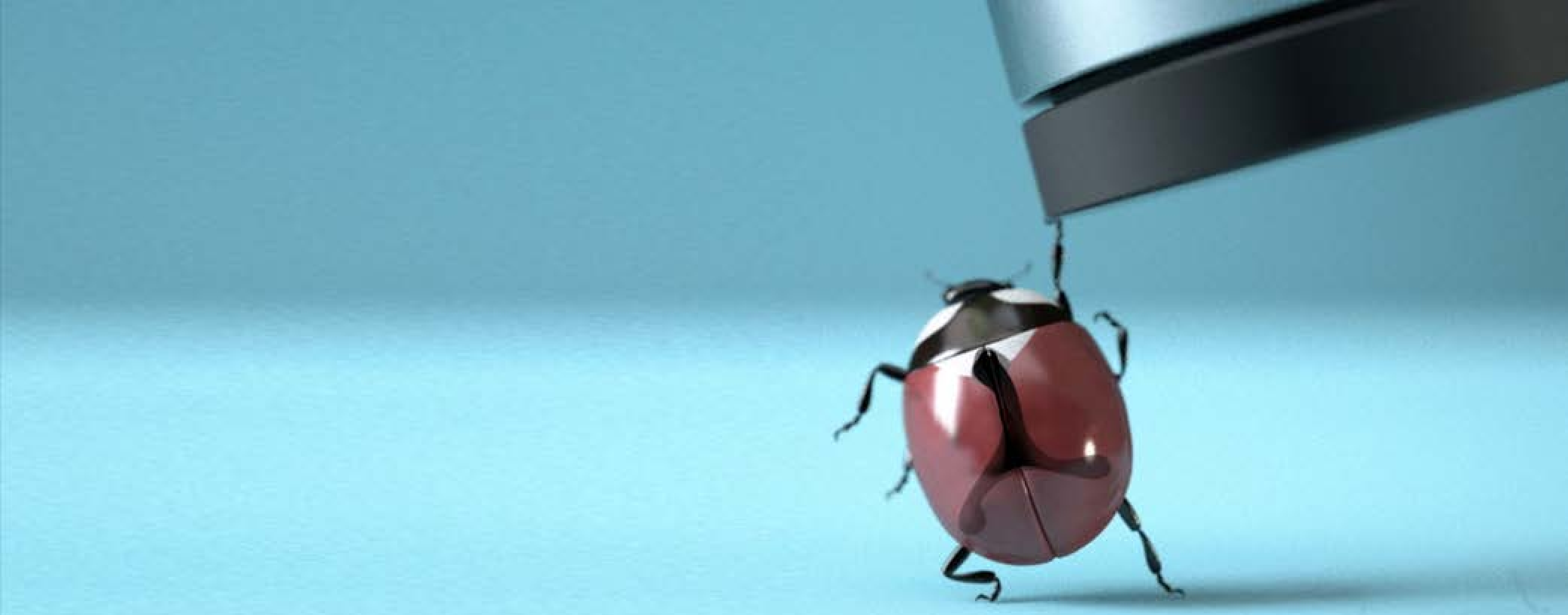


Microstructure modelling in ICME settings

G.J.Schmitz, B.Böttger and M.Apel

TCSAB users meeting, Stockholm, June 2016

ICME – an emerging discipline

Focus of ICME is on

engineering the properties of a component as a function of the local properties of the material inside the component and along its entire production and service life cycle

The role of microstructures in ICME

There are NO (!!) processing-property relationships
but
- **properties are determined by microstructures**
- **microstructures are determined by processes**

Processes are often strongly affected by microstrutures

Microstructures are not static, but evolve under operational conditions

Determination/prediction of materials/component properties requires understanding of microstructures and the description of their evolution

Microstructures provide a natural bridge between continuum scale process models and electronic/atomistic/mesoscopic models

History of ICME

In view of the

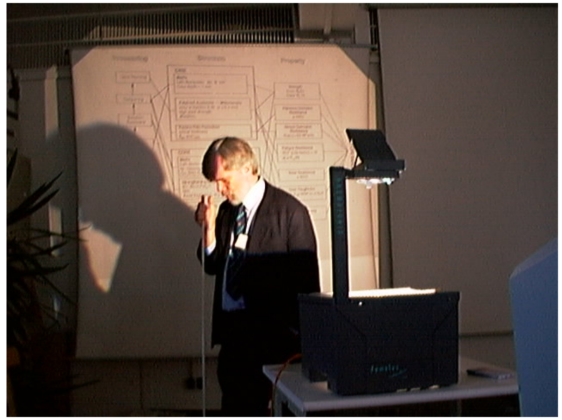
„C“

in ICME:

ICME history starts about the 1960s

i.e. about 50 years ago

Computational Thermodynamics (phase equilibria)



„I disliked computers. Thus I started studying metallurgy, because I thought this subject would be too complicated to be ever put on a computer……"

Bo Sundman, one of the creators of Thermo-Calc

The CALPHAD method

CALculation of PHAse Diagrams

Experimental Information → Models for the thermodynamic properties of each phase G(T, P, y)

Empirical rules → Models for the thermodynamic properties of each phase G(T, P, y)

Fundamental theories → Models for the thermodynamic properties of each phase G(T, P, y)

Models for the thermodynamic properties of each phase G(T, P, y) → Database for model parameters

Database for model parameters → Predictive calculation of: thermodynamic properties, equilibrium states, phase diagrams

www.calphad.org

1969 Formation of CALPHAD.

1971 Sub-lattice model for 2 comp. (Hillert and Steffansson, KTH).

1977 Development of Thermo-Calc starts

Theories of phase transitions/ Phase-field models

van der Waals (1893)

Korteweg (1901

Landa

Cahn

Halpe 7)

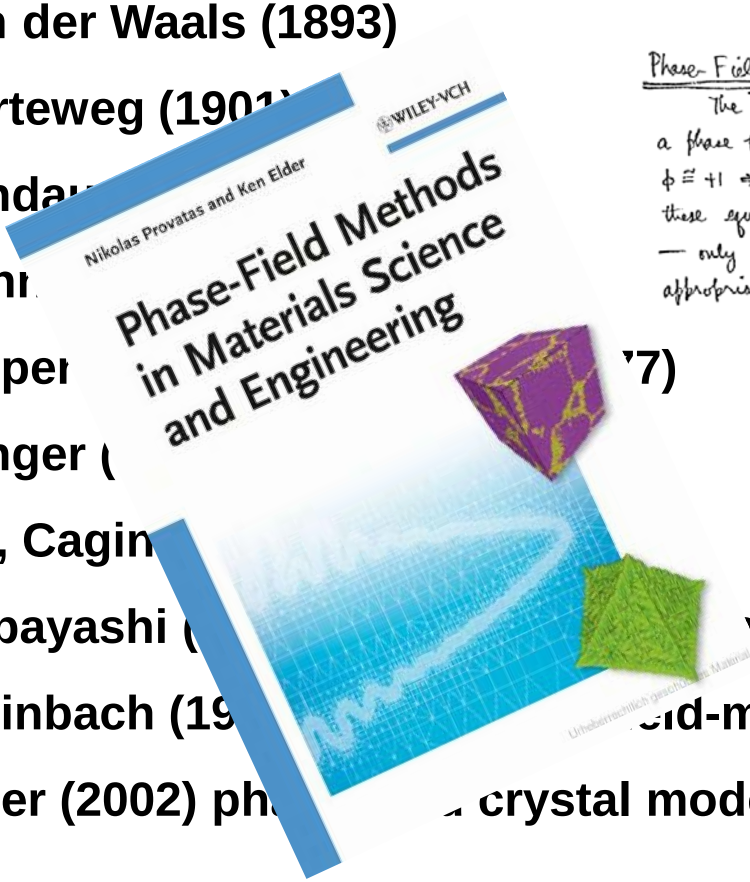
Langer (

Fix, Cagin

Kobayashi (se field

Steinbach (19 eld-model

Elder (2002) ph crystal models



2010

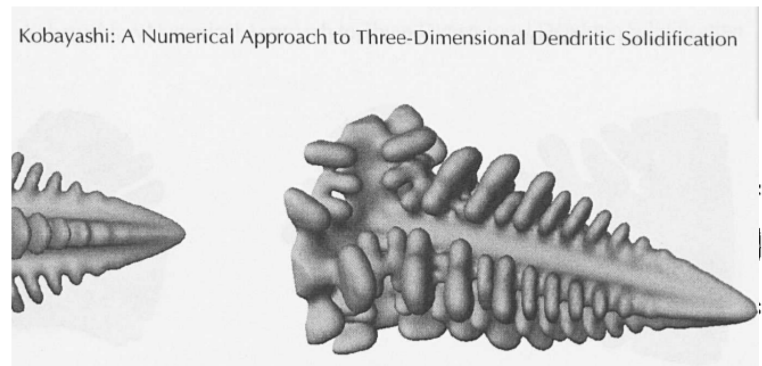
J.S.L 8/78 ①

Phase-Field Model

The idea is to set up the simplest possible equations of motion for a phase field $\phi(\vec{x},t)$ which will identify the phase (e.g. $\phi \cong -1 \Rightarrow$ solid, $\phi \cong +1 \Rightarrow$ liquid) at each point $\vec{x}$ and time t. We don't care whether these equations are a realistic microscopic model of any physical system — only that they reduce to our previous free-boundary problem in appropriate limits.

