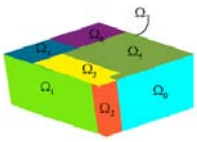
Source: Oosterling; van den Berg; Renevier, Meisel; Leopold: **ICMCTF 2002**

State-of-the-art

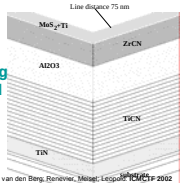




Domain Decomposition Method



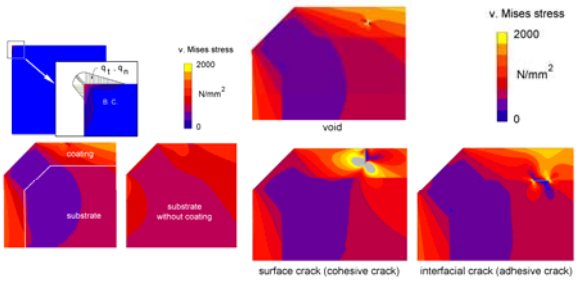
Total Cutting length: 11.700 m
130 days manufacturing with one MoS_2 – coated cutting insert !!!



Source: Oosterling, van den Berg, Reneiver, Meijer, Leopold, ICMCTF 2002

State-of-the-art

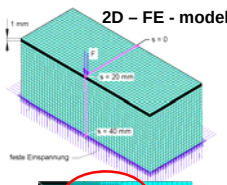
Failure modes



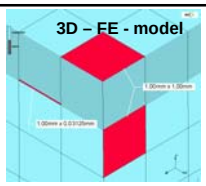
Source: DFG Le 746/22-4

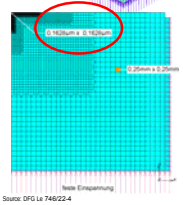
State-of-the-art

2D – FE - model



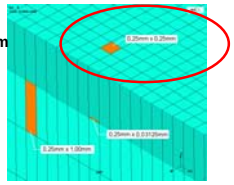
3D – FE - model





Source: DFG Le 746/22-4

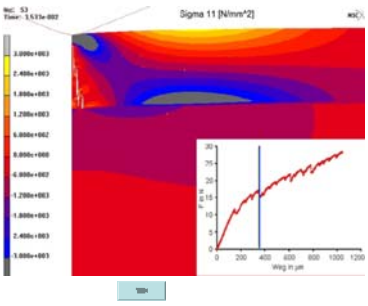
Minimum element size 250nm square



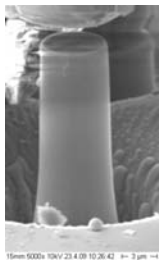
Crack Initiation in Coating-Substrate-Systems

State-of-the-art

FE-Simulation



SEM - Experiment



Source: DFG Le 746/22-4

Source: EMPA

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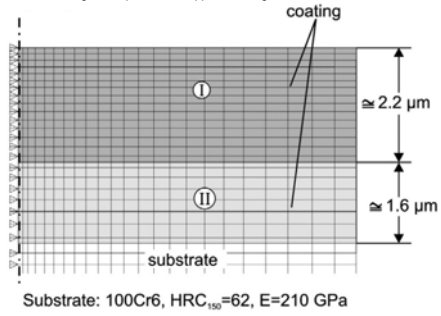
Ball - cratering test imprint on the applied coating and the FEM simulation of its structure.



