VTT Technical Research Centre of Finland Ltd

VTT ProperTune™

Enabling Integrated Computational Materials Engineering for Businesses

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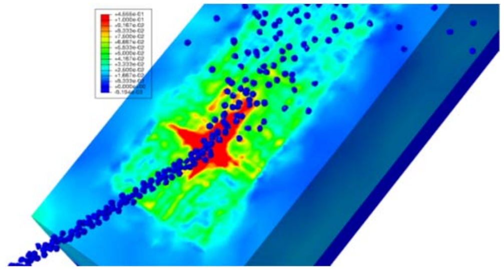
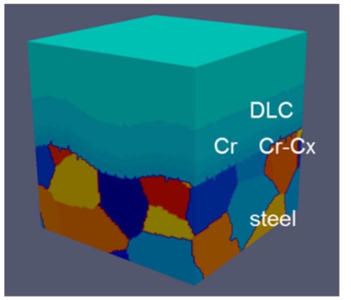
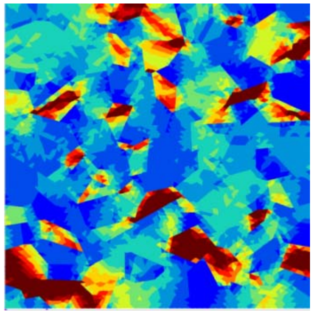
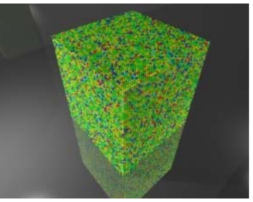
Contents



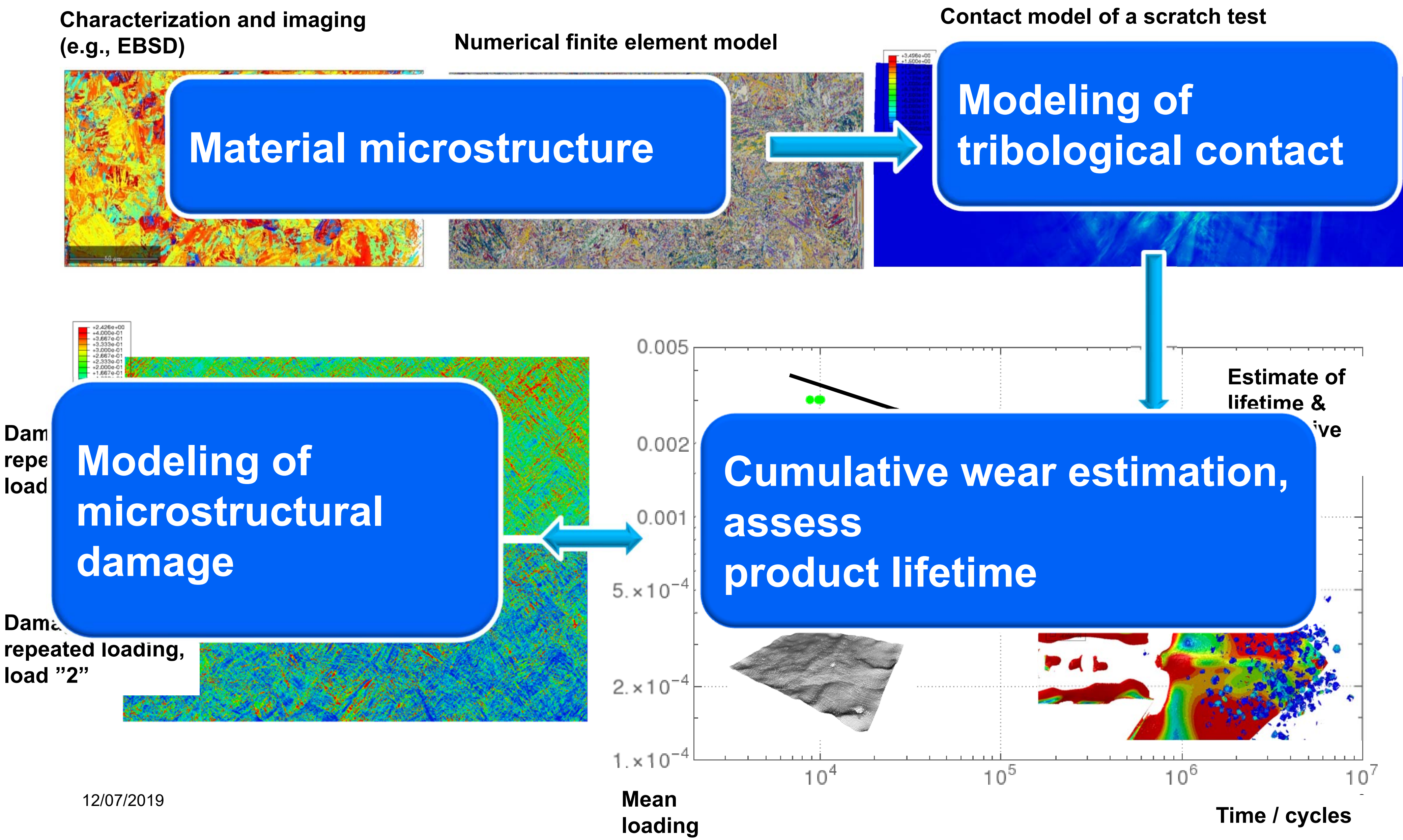


- Brief introduction to core concepts of “VTT properTune”
- Typical uses & how projects make use of “VTT properTune” in R&D&I
- 2 industry use cases:
  - Design of a new wear resistant steel (in collaboration with ArcelorMittal)
  - Optimization of damage tolerant composites & microstructures (in collaboration with Caterpillar)

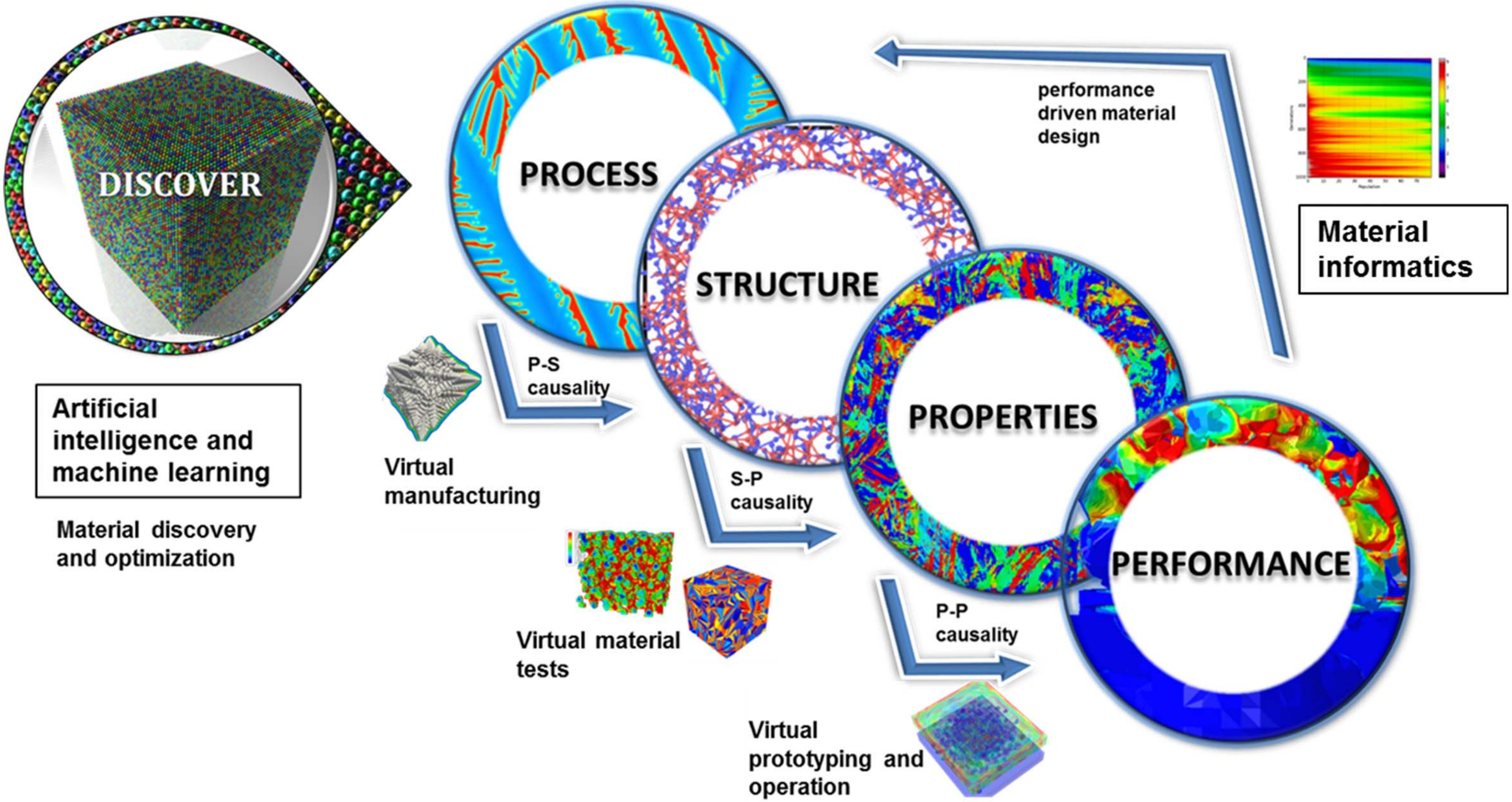




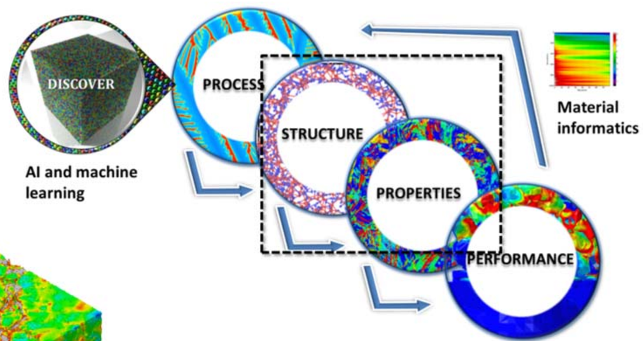
EXAMPLE: Applying VTT properTune to Modeling of Wear Damage and Cumulative Wear

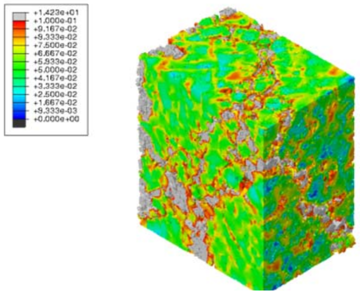


VTT properTune as a tool for "Integrated Computational Materials Engineering"



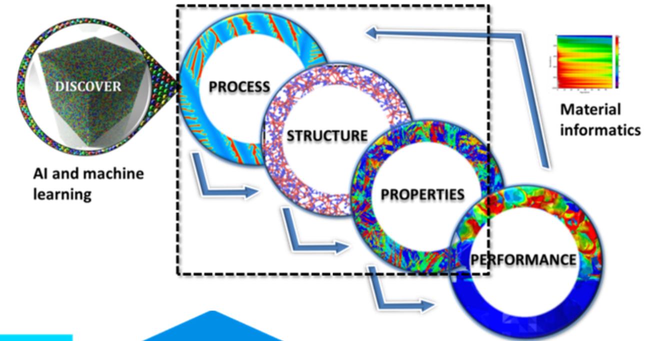
Typical examples and uses of "VTT properTune"