Jim Langer's notes from1978

(kindly provided by A.Karma)



A phase field concept for multiphase systems

I. Steinbach [a,*], F. Pezzolla [a], B. Nestler [a], M. Seeßelberg [a], R. Prieler [a], G.J. Schmitz [a], J.L.L. Rezende [b]

[a] ACCESS e.V., Intzestraße 5, D-52072 Aachen, Germany

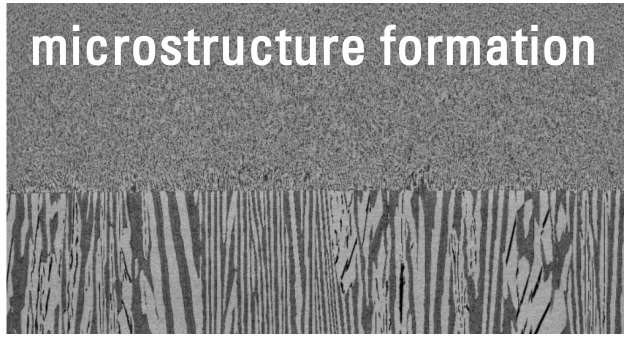
[b] Foundry Institute RWTH Aachen, D-52056 Aachen, Germany

Received 20 November 1995; accepted 30 November 1995

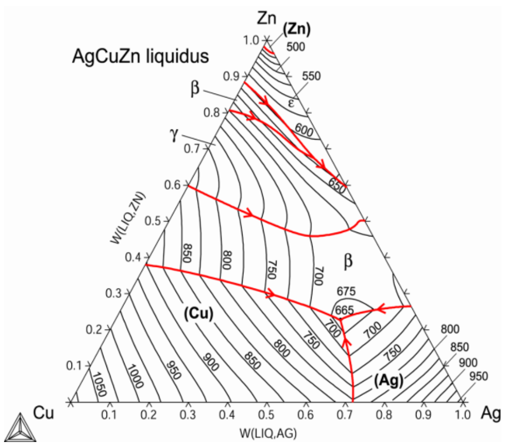
Communicated by H. Müller-Krumbhaar

Physica D 94 (1996)135

Mechanisms of microstructure evolution

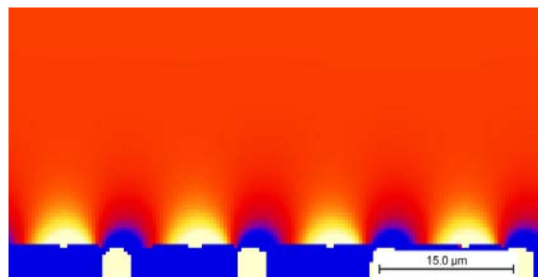


thermodynamics
(energy scale)



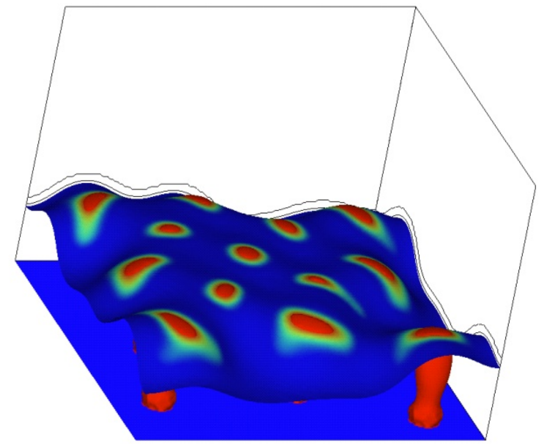
+

transport / diffusion
(time scale)



+

interfaces
(length scale)



TQ interface from TCS

diffusion solver

phase field method

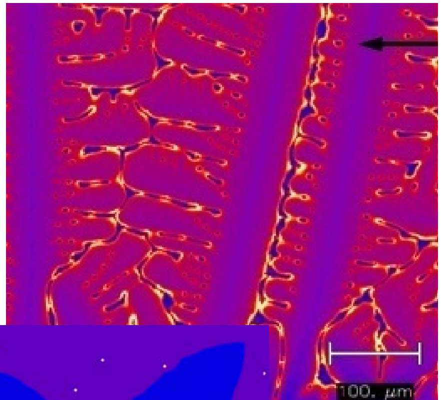
micress®

www.micress.de

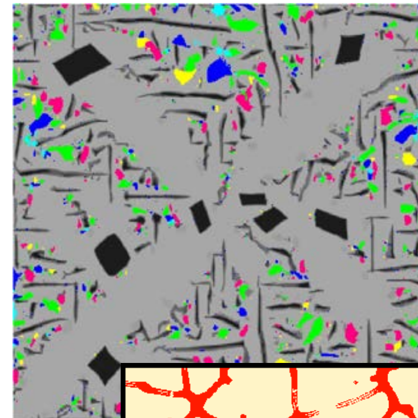
RWTH AACHEN UNIVERSITY

access

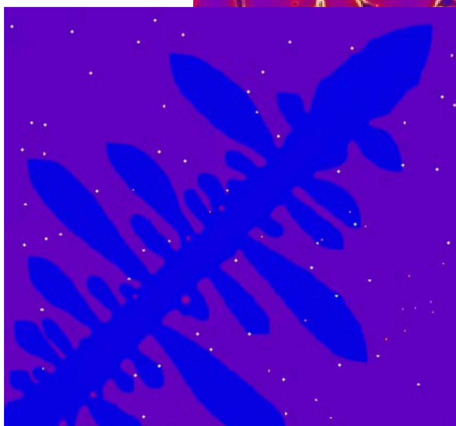
multi-phase-field simulations of microstructure evolution in technical alloy grades



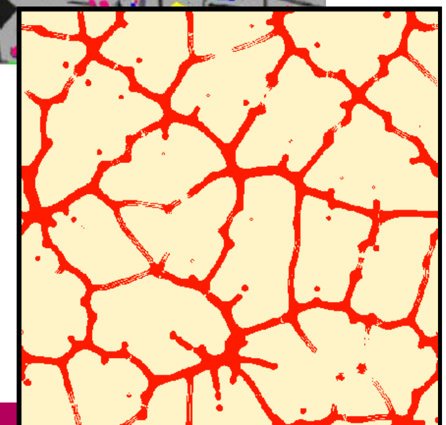
Steel
(e.g. stainless steel)



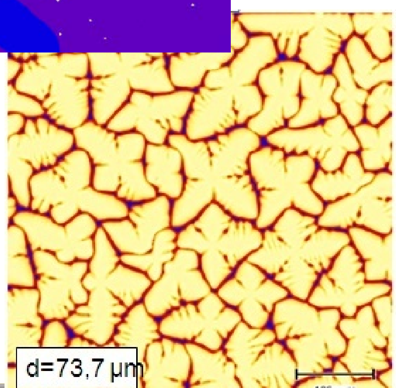
Al-alloys
(e.g. KS 1295)



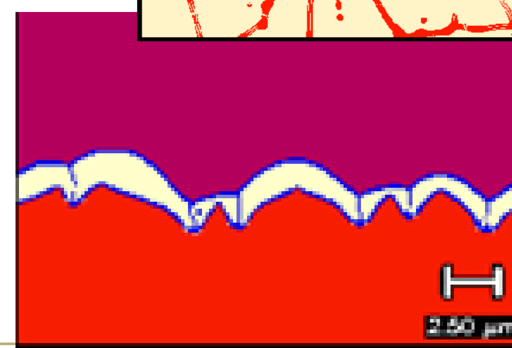
cast iron
(e.g. GJS)



Mg-alloys
(e.g. AZ 91)



Superalloys
(e.g. IN 718)