Substrate: 100Cr6, HRC_{150}=62, E=210 GPa

Source: K.-D. Bouzakis , A. Asimakopoulos, M. Batsiolas Surface & Coatings Technology 202 (2008) 5929–5935

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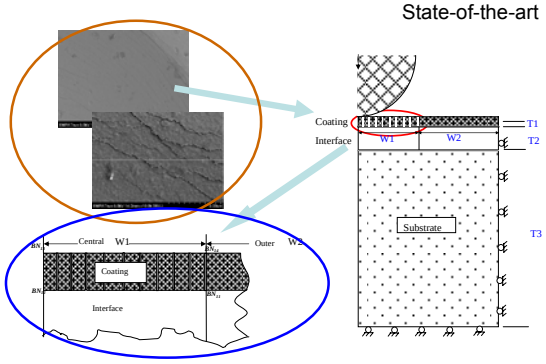

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Macro-Level Damage Module

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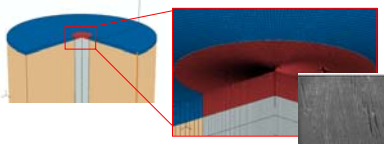
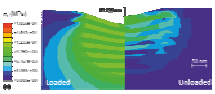
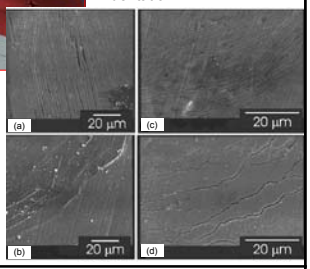


FE model for a single layer coating system under indentation





SEM analysis of the circular cracks observed after the 50N indentation on samples coated with TiN

J. Feng, Y. Qin, R. R. Koodakal and J. Michler:
A NEW TECHNIQUE TO INVESTIGATE THE LOAD-BEARING CAPACITY OF A COATING ON TOOL STEEL

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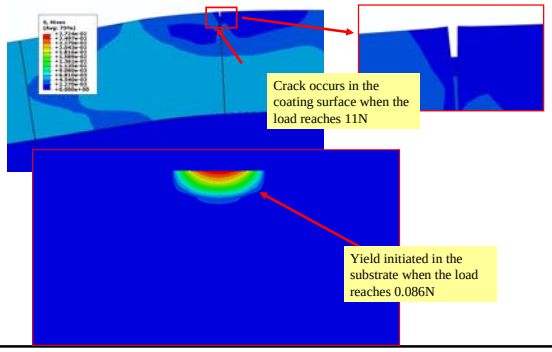
Load Bearing Capacity for Multi-layered Surface System

State-of-the-art



Crack occurs in the coating surface when the load reaches 11N

Yield initiated in the substrate when the load reaches 0.086N

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Chip Formation Simulation to determine the loads at the coatings

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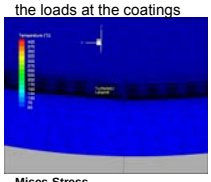
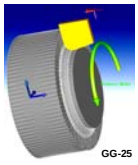
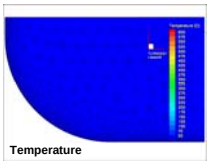


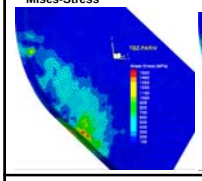


GG-25

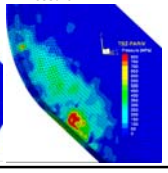


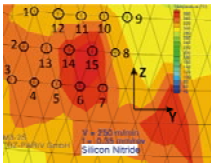
Temperature

Mises-Stress



Pressure





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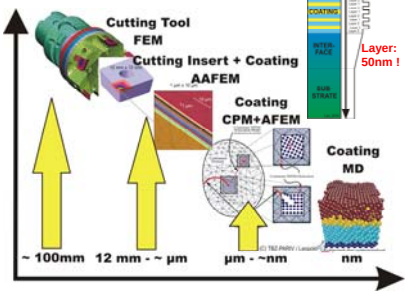
Why do we need Multiscale Modeling?