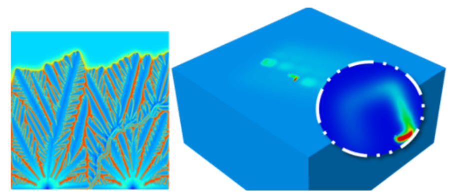




WC-Co microstructure

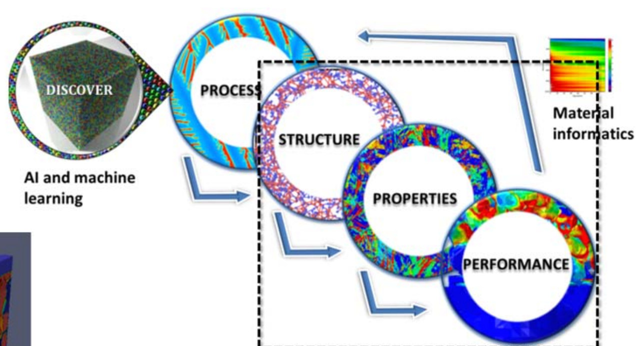
STRUCTURE-PROPERTIES:
Effect of microstructure on strength and engineering material properties

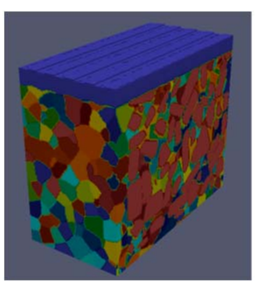




Alloy design for additive manufacturing

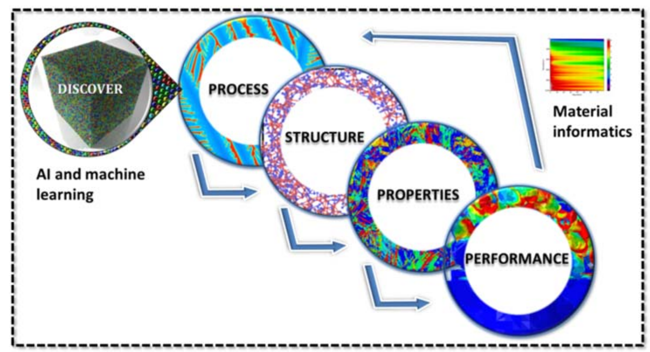
PROCESS-STRUCTURE-PROPERTIES:
Alloy and manufacturing process design for targeted material properties



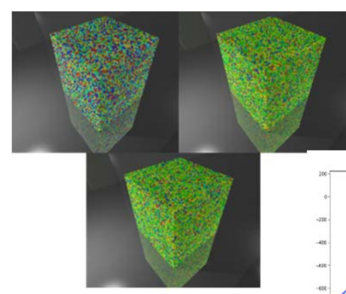


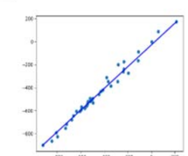
Coated thermomechanically loaded hard material solution

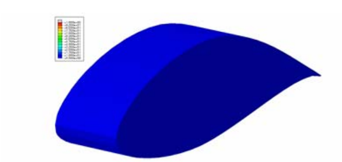
STRUCTURE-PROPERTIES-PERFORMANCE:
Effect of microstructure and micromechanics on fatigue, thermomechanical and wear performance and product lifetime



AI/Machine learning PSPP: Material/material solution discovery, design and optimization



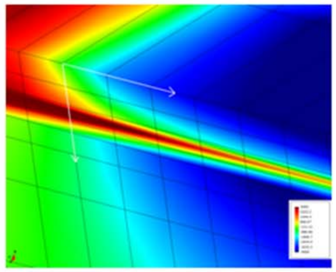




ML driven optimization of erosion resistance

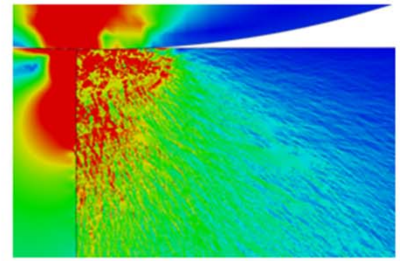
Thin films and coatings

TiN, DLC, MoS2, TS, laser, welded coatings



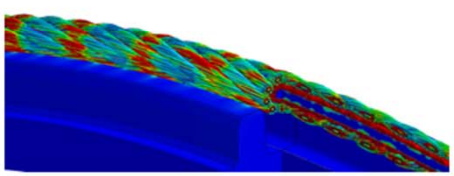
Composite/Hard materials

Cemented carbides, cermets, PM materials and composites, rock materials



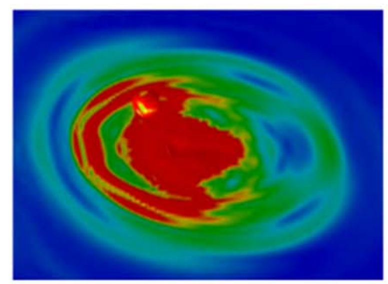
Metals

Wear resistant steels, very high strength steels, steels for machinery, welds, dissimilar metal joints, copper, cast irons, additive manufacturing



Soft materials

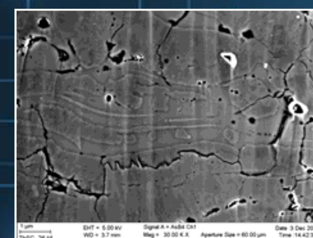
Nanocomposites, polymer composites, elastomers, biomaterials

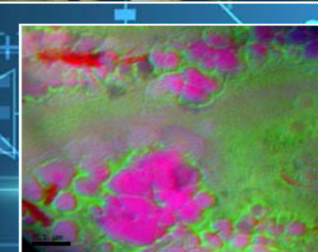


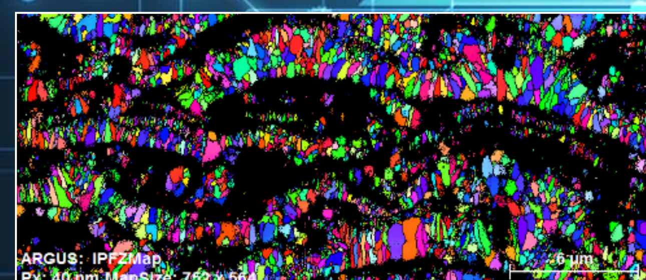
VTT

From material microstructure to full scale components and systems

- **Tools to create the microstructure:**
  - SEM, FIB, EBSD, µ-CT, TEM, APT
- **Tools to characterize the properties:**
  - Nanoindentation, AFM and SPM for mechanical property mapping
- **Tools to validate the models:**
  - Laboratory or component/ system level testing







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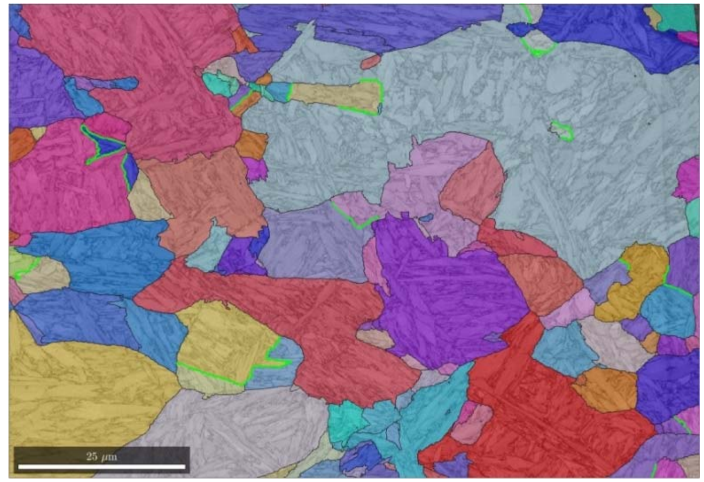
Use case 1: Design of a new wear resistant steel (in collaboration with ArcelorMittal)

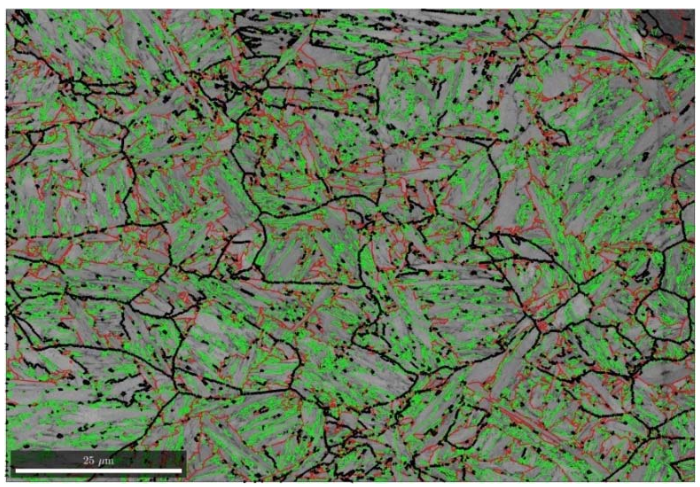
ArcelorMittal

Microstructural modeling: model generation

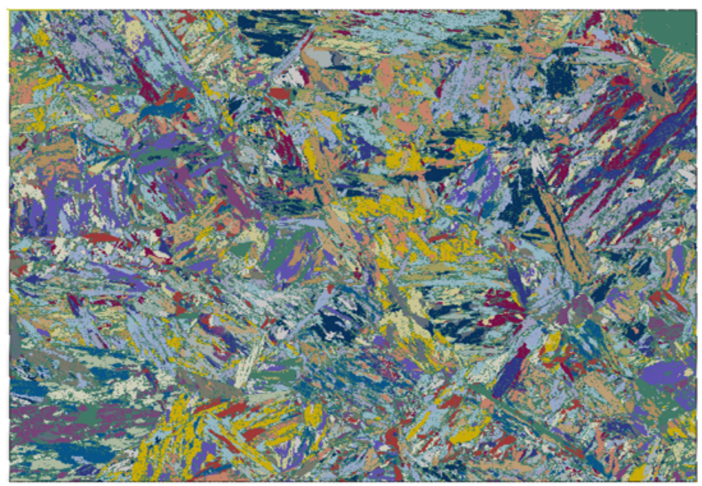
Martensitic steel microstructure



Prior austenite grains reconstructed



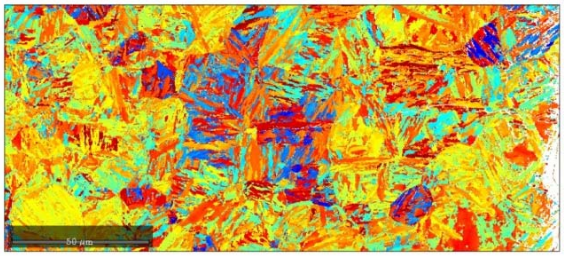
Hierarchies, such as block boundaries (green) and packet boundaries (red)



Computational microstructure

Merger of advanced characterization and modeling means provides quite a realistic description of steel at the microstructural level

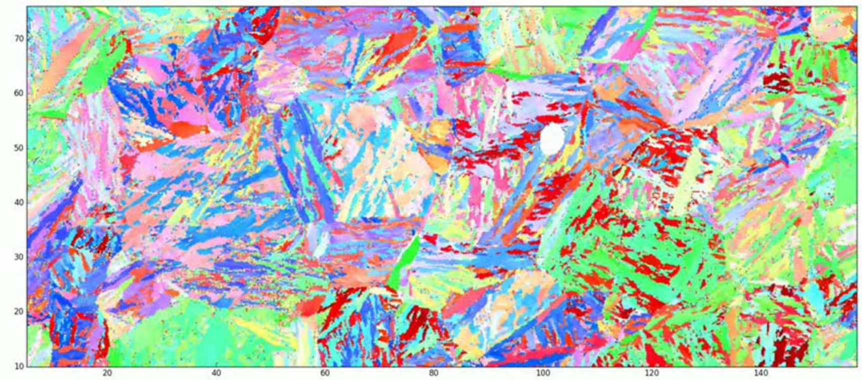
Microstructural modeling: model generation