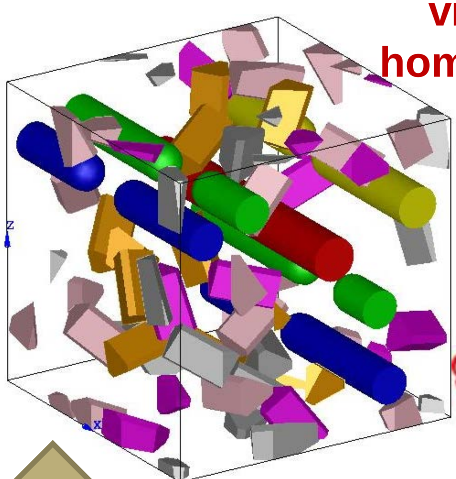


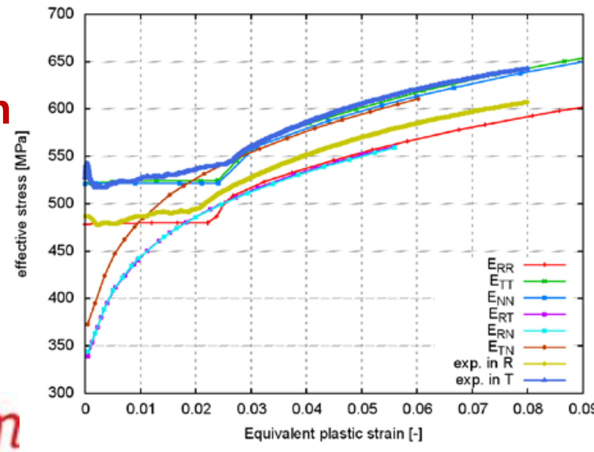
Solders
(e.g. SAC)

eventually: derive properties from simulated microstructures

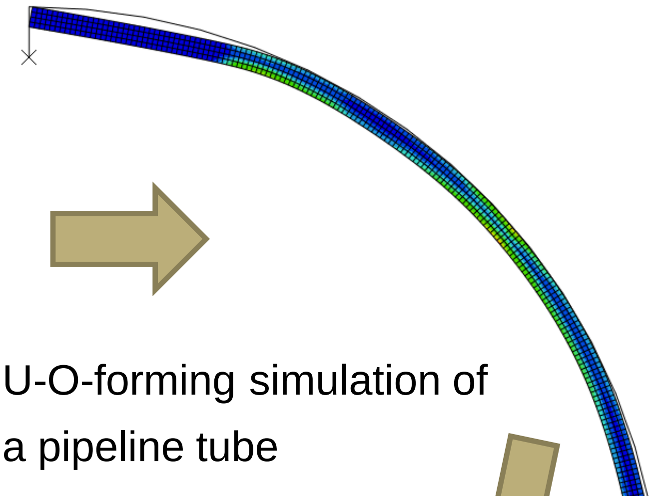
RVE: pearlite in ferrite matrix

virtual test/ homogenization

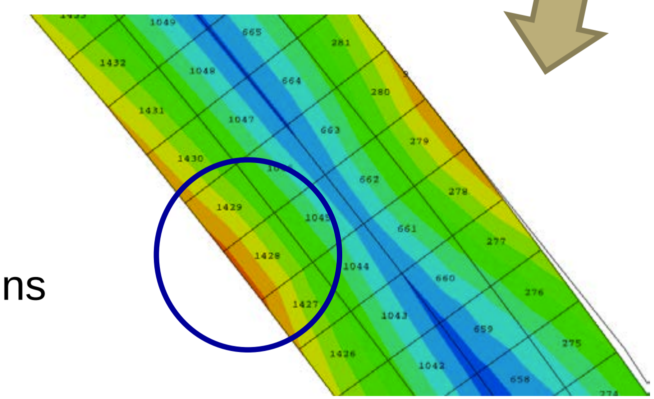




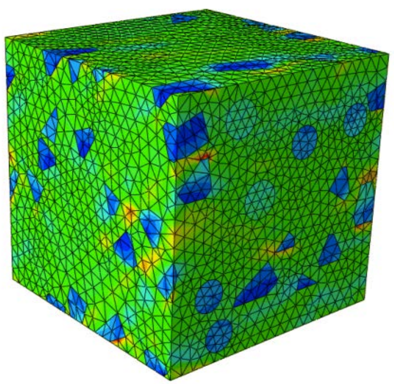
effective anisotropic flow curves



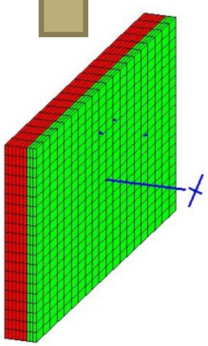
U-O-forming simulation of a pipeline tube



localization in critical regions:
applying local macrostrains on the RVE



equivalent plastic microstrain



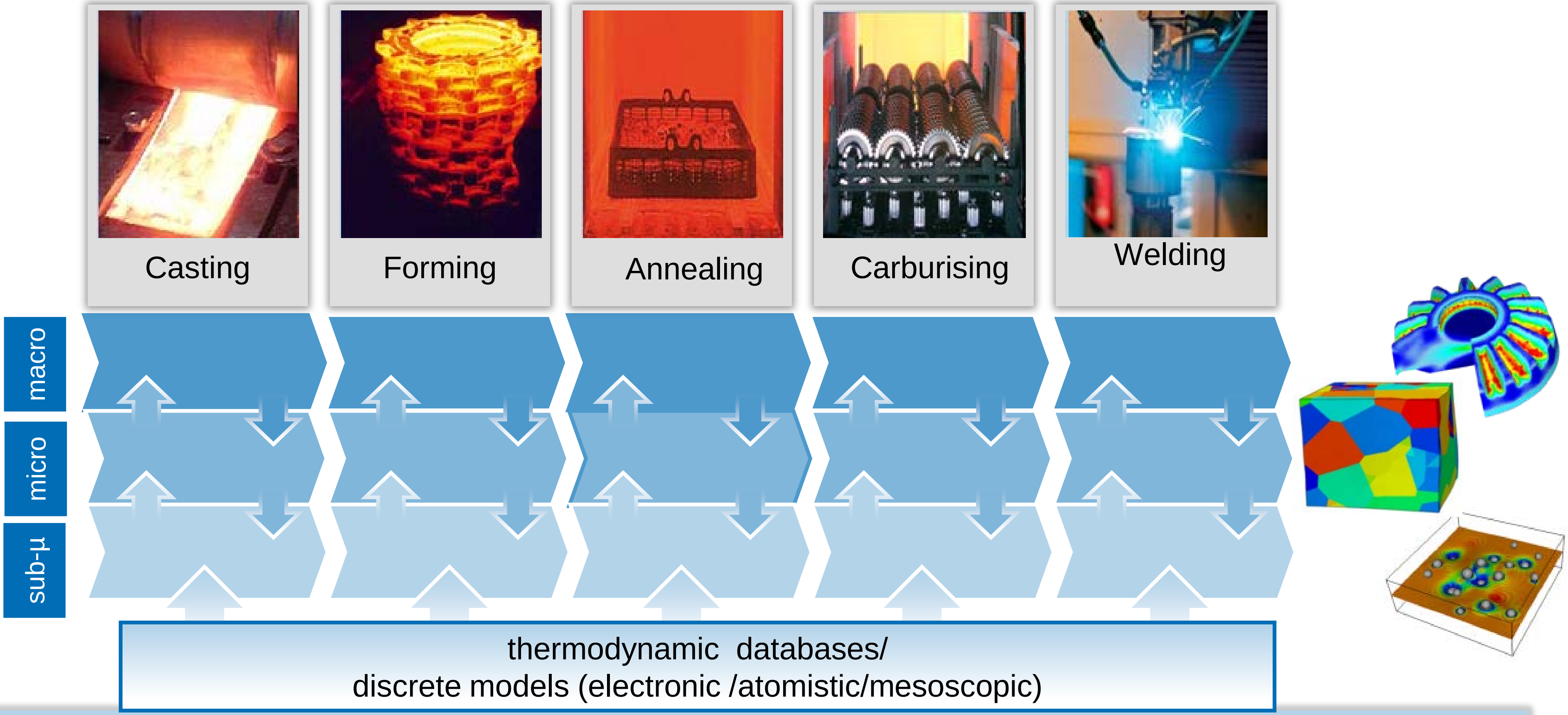
Ferrite-Cementite bilamella

G. Laschet, P. Fayek, T. Henke , H. Quade, U. Prahl:

Derivation of anisotropic flow curves of ferrite–pearlite pipeline steel via a two-level homogenisation scheme