Arch of Galerius

Few Millimeter



Source: http://commons.wikimedia.org/wiki/File:THES_Arch_of_Galerius_E_face.jpg

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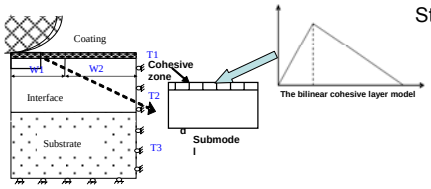
State-of-the-art

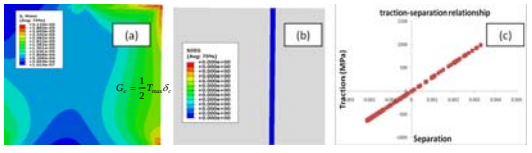


$$G_c = \frac{1}{2} T_{\max} \delta_c$$

G_c Critical Energy-release rate

T_{max} maximum traction

δ_{max} is the characteristic cohesive-zone length



(a) Mises stress; (b) Damage coefficient; (c) Traction-separation relationship for a cohesive element in the coating.

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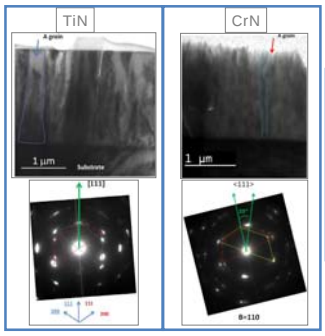
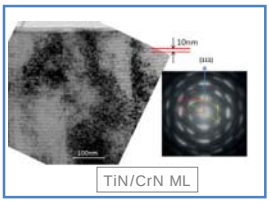
Why do we need Multiscale Modeling?



Microstructure



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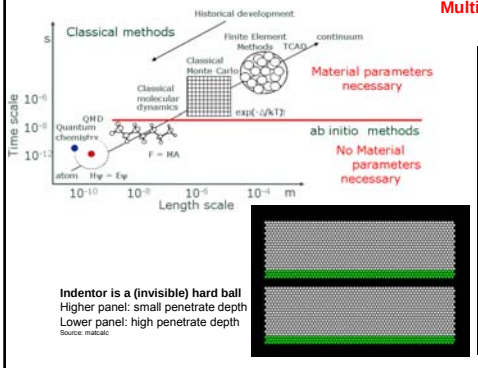
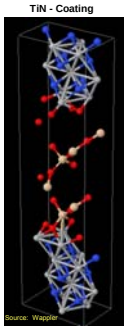
Multiscale problem



Indentor is a (invisible) hard ball
Higher panel: small penetrate depth
Lower panel: high penetrate depth
Source: matcalc

TiN - Coating



SiO_2-Substrate

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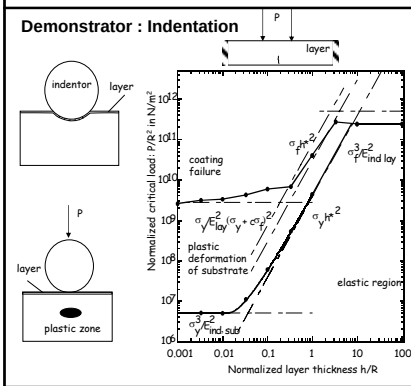
Demonstrator : Indentation



J. Michler, E. Blank
Thin Solid Films 381 (2001) 119-134

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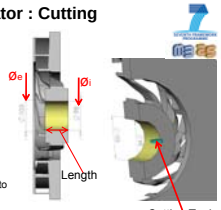
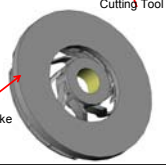
Demonstrator : Cutting

Initial cutting inserts
SPMR 120308 (hard metal without coating)

- Machining Process: **TURNING** (internal)
- Internal Diameter: Ø98 mm goes to
- External Diameter: Ø103 mm
- Advance Speed: 0.4 mm/rpm
- ω: 76 rpm
- Length: 60 mm





Electromagnetic Brake
CC-270

Source: Fundiciones del Estanda S.A.