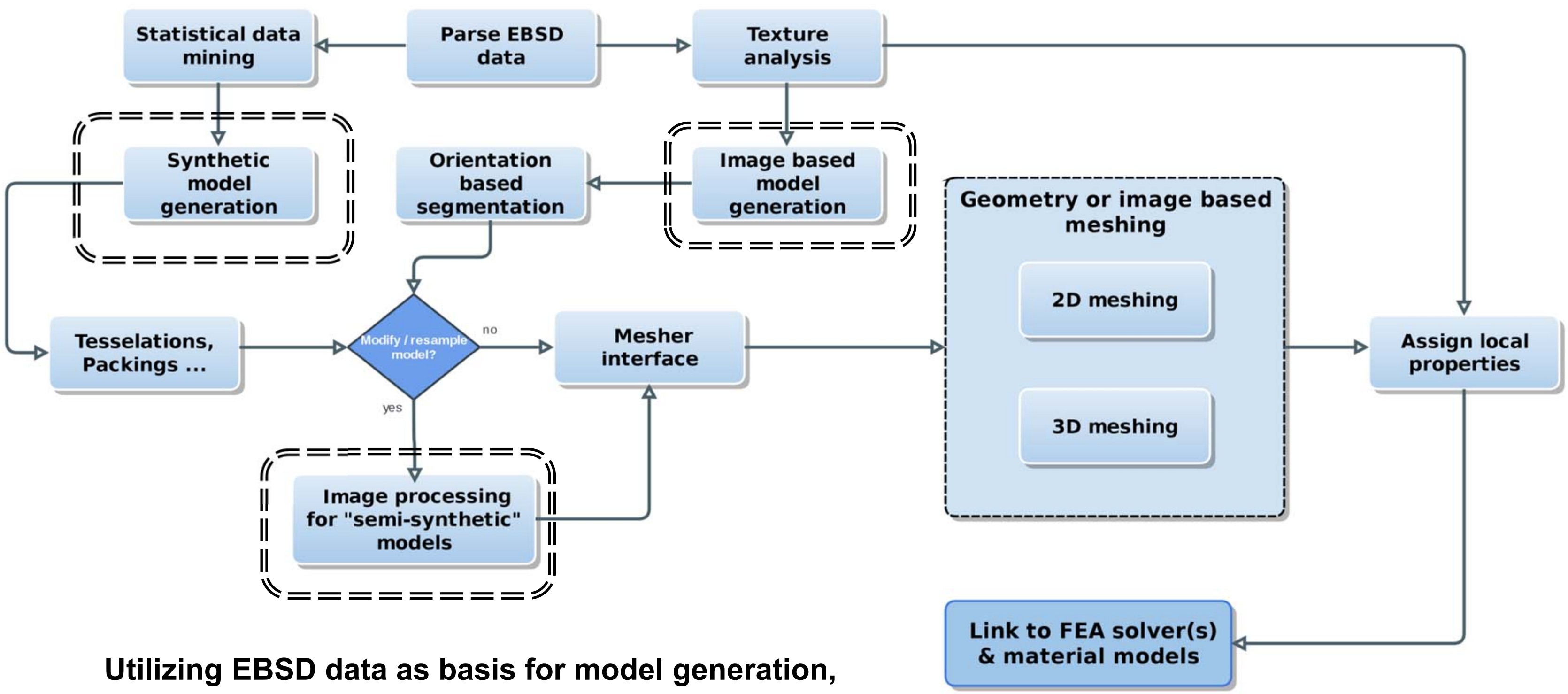
EBSD orientations from characterization

Material plot from finite element model

3D microstructural model geometry from a stack of 2D images

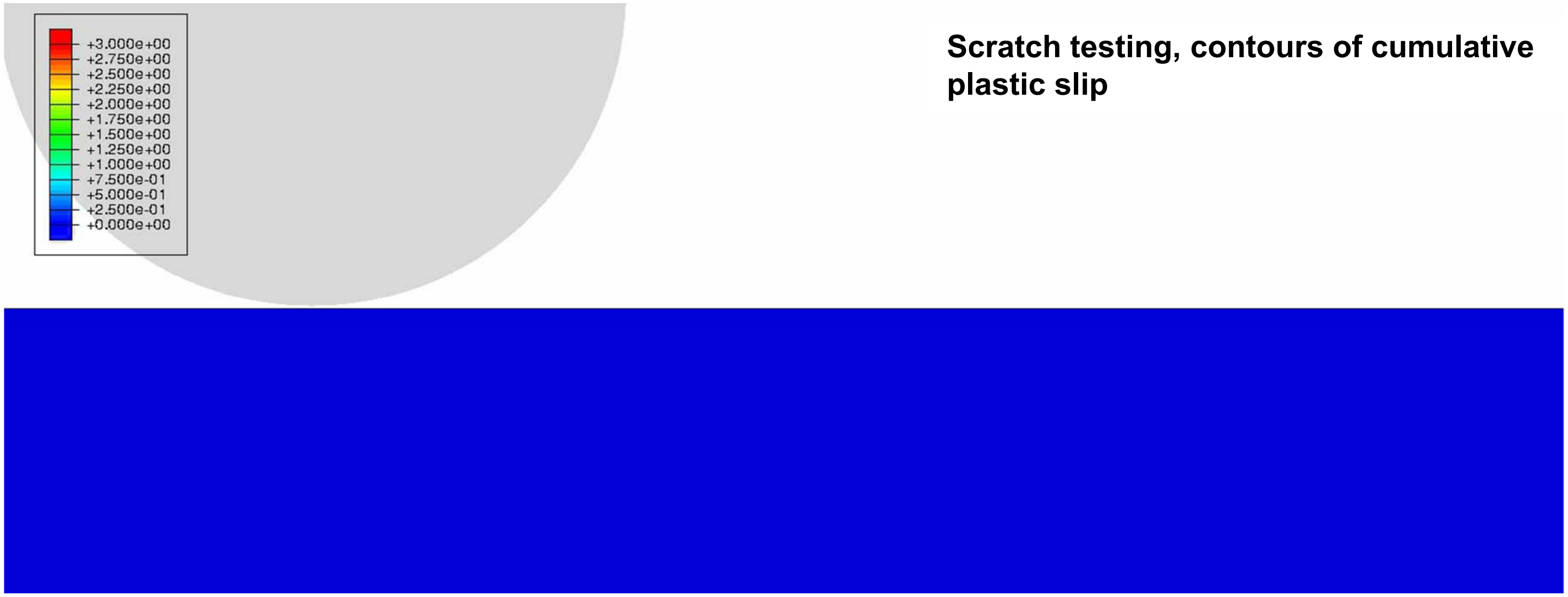


Example of a martensitic steel microstructural model

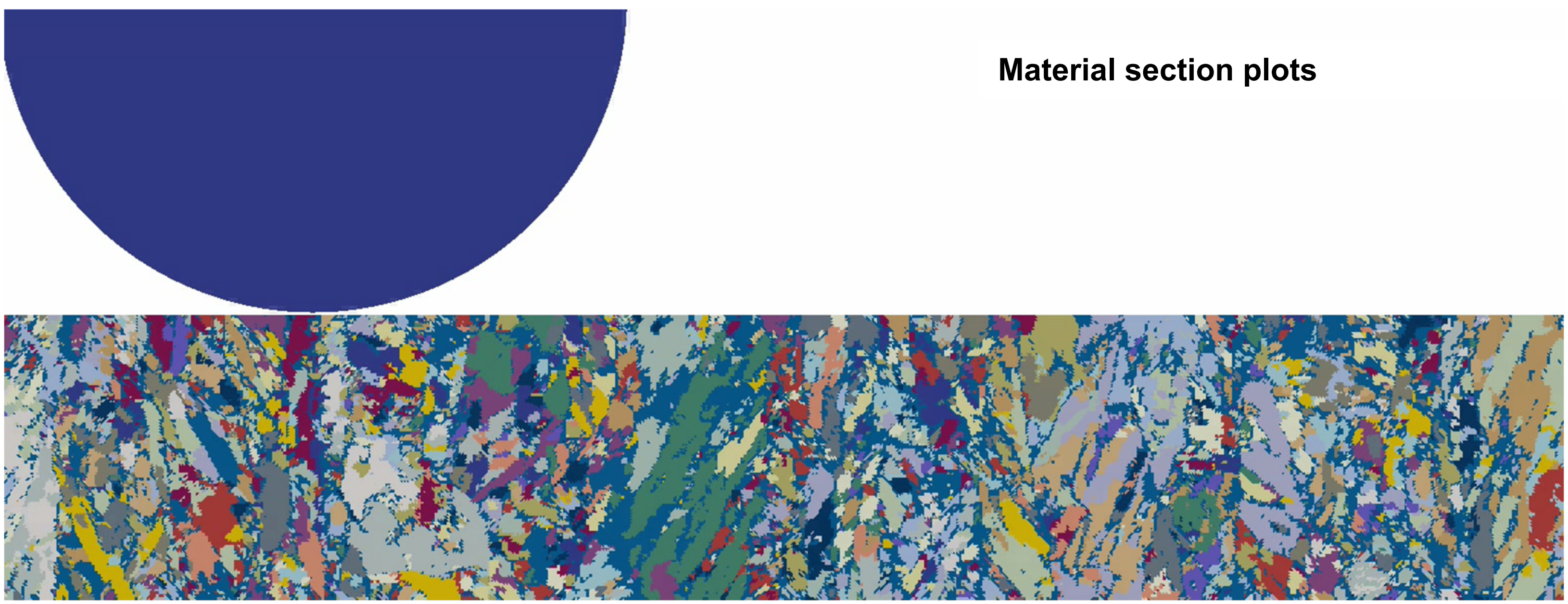


Utilizing EBSD data as basis for model generation, either statistical or directly imaging based model