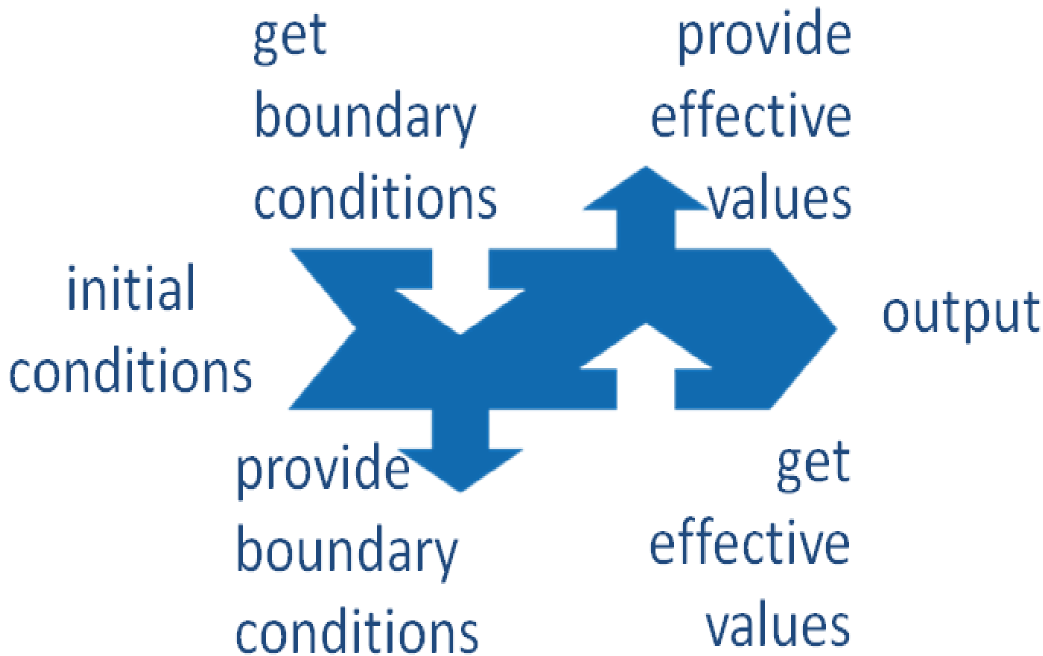
Materials Science & Engineering A 566 (2013) 143–156

Vision: plug & play for ICME



Comprehensive, standardized, modular and extendable modeling environment being efficiently adaptable to a specific material, process-chain and product

The basic platform module:



Example: Microstructure Simulations

e .g.
$T(t)$, $c_i(t)$

e.g. average λ_2,
grainsize distribution
fs(T),etc.

μ -structure (in)

μ -structure (out)

Temperature T ,
concentrations $c_{i,}$
Phase fractions Φ_i

e.g. local equilibrium
interfacial energies
precipitate size distributions
…

example: solidification ..(without flow)

Data source	Thermo-Calc Software	**Experimental data**	**Estimated values**
Data	H (T), c_p(T), ρ_{solid}(T), ρ_{liquid}(T)	λ_{solid}(T),λ_{liquid}(T)	
Process	Temp_1D, STAR-Cast, SimWeld, MAGMA	**& many others**	
Boundary conditions	T (t), c_i(t)		**Estimated values**

example: solidification ..(without flow)

Data source	Thermo-Calc Software	**Experimental data**	**Estimated values**
Data	$H\ (T), c_p(T), \rho_{solid}(T), \rho_{liquid}(T)$	$\lambda_{solid}(T), \lambda_{liquid}(T)$	
Process	Temp_1D, STAR-Cast, SimWeld, MAGMA		& many others
Boundary conditions	$T\ (t), c_i(t)$	**e.g. SDAS/ λ_2** (secondary dendrite arm spacing)	**Effective property**

provide boundary conditions

get effective data

Temperature T ,

concentration of alloy elements c_{i},

Phase fractions Φ_i

Partitioning of alloy elements
Diffusion matrix/mobility data
driving force dG
tranformation enthalpy
equilibrium phase fractions Φ_i

Interfacial energies
Precipitate size distributions

Thermo-Calc Software

DICTRA

TC-Prisma

get initial conditions

Source	Tools	Output
preceeding simulation	micress, DAMASK Düsseldorf Advanced Material Simulation Kit	**restart-file**
digital experimental data e.g. CT scans, SEM/EDX,LOM, EBSD stacks	ParaView, DREAM3D	**vtk-type-file**
experimental data e.g. images	GIMP + pgm2txt, DREAM3D	**ASCII text**
synthetic microstructures e.g. voronoi tesselation designed structures, assumptions	e.g. (paint) or .dri, DREAM3D	**HDF5 files**
microstructure database	MRL	

provide output

restart-file

„mcr“-files

vtk-type-files

HDF5 files

ASCII files

DAMASK
Düsseldorf Advanced Material Simulation Kit

micress

DP_MICRESS

ParaView

DREAM3D

mesh2xx + ABAQUS

HOMAT

MRL

gnuplot 4.6 , , etc.

subsequent simulation

2D visualisation / analysis
e.g. virtual EDX

3D visualisation/analysis
e.g. virtual EDX/ virtual EBSD

virtual testing

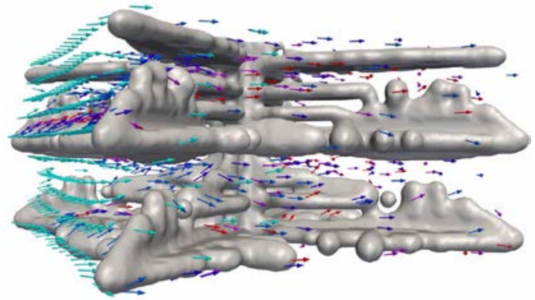
effective properties

store µ- structure in database

average values/ other data
e.g. average grain size, phase fractions, cooling curves

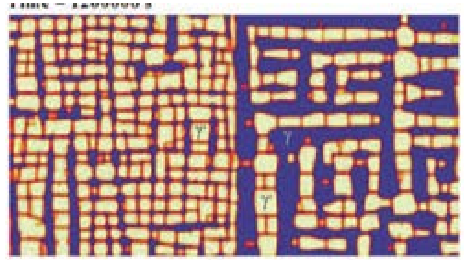
Some recent trends in microstructure simulations of technical alloys (1/3)

Coupling with flow



B.Böttger , R.Berger
3D dendrites in IN 718
unpublished

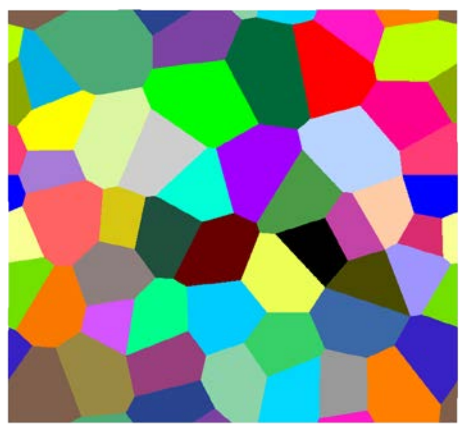
Coupling with elastic stresses



L.Zhang, I. Steinbach, Y.Du
Int. J. Mat. Res. 102(2011)4 p375 ff

Linking with crystal plasticity FEM

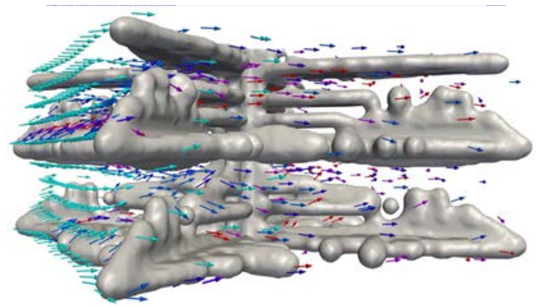
(courtesy O.Güvenç)



O. Güvenç, M. Bambach, and G. Hirt
steel research int. 85 (2014) No. 6
DOI: 10.1002/srin.201300191

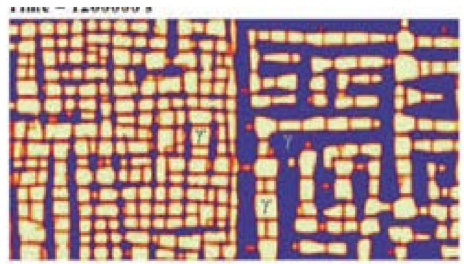
Some recent trends in microstructure simulations of technical alloys (1/3)

Coupling with flow



B.Böttger
3D dendrites in IN 718
JOMM 68 1 (2016) 27-36

Coupling with elastic stresses



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Linking with crystal plasticity FEM