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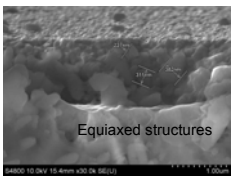
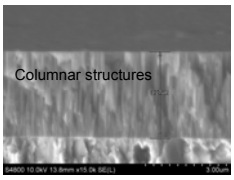
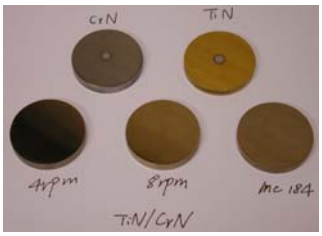
Different structures







Source: Fundiciones del Estanda S.A.

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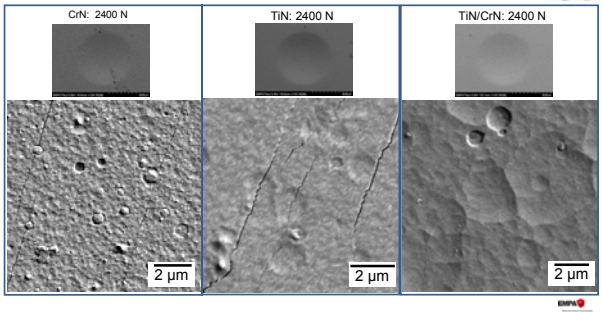
Crack patterns: 5mm ∅ WC sphere



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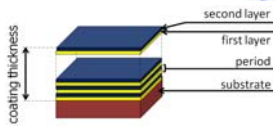
Mechanical Material Properties

Layer Type	Materials	Layer Thicknesses (nm)	Total Coating Thickness (nm)	H (GPa)	E_r (GPa)	ν -
Monolayer	TiN	646		15.7	224.4	0.18
	CrN	1069		17.7	205.6	
	NbN	780		32.1	290.4	
Multilayer	TiN/NbN	16.66 / 16.28	659	15.05	208.5	
	TiN/CrN	18.03 / 17.52	697	15.72	190.8	
	NbN/CrN	19.61 / 18.65	765	18.9	197.6	



	Total thickness [nm]	Number of periods	Deposition temperature [°C]
TiN	1800	1	500
CrN	2000	1	450
TiN/CrN	2000	200	420

EMPA

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Table 1. List of M32S case studies

Partner	Business case	Application field	Selected components	Requested Coating Functionalities	Candidate coatings
DIAD	Rough turning of cast iron (grey cast iron GG25)	Automotive (bars, brake discs, cylinder block, etc.)	Si_3N_4 based ceramic cutting tools	Antiwear	Hard coatings (TiAlCN)
FDE	Turning of quenched and tempered steel (15CrMoV5-10)	Casting dies for railway application	CVD coated Hard metal insert (TiCN, Al_2O_3 and TiN)	Antiwear and oxidation resistance, Increase of tool life	Catodic arc PVD with coatings having a Cr/CrN multilayer structure
POLITO	Cold rolling of precious metals, Cu alloys or Al alloy sheets	Jewels, biomedical, food sector	CrMoV alloyed steel roller mounted on a cold rolling 60 tons mill	Increase of wear resistance of the roller with 30% cost reduction with respect to state of the art solution	Open to suggestions

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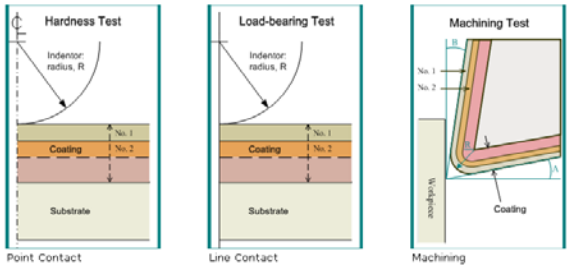
Three typically test methods



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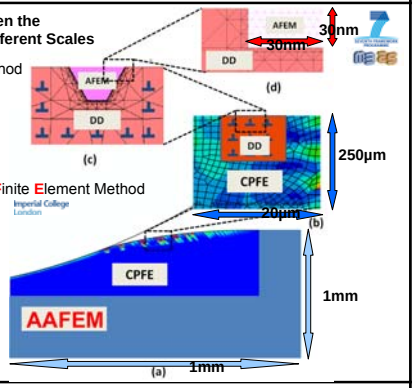
Bridging the Gaps Between the Modelling Activities at Different Scales