Scratch test models, FM450 fully martensitic grade

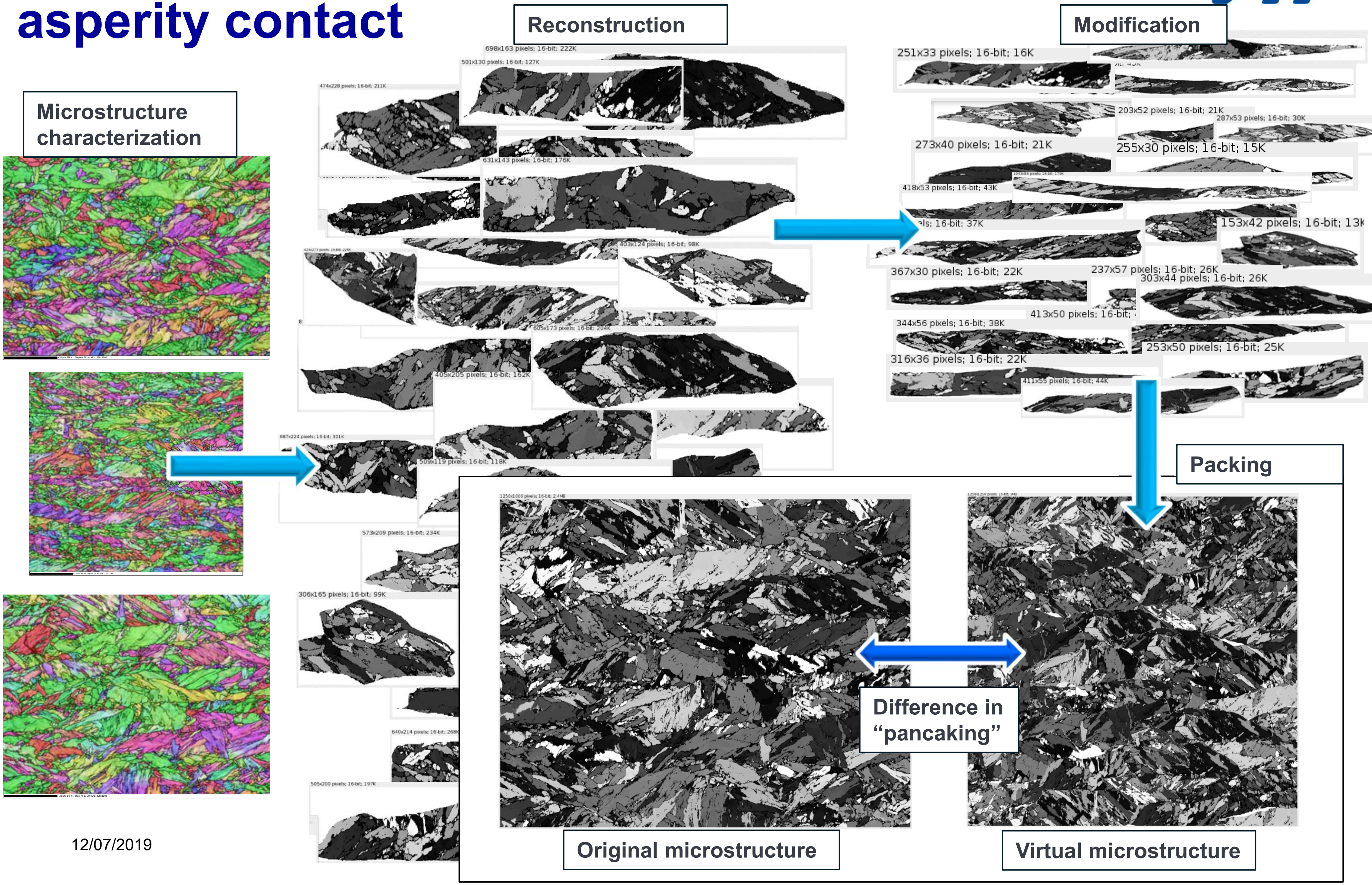


Scratch testing, contours of cumulative plastic slip



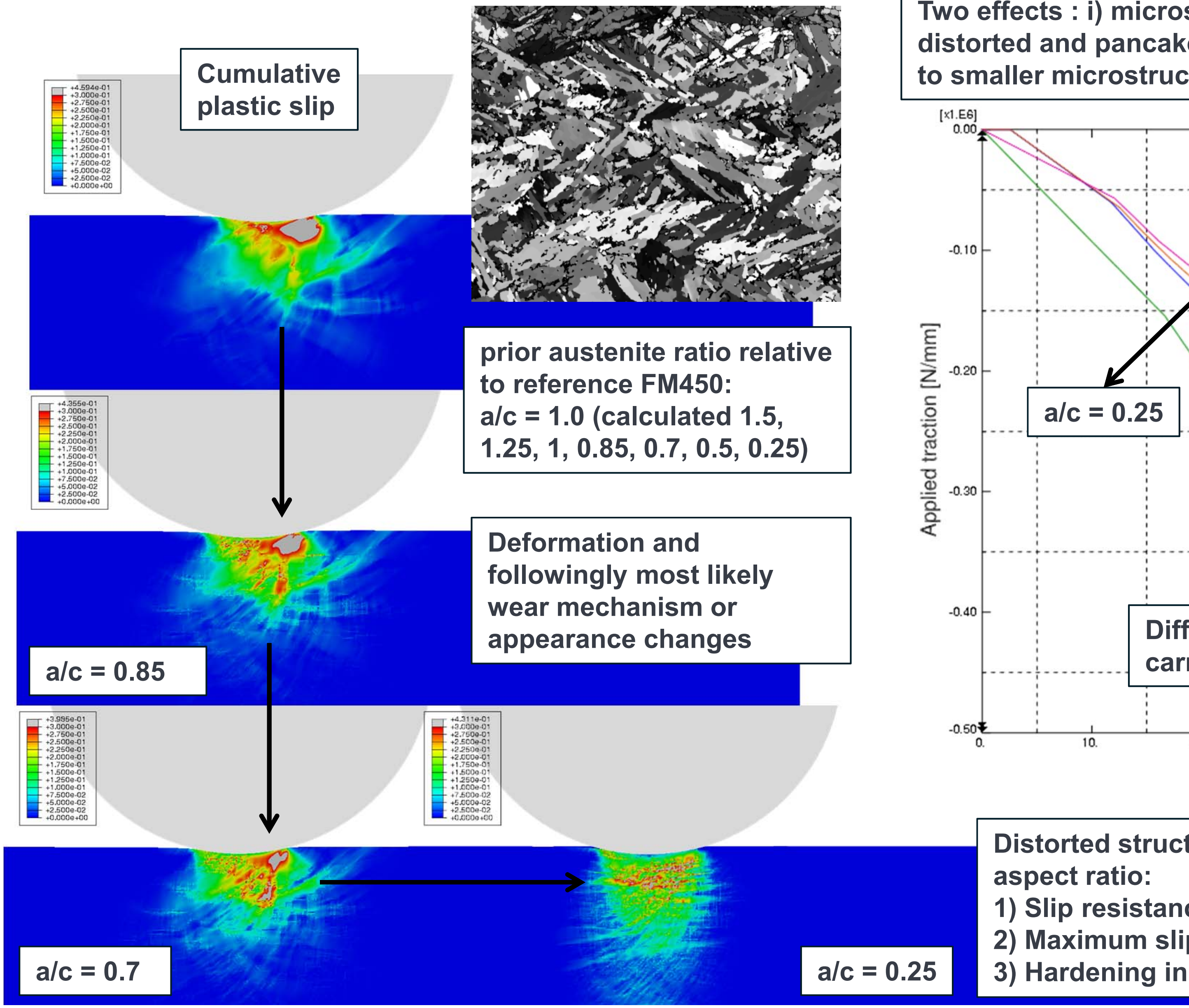
Material section plots

FM450 microstructure design with single asperity contact



FM450 microstructure design with single asperity contact: load carrying capacity

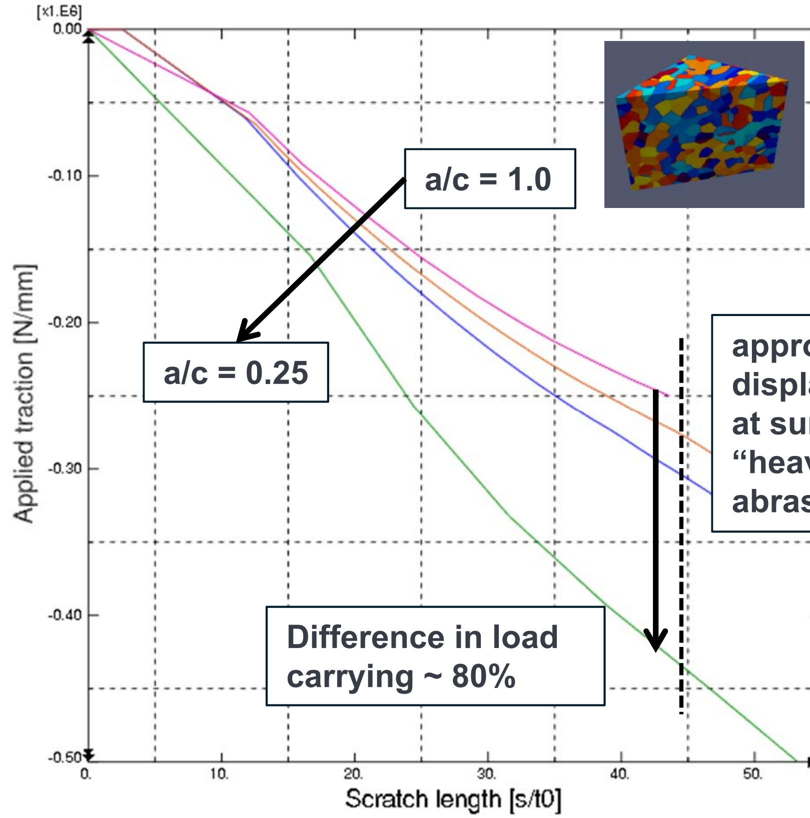
Cumulative plastic slip



prior austenite ratio relative to reference FM450:
a/c = 1.0 (calculated 1.5, 1.25, 1, 0.85, 0.7, 0.5, 0.25)

Deformation and followingly most likely wear mechanism or appearance changes

Two effects : i) microstructure morphology becomes more distorted and pancake like, ii) strengthening/hardening due to smaller microstructural features

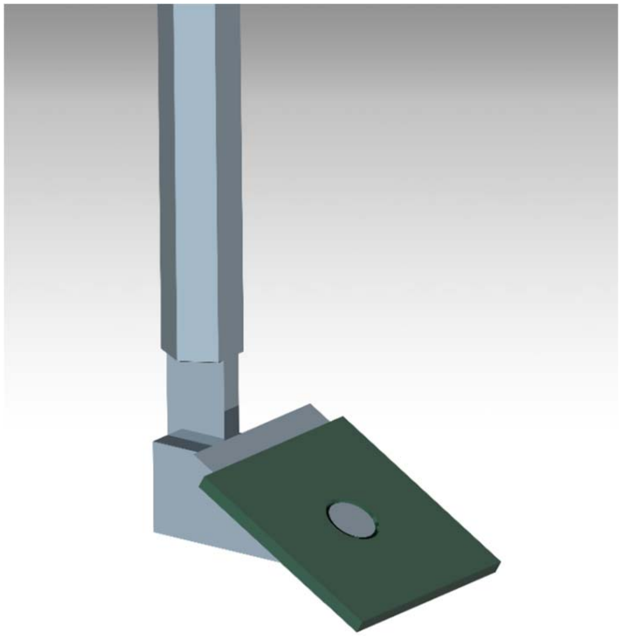


approx. 6 μm displacement at surface, “heavy abrasion”

Difference in load carrying ~ 80%

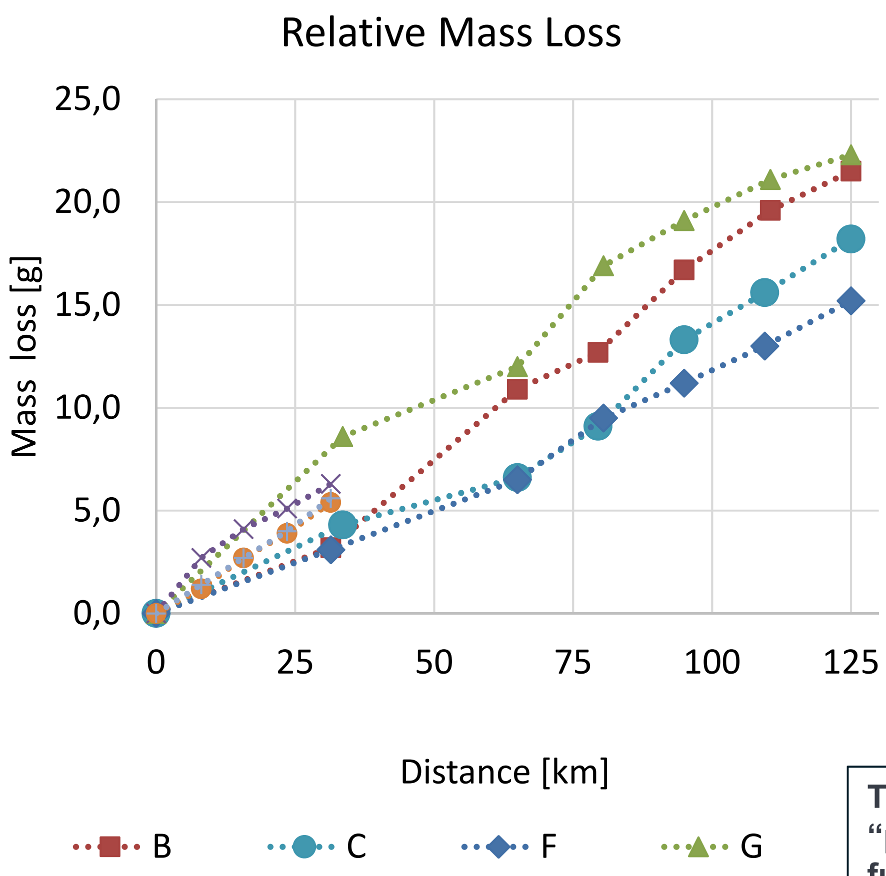
Distorted structure with high prior austenite grain aspect ratio:
1) Slip resistance greater due to morphology,
2) Maximum slip localized to smaller material volume,
3) Hardening increases load carrying capacity.