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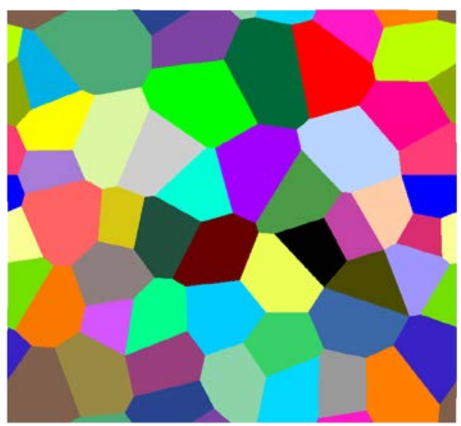
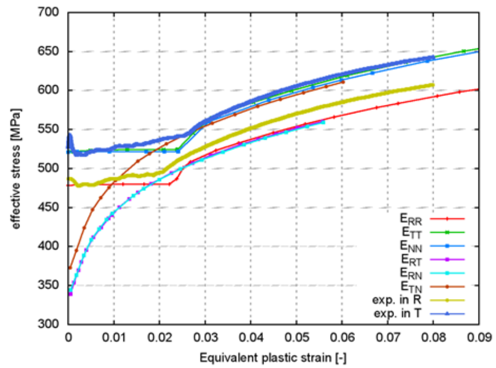


O. Güvenç, M. Bambach, and G. Hirt
steel research int. 85 (2014) No. 6
DOI: 10.1002/srin.201300191

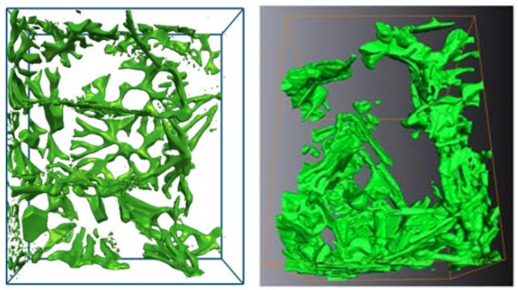
Some recent trends in microstructure simulations of technical alloys (2/3)

Determination of effective properties



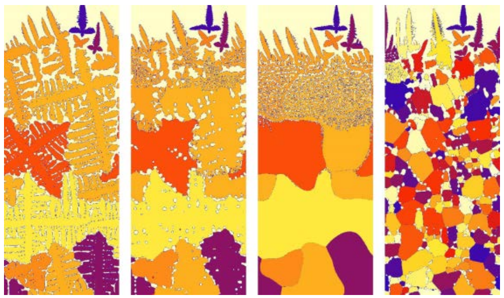
G. Laschet, P.Fayek, T.Henke , H.Quade, U.Prahl
Materials Science & Engineering A 566 (2013) 143–156

Modelling of faceted growth



Janin Eiken, Markus Apel, Song-Mao Liang, Rainer Schmid-Fetzer:
Acta Materialia 98 (2015)152–163

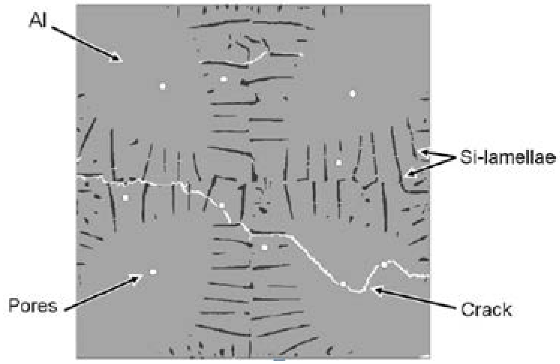
Modelling of joining processes



G.J.Schmitz, B.Böttger and M.Apel
On the role of solidification modelling in "ICME"
Materials Science and Engineering 117 (2016) 012041 doi:10.1088/1757-899X/117/1/012041

Some recent trends in microstructure simulations of technical alloys (3/3)

Modelling of failure and fatigue



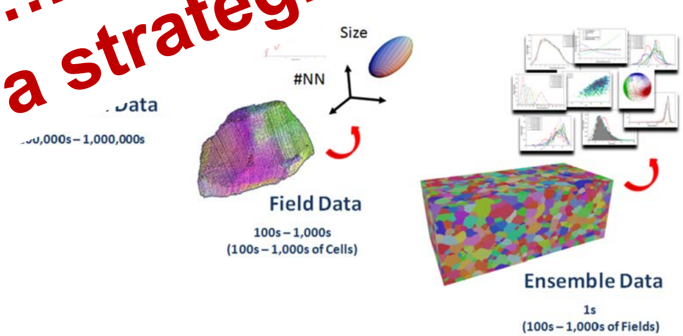
G. Lasko, M. Apel, A.Carré, U. Weber and S. Schmauder
Adv. Eng. Materials 13 (2012)1
DOI: 10.1002/adem.201100188

information exchange with experiments

M.Apel
...he 3rd World
... on ICME
...iley TMS (2015) p165-172
(ISBN 978-1-119-13949-2)

Interoperability of software tools

...in a plug&play mode of operation is a strategic interest of MICRESS!



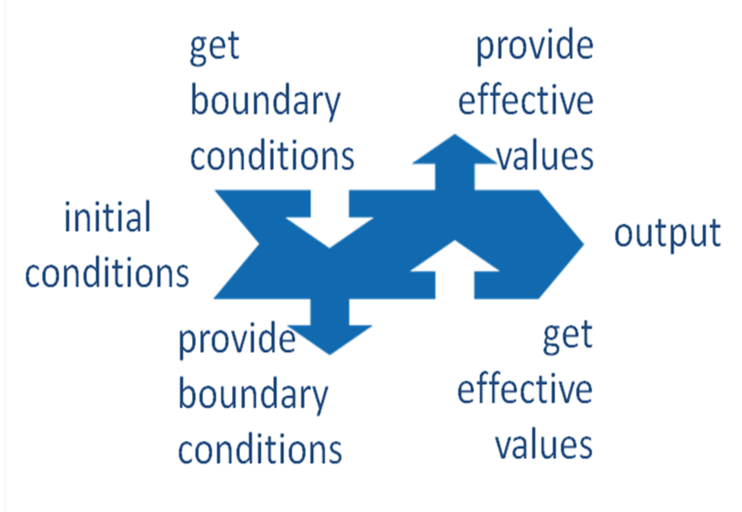
ongoing work:

Can HDF5 provide the basis for an emerging standard for describing microstructures?
JOMM 68 1 (2016) 77-83

Plugs and sockets for plug & play: benefits of standardization

Have you ever tried to get

that one

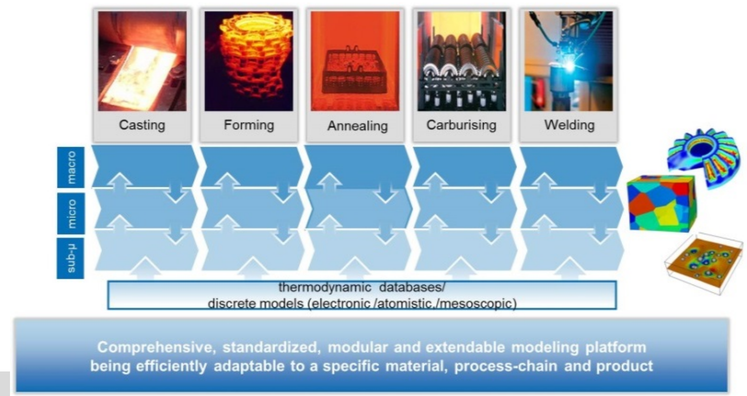


into that one?

The European Materials Modeling Council

- EU project ICMEg -

EMMC



consortium: 11 partners, 6 countries

vision: plug&play in ICME

approach: global, open standards

How to do in practice? Read more:

ICMEg - the Integrated Computational Materials Engineering expert group - a new European coordination action

Integrating Materials and Manufacturing Innovation 2014, **3**:2 doi:10.1186/2193-9772-3-2

Georg J Schmitz (G.J.Schmitz@access.rwth-aachen.de)
Ulrich Prahl (Ulrich.Prahl@iehk.rwth-aachen.de)

www.icmeg.eu
www.icmeg.info

Huge variety of existing codes

different scales; different objectives; different properties; different materials

only common denominator: MATERIAL

What is a material ?

Any material is

„a number of atoms arranged in a volume“

The number of atoms may be large and they typically will belong to several chemical elements

The European Materials Modeling Council

What is a material in terms of keywords?