Atomic Finite Element Method

Crystal Plasticity Finite Element Method

Advanced
Adaptive
Finite
Element
Method



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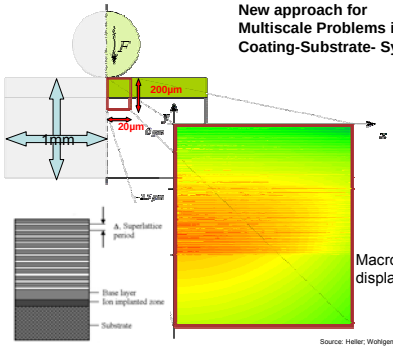
AAFEM Module for Super Lattice Coatings

New approach for Multiscale Problems in Coating-Substrate- Systems



100 several 50 nm layers simulated starting with **TiN** and finished with **CrN** at the interface from coating to substrate

model with highest number of elements (***superlattice – TiNCrN_170)*** with 889105 elements

Macro submodelling to export displacements to CPFE subdomain

Source: Heller; Wohlgemuth; Meyer; Leopold – CIRP CMMO 2011

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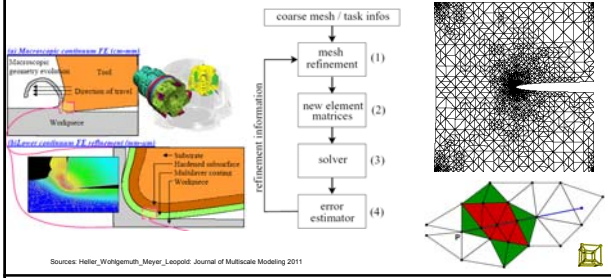
Macroscopic and lower Continuum FE refinement

The Solver: PCGM
example: hierarchical basis preconditioner
very cheap and quick



Sources: Heller_Wohlgemuth_Meyer_Leopold Journal of Multiscale Modeling 2011

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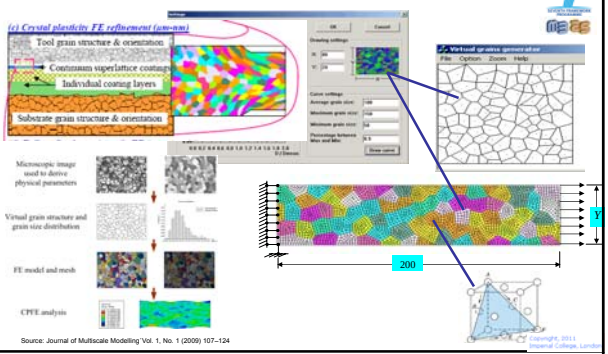
Micro-Mechanics Modelling based on Crystal Plasticity FE refinement



Source: Journal of Multiscale Modelling Vol. 1, No. 1 (2009) 107–124

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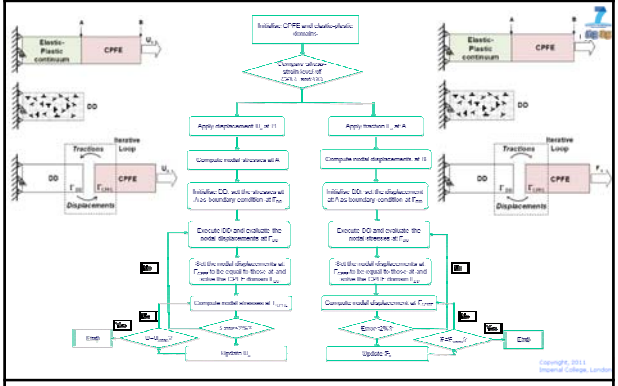