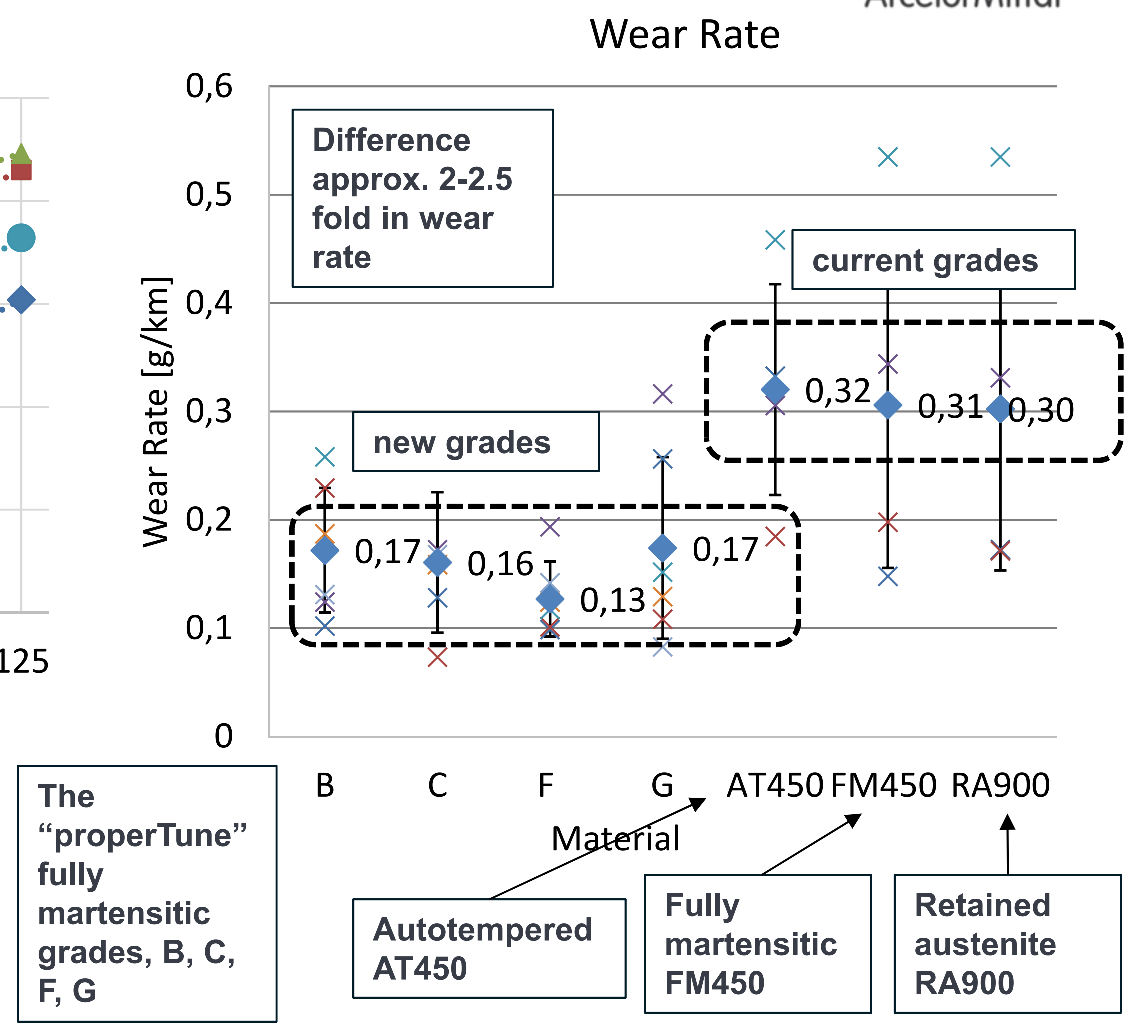
Testing of new steel grade(s) by TUBS in full scale wear test arrangement



The tine ran typically for some 100-200 km in a “tillage simulator”, roughly 8 m diameter track where the soil/abrasive characteristics can be controlled and adjusted.

Testing of new steel grade(s) by TUBS in full scale wear test arrangement

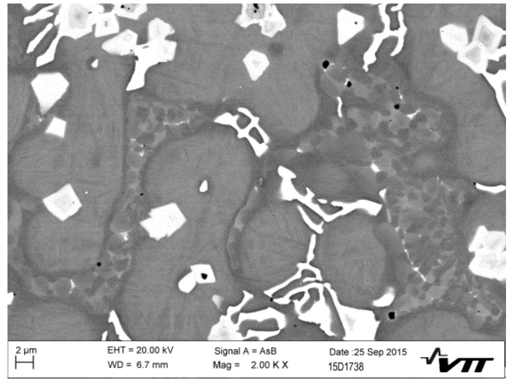




Use case 2: Optimization of wear resistant composites & microstructures (in collaboration with Caterpillar)

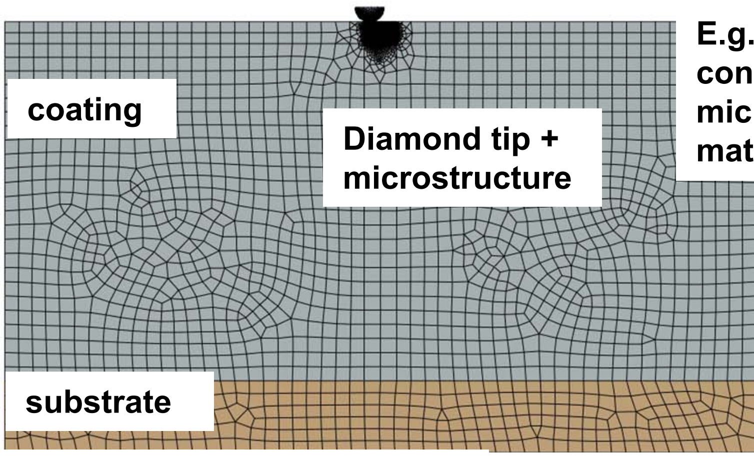
Models & different analysis cases

- Model types, two microstructural regions of interest:
  - Coating contact surface microstructural model
  - Coating-to-substrate interface microstructural model

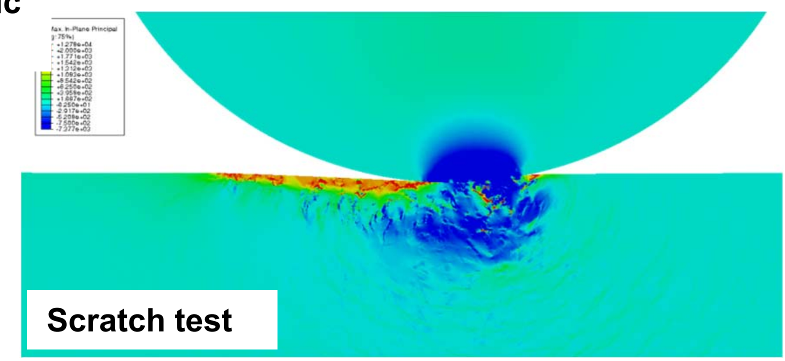


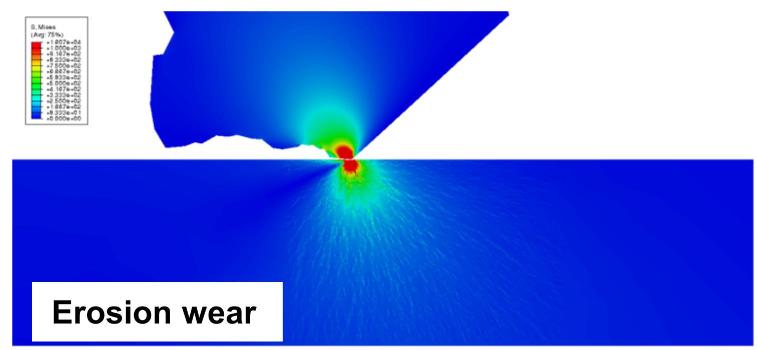
E.g. carbide and boride containing composite microstructure with martensitic matrix

- Wear load cases:
  - Compression, indentation, scratch test
  - Erosion wear (small abrasives)
  - Impact wear (larger abrasives)
  - Steel ball impact (validation)

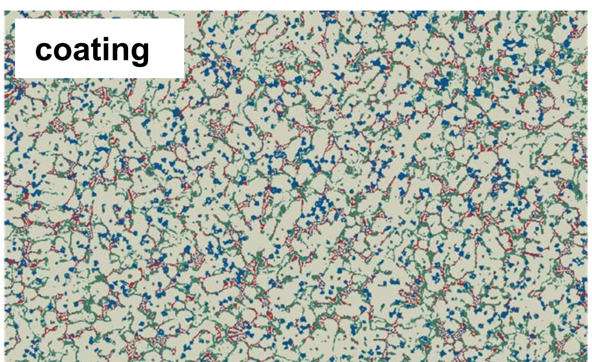


Coating contact surface microstructural model layout



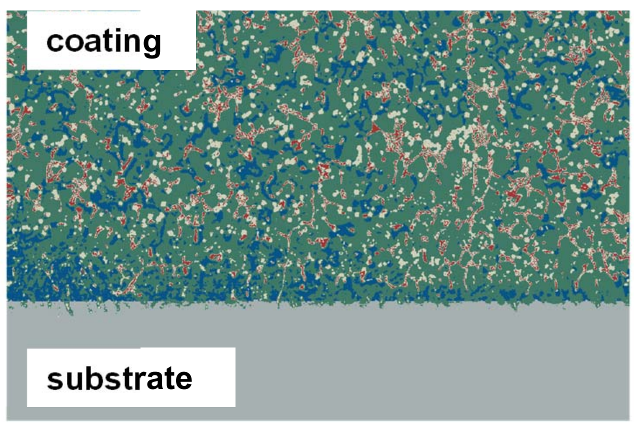


Coating contact surface microstructure:



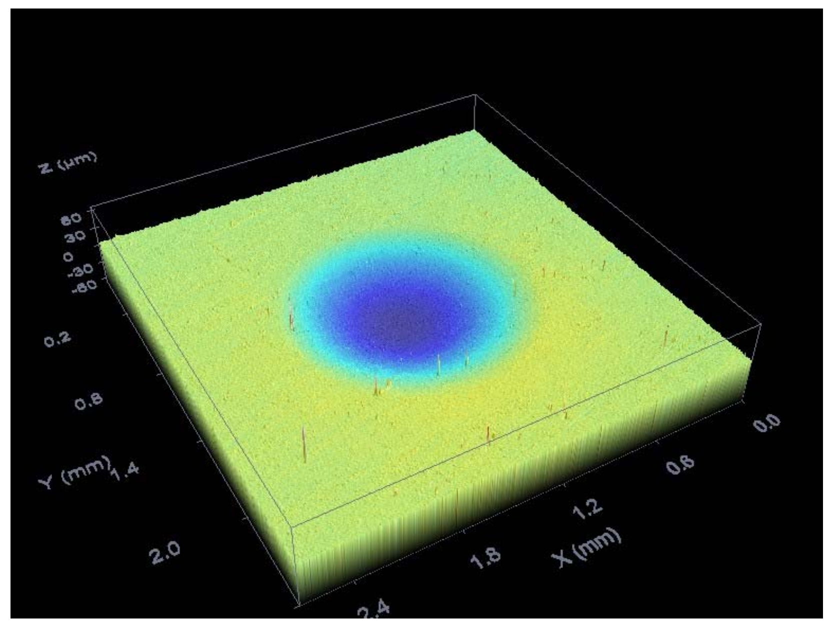
Microstructures of FEA models

Coating-substrate interface microstructure:

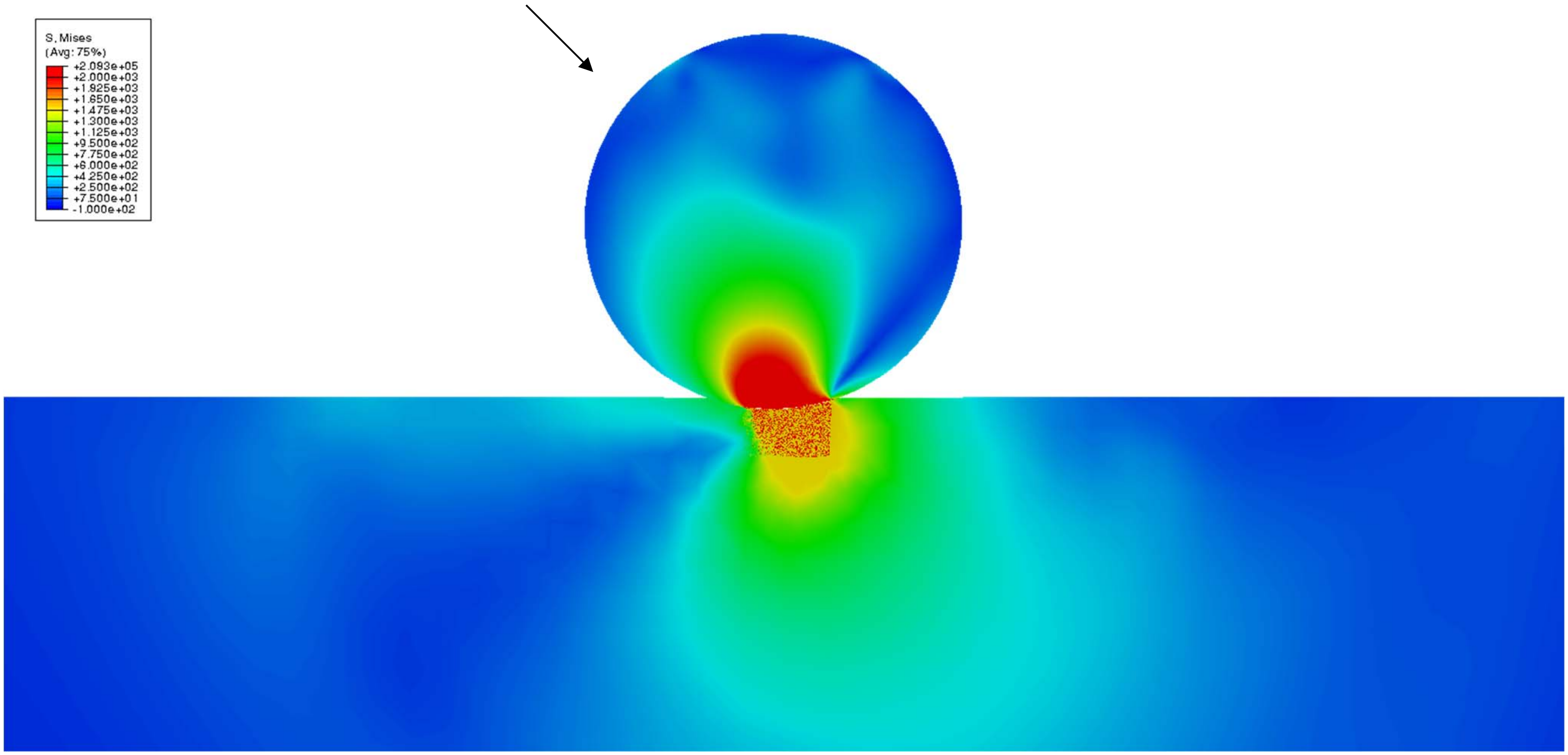


Validation and performance tests

- Steel ball and WC-Co ball impact tests with different impact energies (3 sets of 6 different energies from 0.5 to 2.2J) performed – Experimental results are used to validate the models
- Ball velocity recorded with high speed camera just before impact
- Craters analysed with 3D-profilometer and more detailed analysis performed with SEM or FIB-SEM

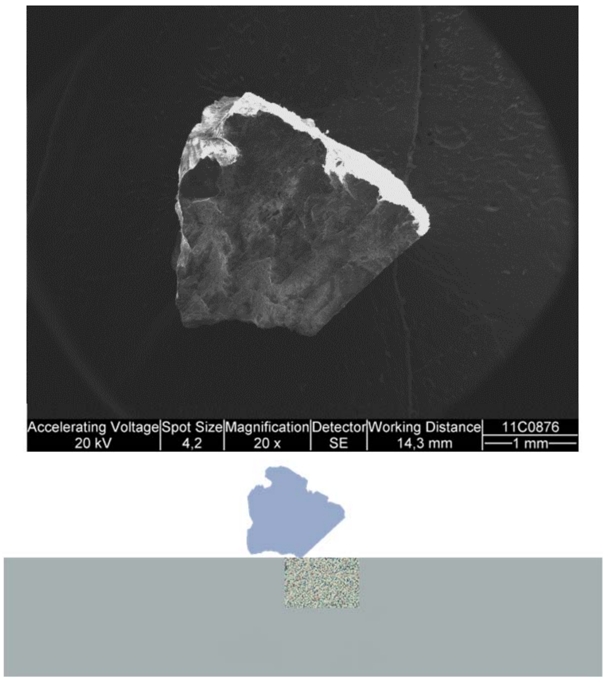


Verification case via impact wear like loading

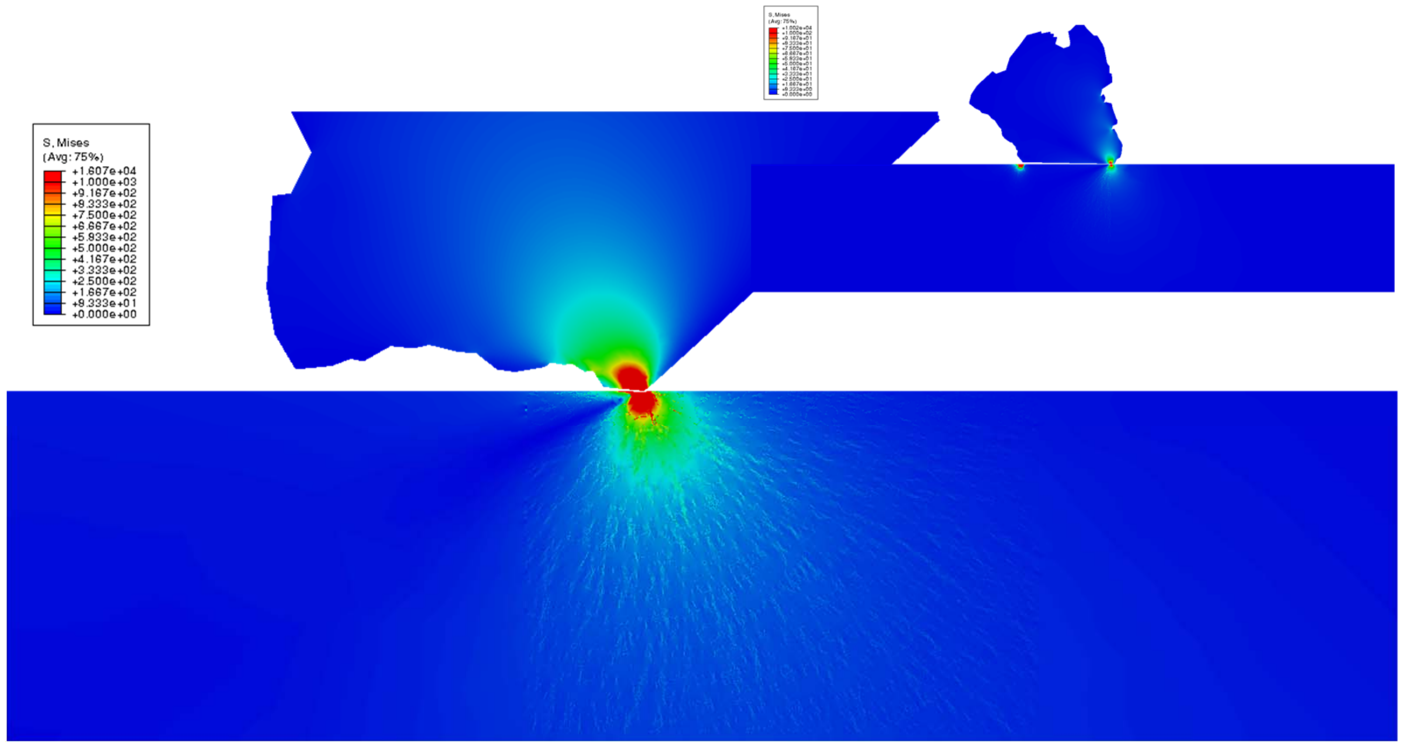


Steel ball impact test for simple validation of the model, model maximum remaining displacement for experimental impact velocity and angle 58 μm, which is well in line with the experimental results (considering scatter of both experiments + models, and the fact that in current work still utilizing 2D modeling). Experimental results between 43 to 53 μm