Any material is

„*a* NumberAtoms

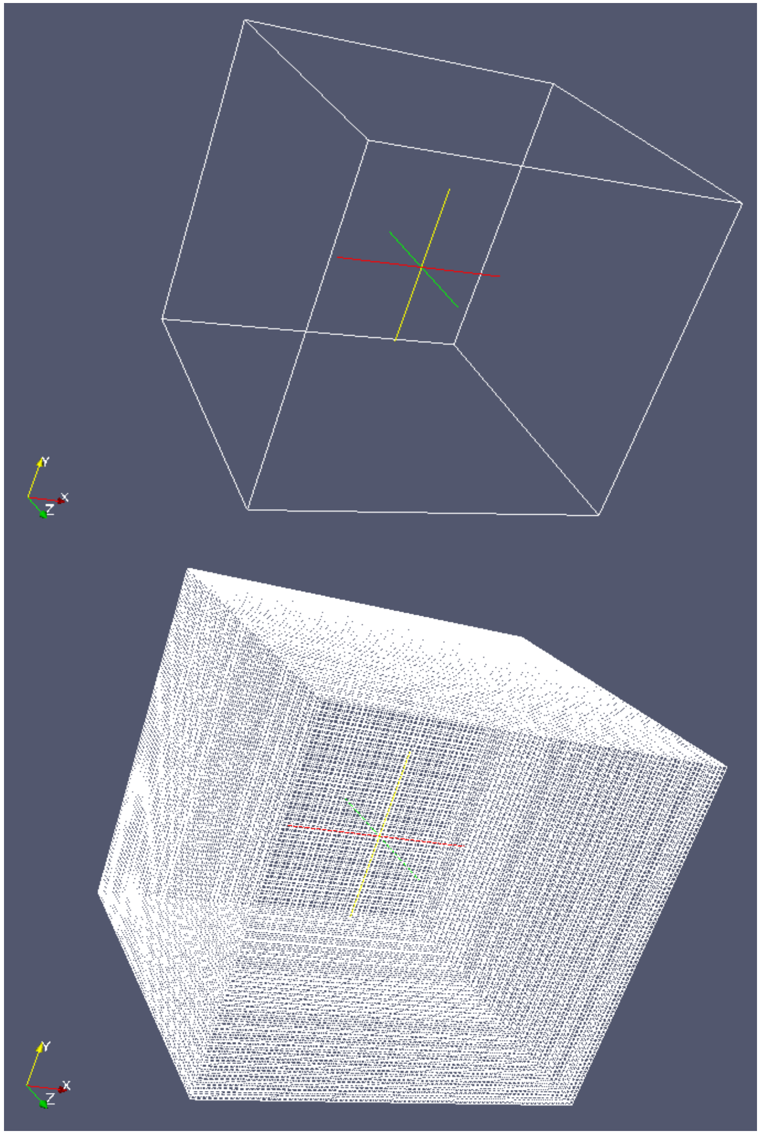
***arranged in a* Volume"**

The **NumberAtoms** may be large (**NumberMoles)** and they typically will belong to a **NumberChemicalElements**

What is a material ?

- Volume
  - must be large enough to host the number of atoms
  - should be large enough to be representative for the „material“
- Atoms are described by electronic and atomistic models

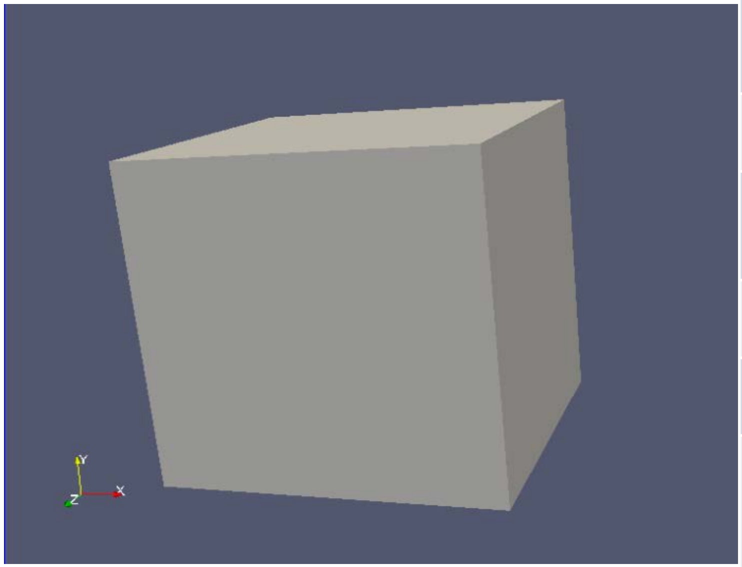
Position/Volume/Orientation of RVE



Keyword	Example
ReferenceFrame	(component frame CF)
RVEID	Identifier
Position	= (x_0 y_0 z_0) (in ComponentFrame)
Centroid	= (x_1 y_1 z_1) (in RVE Frame)
Origin	Position-Centroid
Orientation	Orientation e.g Euler Angles or Quaternions (w.r.t CF)
Volume	NumberCellsX*CellSizeX NumberCellsY*CellSizeY* NumberCellsZ*CellSizeZ or lenghtX*lenghtY*lenghtZ
Surface	separate slides…

Note: RVE may have arbitrary shape
Discretisation needs NOT to be voxel type

Generic microstructure: Atoms in an RVE



Keyword	Example
NumberChemicalElements	2 (Al and Cu)
ChemicalElementID „CEID“	=1 (for Al) (=2 (for Cu))
ChemicalElementName(CEID)	= Al, CU
NumberMoles(CEID)	= see „composition“
NumberMoles	all Atoms
Mol(CEID)_Fraction	(NumberMoles(CEID) /NumberMoles)
Composition	Vector of all Mol_Fractions for all CEID

Note: „Properties“ are introduced via CEName e.g. MolecularMass Al = 27g/mol

Some further keywords: NumberConstituents, NumberIsotopes, NumberAtoms ConstituentID, ConstituentName(ConstituentID), IsotopeID, IsotopeName(IsotopeID)

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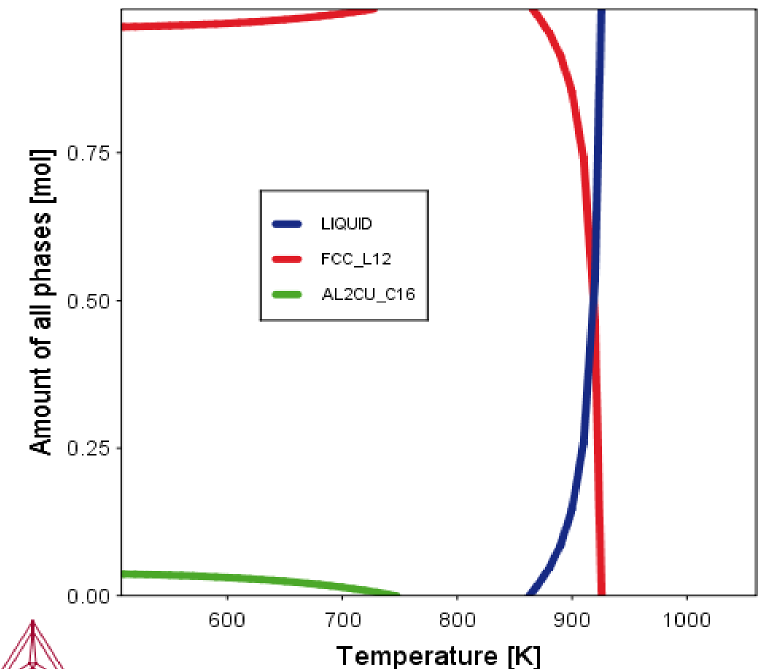
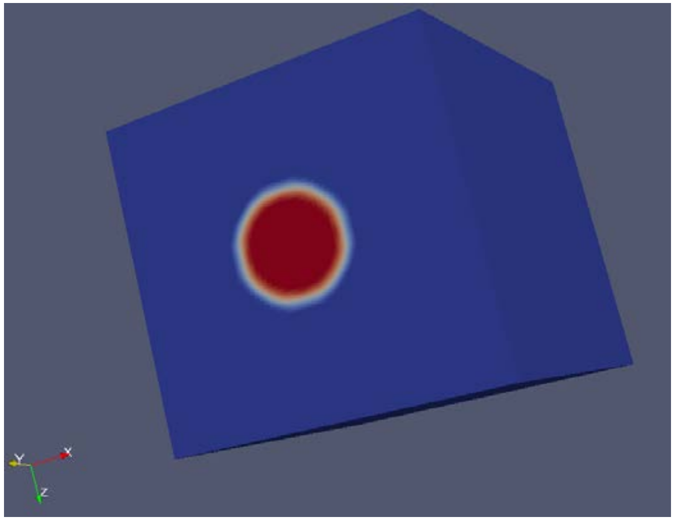
Generic microstructure: Phases in an RVE