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Simulation of the TiN film growth on TiN(001)

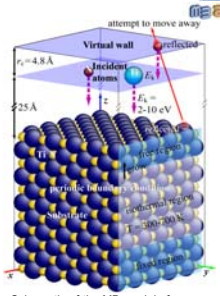
MD-Simulation

Potentials

Interaction	MEAM Potential
Ti-N	Ours
N-N	Lee's[9]
Ti-Ti	Kim's[10]

Parameters of MD model

Model	Description term	Value
	$l_x \times l_y \times l_z$ N_{sub}	[100]×[010]×[001] 1100
	d_{res}	3 ML
	d_{free}	3 ML
	r_{iso}	$\frac{1}{2}a_T$/100adatoms
	T	300-700 K
Incident atom	direction	normal to substrate
	E_k	2-10 eV
	H	20 Å, move up at r_{iso}
	R_{dep}	1 atom/ps
	N_{dep}	500
Virtual wall	h	4.8 Å, move up at r_{iso}



Schematic of the MD model of atomic deposition

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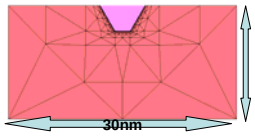
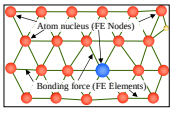
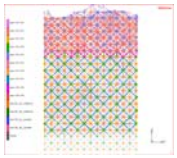
Atomic FEM

Inter-atomic potential - Lennard-Jones potential

$$U_{tot}(x_1, x_2, ..., x_N) = \sum_{i<j}^{N} U(x_j - x_i)$$







Atoms = FE nodes (several sets depending on type in the MD model)
Automatic generation of CBUSH elements (user selected max. length)

Limitations:
AFEM < 100,000 nodes
(Max. AFEM domain size: 0.03μmx0.03 μm)
Min. element edge size in CPFEM: 1.. 100 Å

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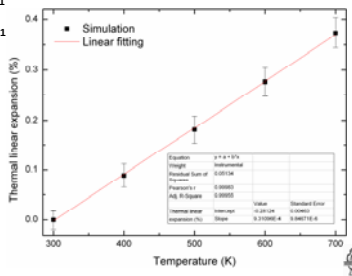
Validity of the potential

MD-Simulation

Thermal linear expansion coefficient

Simulation 9.31×10^{-6} K^{-1}

Experiment 9.35×10^{-6} K^{-1}



Thermal linear expansion of TiN.

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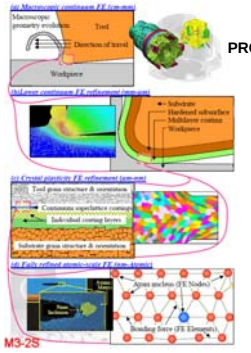

PROJECT M3-2S (NMP3-SL-2008-213600)

Project Partner:
University of Birmingham (UK)
Asociacion De La Industria Navarra (ES)
DIAD (IT)
Fundiciones Del Estanda (ES)
Wilde FEA Ltd (UK)
TBZ-PARIV GmbH (DE)
Swiss Federal Laboratories for Materials Testing & Research (CH)
Fraunhofer IWU (DE)
Harbin Institute of Technology (PRC)
Politecnico di Torino (IT)
University of Strathclyde (UK)
Imperial College of Science, Technology and Medicine (UK)

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SUMMARY

- „Conventionally" Finite Element Simulation can be applied for deformation and stability analysis of coating-substrate-systems
  That's "state-of-the-art"
- "Virtual" Cutting Tool Design and "Virtual" Machining is an important topic in manufacturing
- New workpiece materials are responsible for new demands in coating-substrate-structures
- In addition to "homogeneous" coatings – more and more structured coatings are developed
- This new type of coatings are "non-homogeneous" and "non-isotropic"
- Subdomain techniques : Continuum-mechanically methods + ab-initio methods can be used in the near future

Thank you for your Attention!