Modeling results, dynamic impact analyses

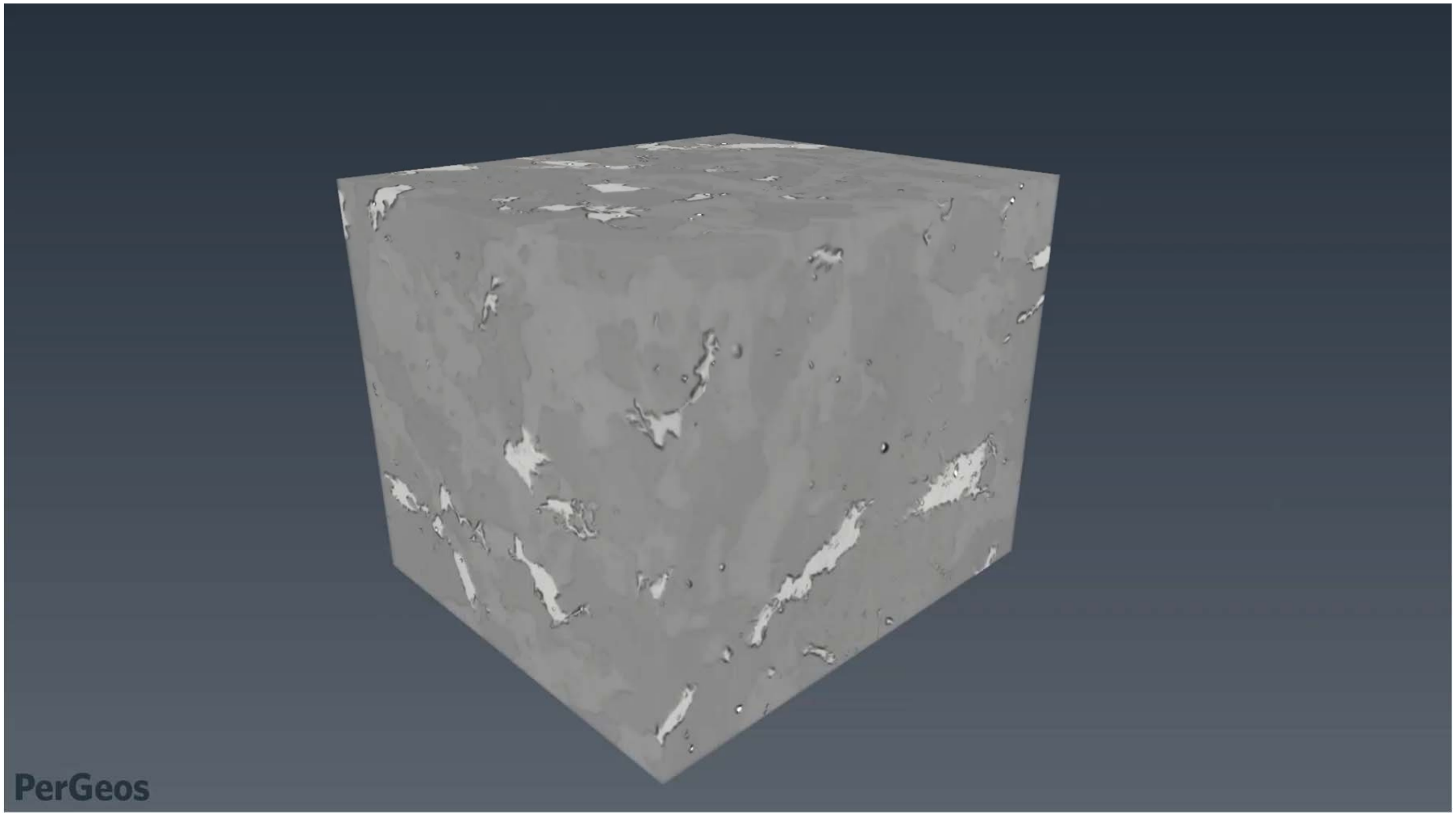


Impact of a small abrasive and microstructure (“local” hard granite)

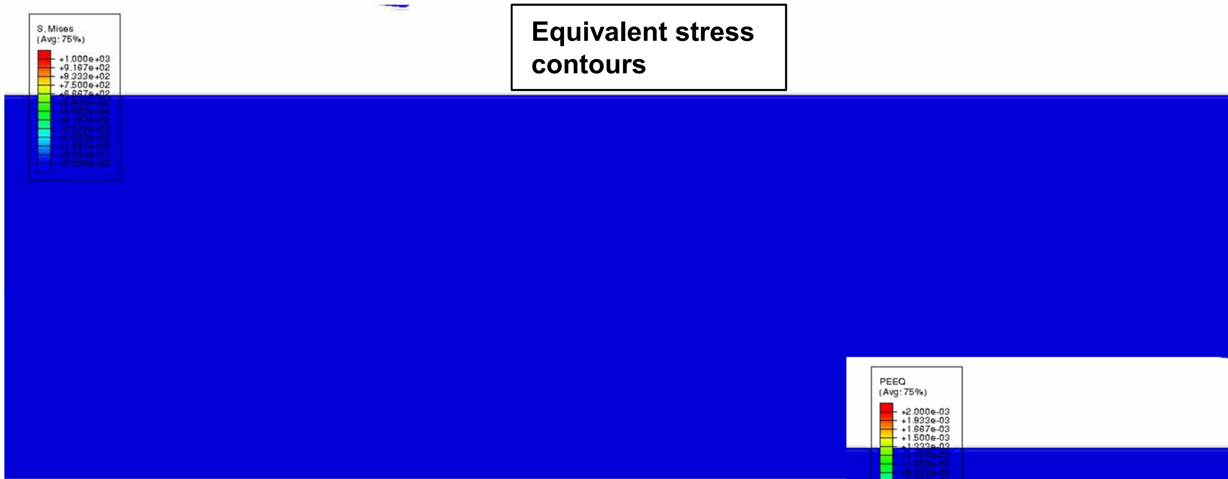


Impact of the small abrasive on the surface at 15 m/s, equivalent stress contours