Keyword	Example
PhaseType	Multiphase solid liquid
NumberPhases	in the RVE = 3
PhaseID	= 3 , 1 and 2
PhaseName(PhaseID)	= Liquid = α- Al = Al_2Cu
Volume(PhaseID)_Fraction	Volume(PhaseID) /Volume(RVE)

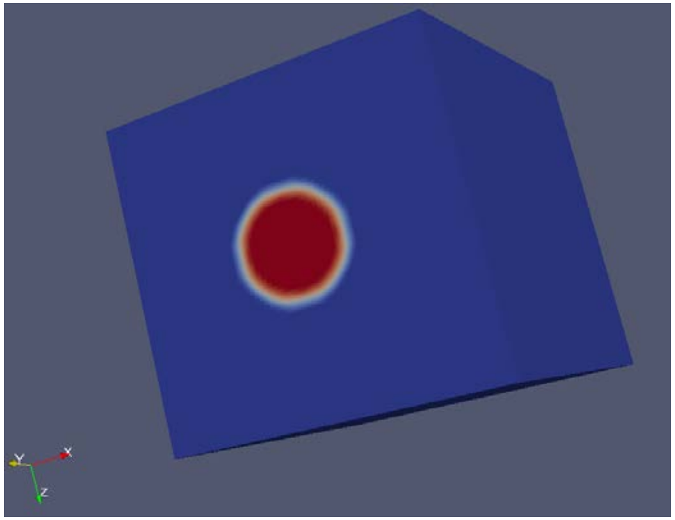
Note:
Equilibrium volume fractions of phases can be calculated for given composition and conditions, but NO information about spatial distribution of the phases in the RVE

Generic microstructure: Ensembles/Phases I



Keyword	Example
PhaseID	1
PhaseName	α- Al
Volume	Volume of this phase
Centroid	Centroid of this phase
Orientation	…
NumberChemicalElements	2 (Al and Cu)
ChemicalElementID „CEID“	=1 (for Al) (=2 (for Cu))
ChemicalElementName(CEID)	= Al, CU
NumberMoles(CEID)	= see „composition“
NumberMoles	all Atoms in PhaseID
Mol(CEID)_Fraction	(NumberMoles(CEID) /NumberMoles)

Generic microstructure: Ensembles/Phases II



Keyword	Example
CrystalStructure	solid-solution FCC
CrystalSymmetry	cubic
Crystalline_Fraction	1
LatticeConstants	e.g. numbers, xyz or CIF file information

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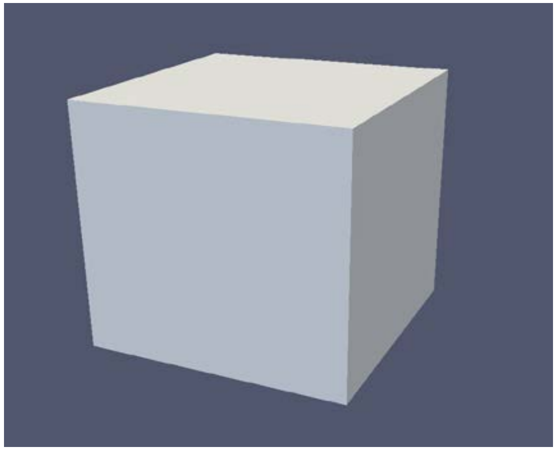
An RVE from the engineering perspective



- homogeneous and isotropic piece of materi
- „effective“ (i.e. homogenized/average
- Different RVEs at different positi ent
- „Properties“ typically taken f atabases
- Microstructure determi es: statistical information abou e features thus is highly desirable an available e.g.

  – ize (Hall-Petch relation)
  – nisotropy)
  – ondary dendirte arm spacing (permeability, strength,..)
  – Phase fractions (precipitation hardening)
  – Phase composition…(solution hardening)
  – Dislocation densities..(work hardening)

Application Engineers view of a material:
a name + related properties

Keywords for spatially resolved information

How to describe

„arranged"

??????

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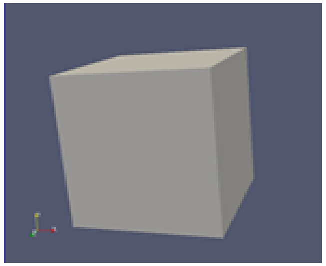
How to describe arranged?

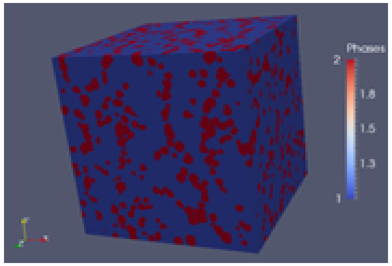
- Atoms may „self arrange“ (see also e/a/m models) and form **objects/features** and **ensembles** of objects/**features** e.g.
  - molecules, particles, precipitates, crystals/grains
  - different phases/crystal structures
  - defect structures….and eventually
  - multiphase, polycrystalline materials

RVE



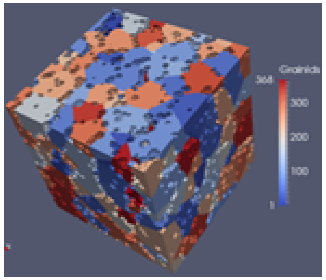
effective material

Ensemble(s)



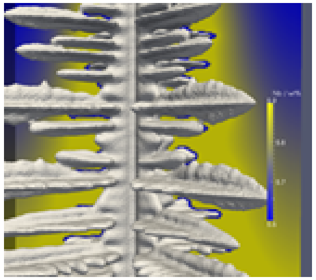
e.g.phases

Feature(s)



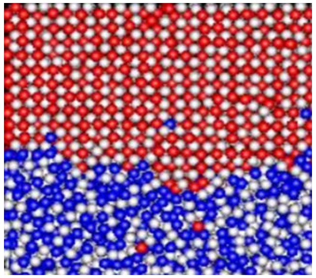
e.g. grains

Fields



e.g. concentration

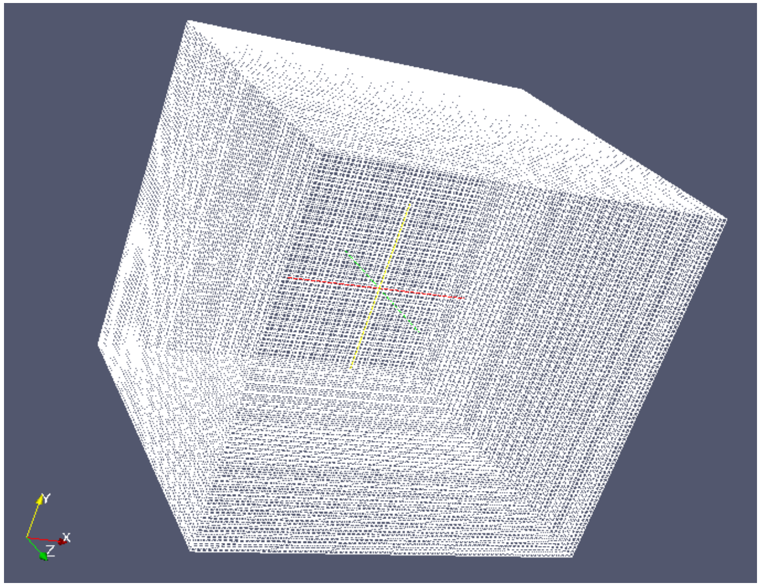
Atoms

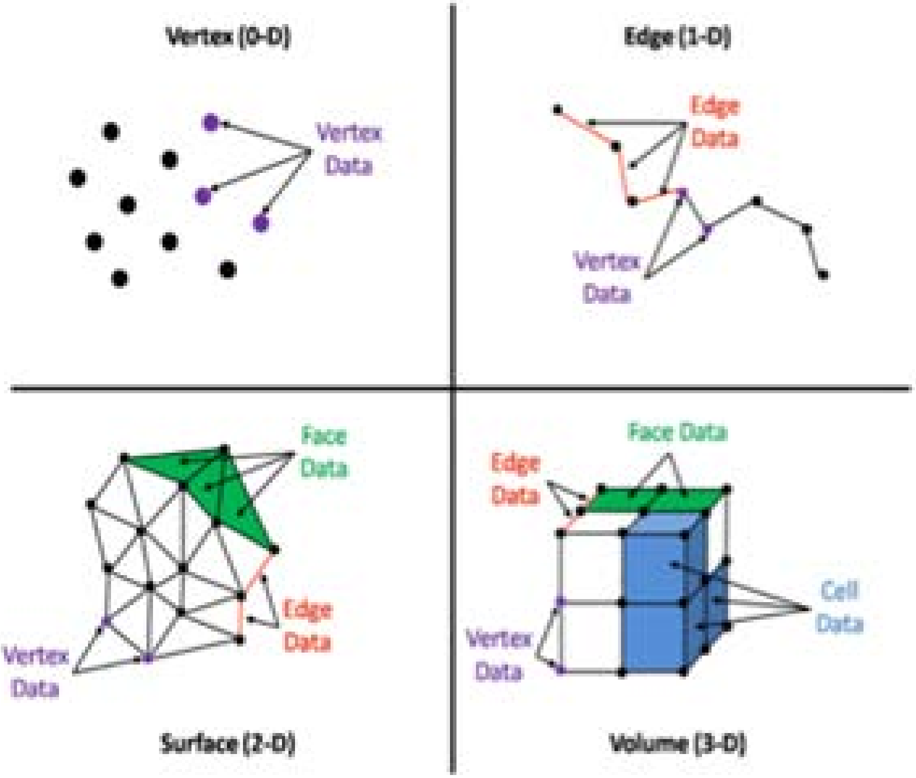


e.g. positions

- Materials reveal an inherent hierarchical structure!