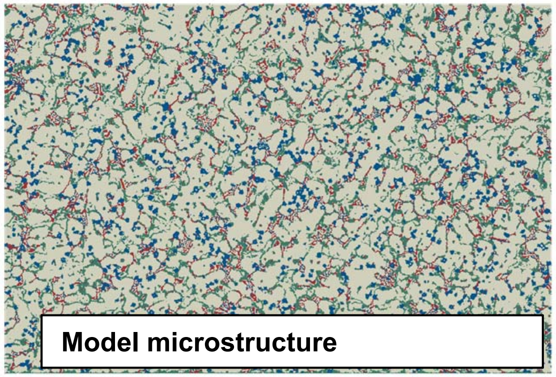
X-Ray Tomography of Granite sample



Summary of results for sliding abrasion and erosive & abrasive conditions

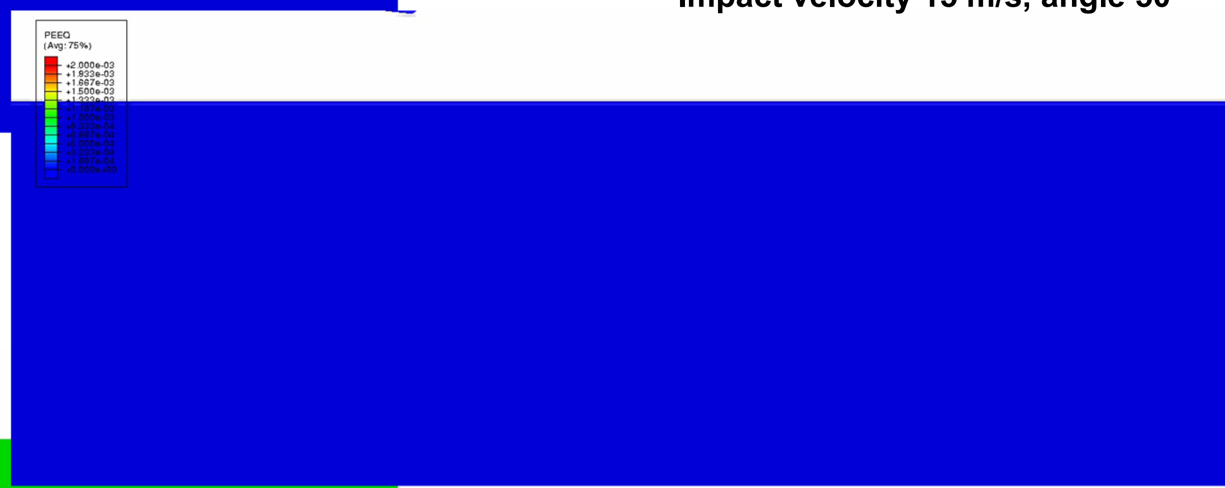


Equivalent stress contours

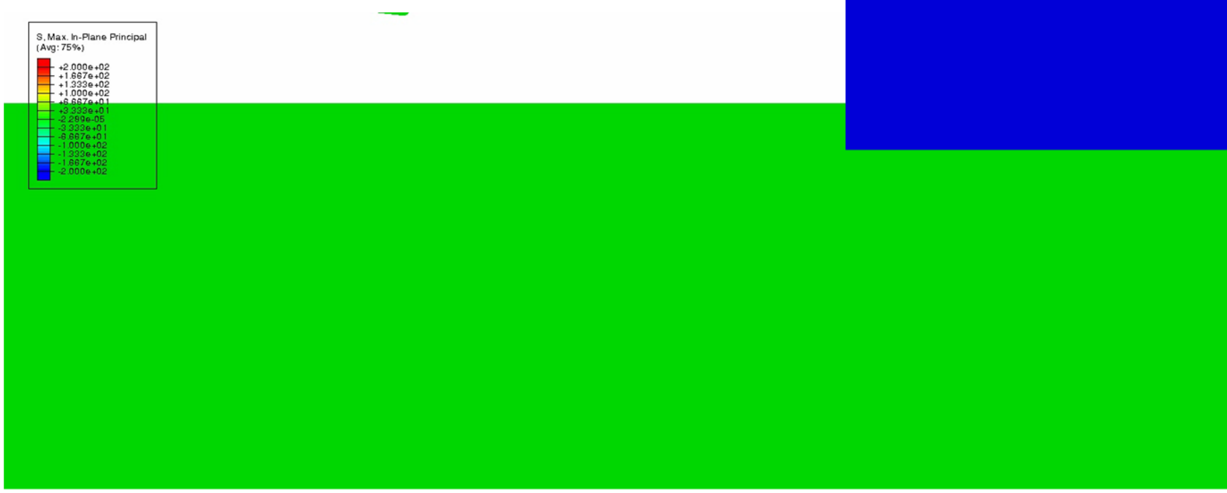


Model microstructure

Contact with small abrasives ~ erosion. Impact velocity 15 m/s, angle 50°



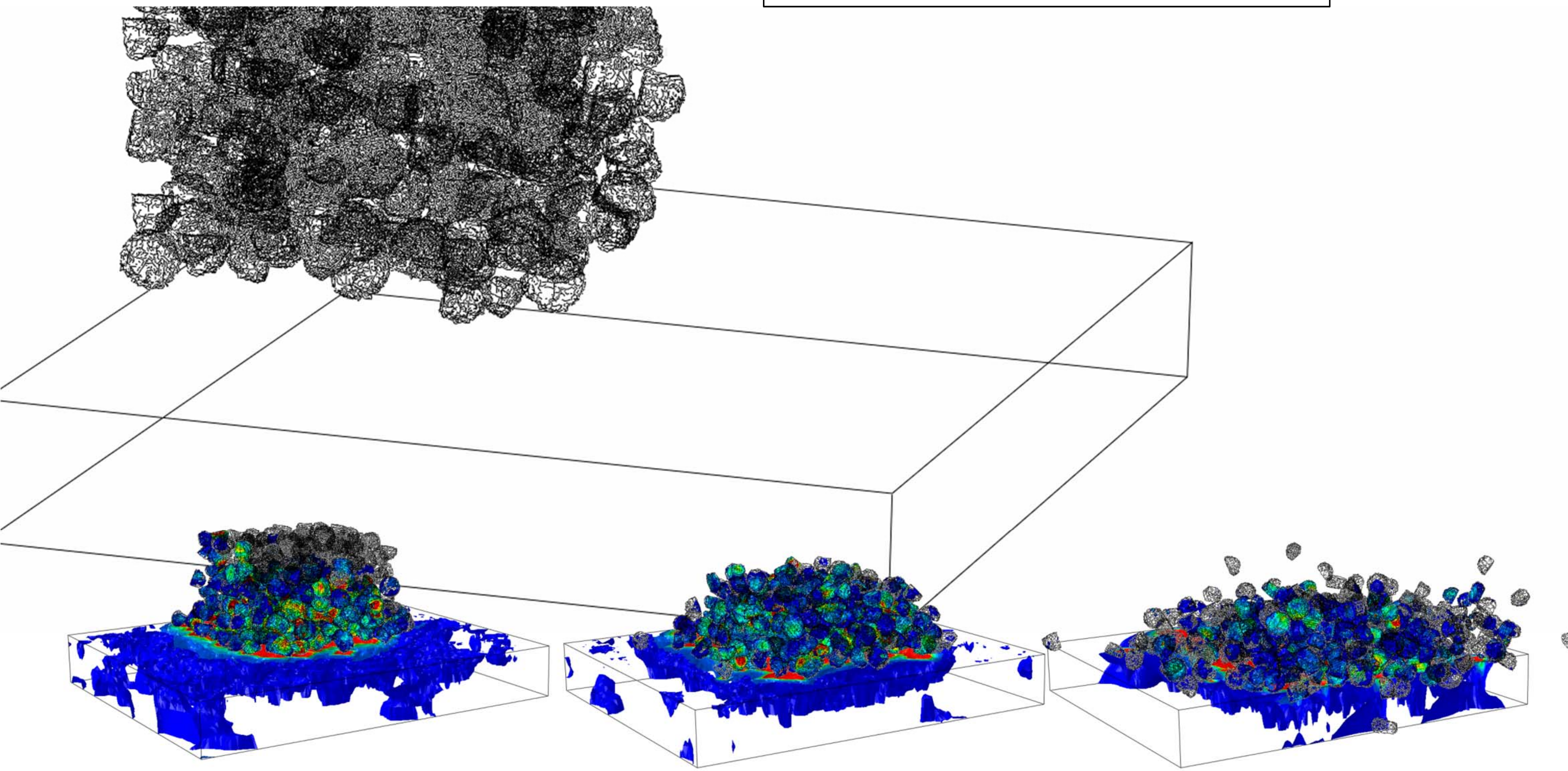
Equivalent plastic strain contours



1st principal stress contours

Modeling abrasive wear loading in 2- and 3-body contacts

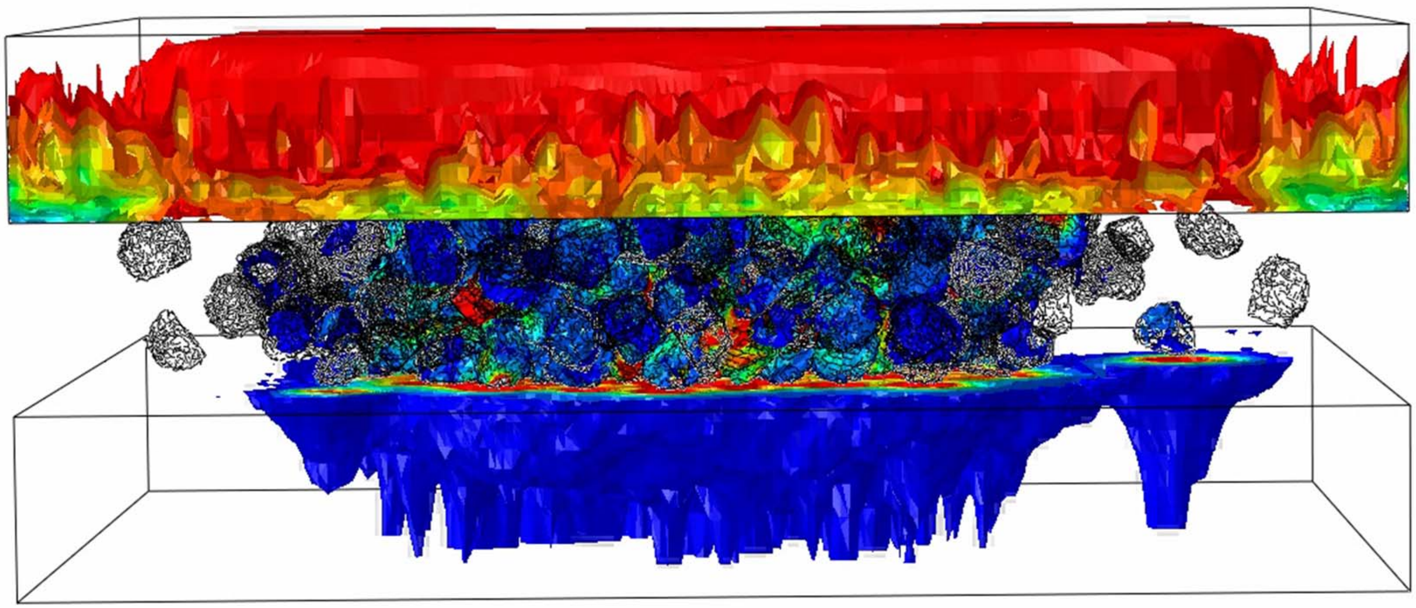
Modeling abrasive wear loading arising from 2- and 3-body abrasion.

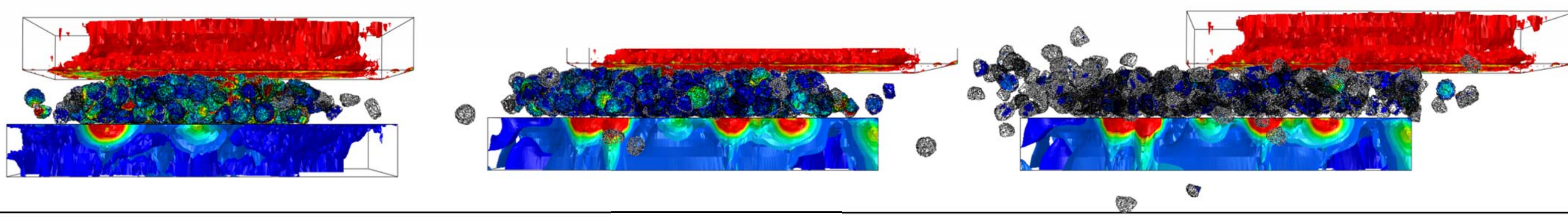


Wear resistance and the “collapse” of a rock column and a velocity of approx. 50 m/s at a nominal angle of 50 degrees.

Modeling abrasive wear loading in 2- and 3-body contacts

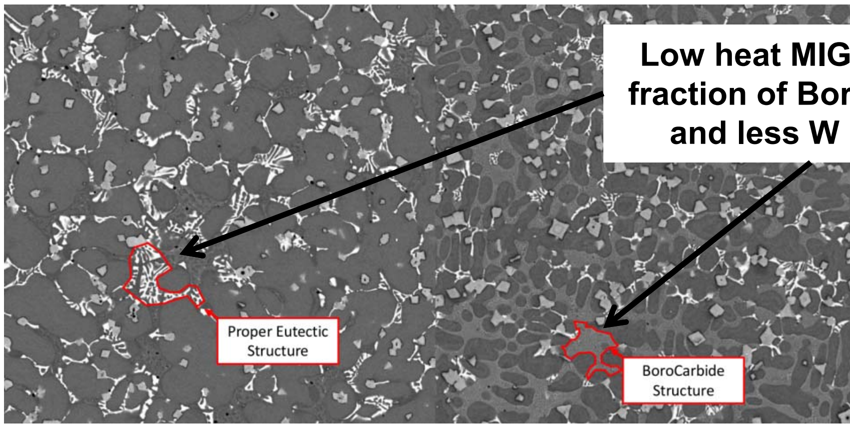
Modeling abrasive wear loading arising from 2- and 3-body abrasion.

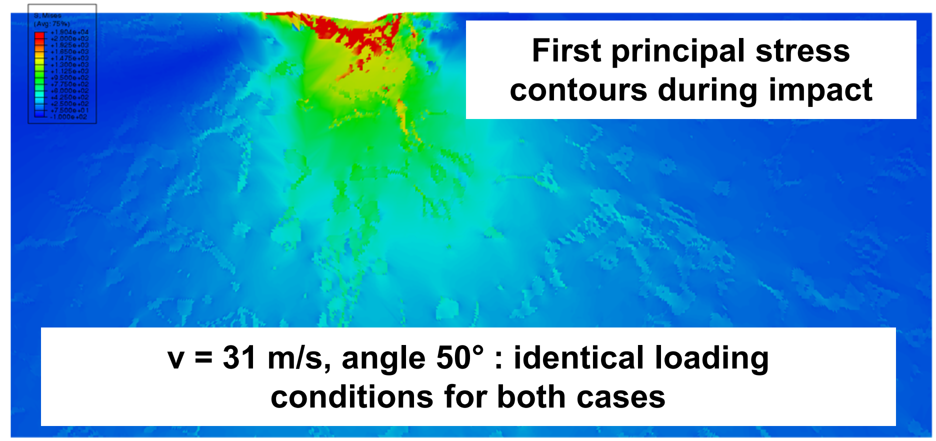


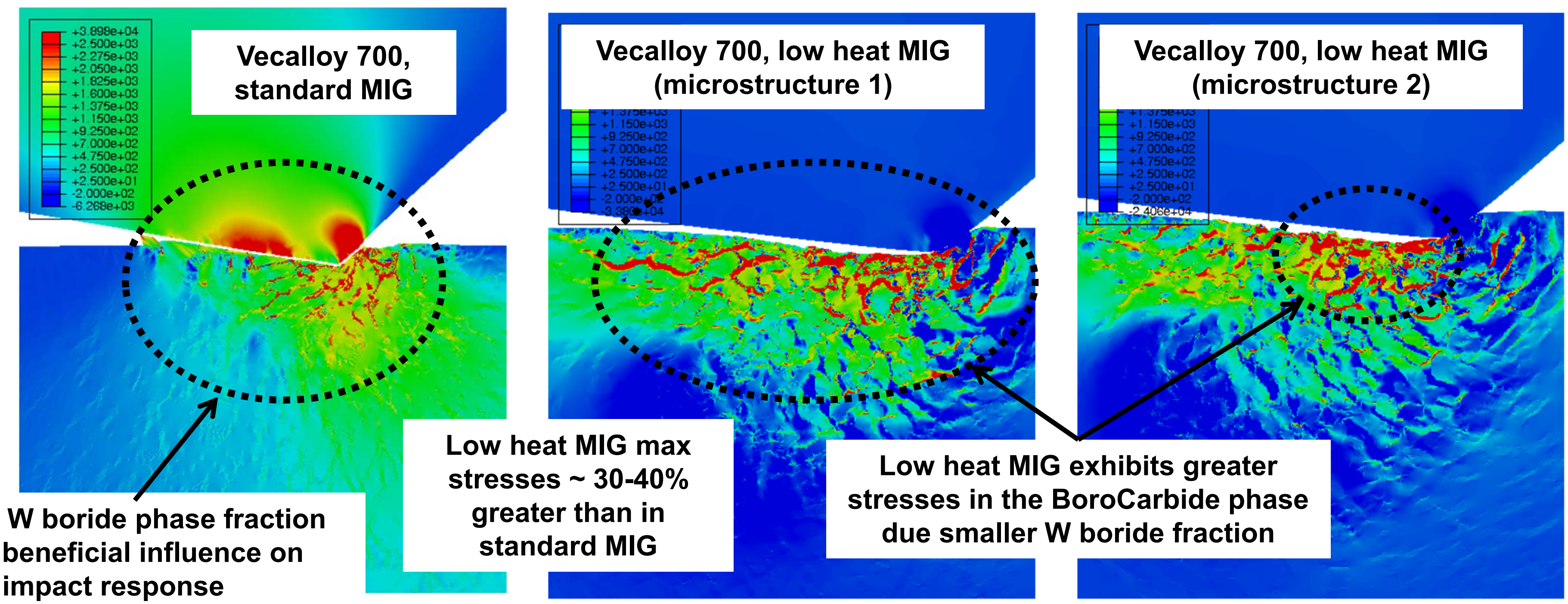


Wear resistant plate moving laterally with a velocity of 10 m/s.

Summary: Comparison of impact resistance of two different microstructures







OUTCOME: Impact resistance retained, resistance to abrasion (G65) improved by 40%.

References