continеous fields (x,y,z,t_0): structuring space





Note: RVE may have **arbitrary shape** ,
Cells may have **arbitrary shape** and may be defined by vortices, edges and faces

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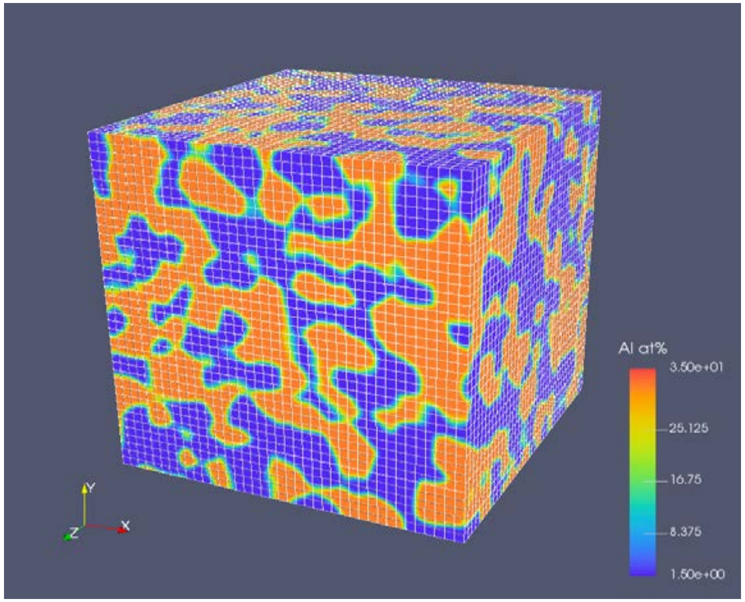
Continous Fields (x,y,z,t_0)



Keyword	Example
CellID	defines position of Cell
Mol_Fraction(CEID)	e.g. at% Al
Composition	
Orientation	….
Strain	….
Defect_Density(type)	….
FlowVelocity	…..
FeatureID	next slide

Further:
Fields corresponding to any other keyword in case spatial variations are relevant

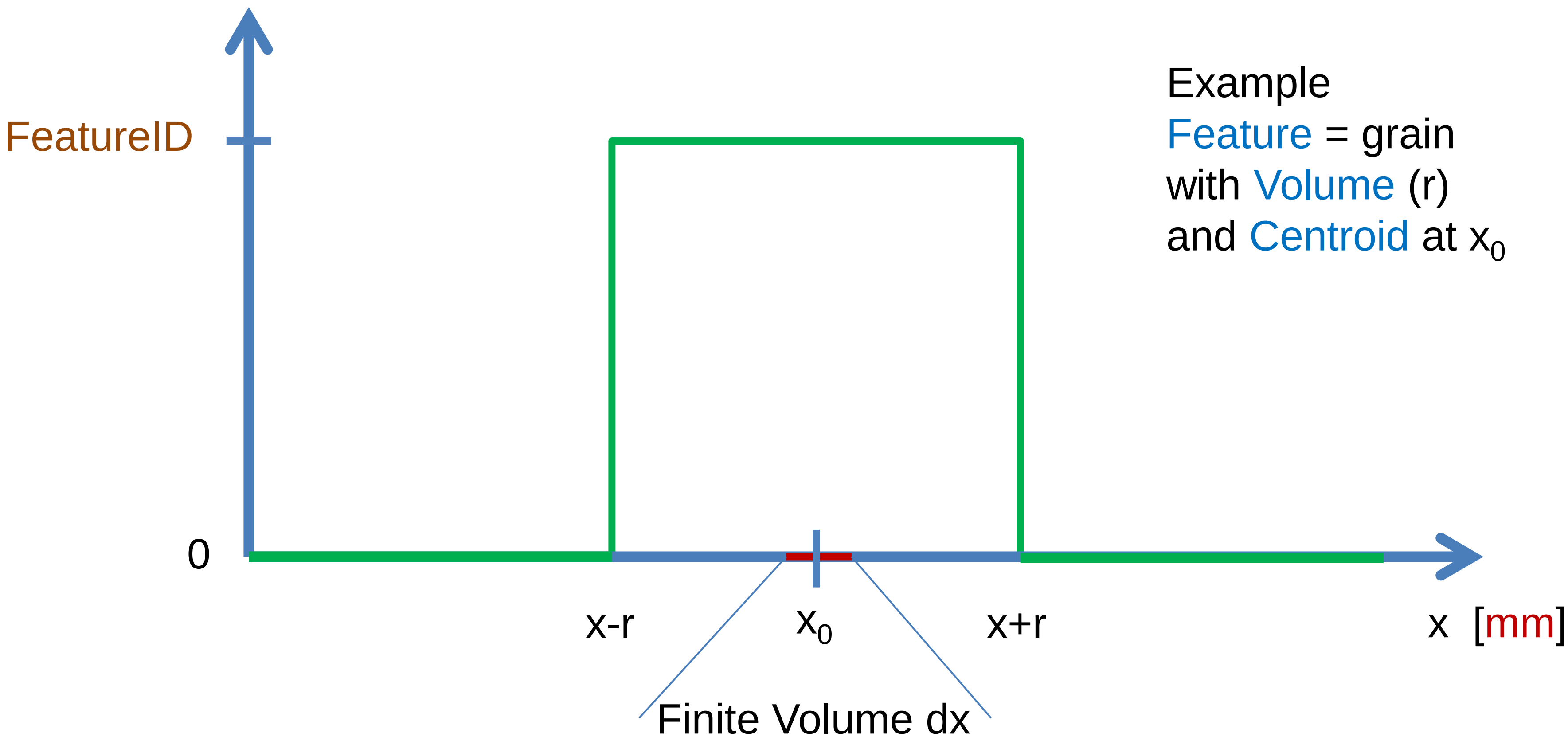
Describing features by fields

: feature indicator function (**<u>….a FIELD)</u>**

= 0 if feature is absent

= FeatureID if feature is present

1D space



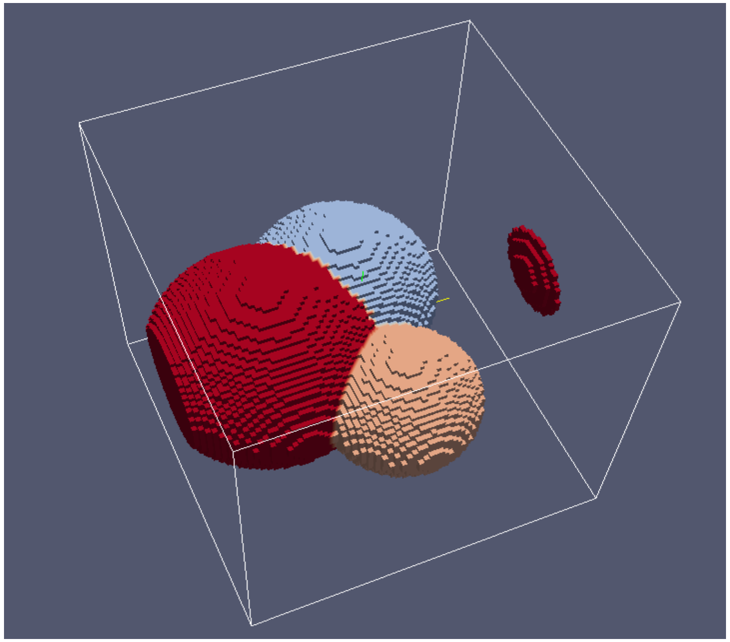
Example

Feature = grain

with Volume (r)

and Centroid at x_0

Generic microstructure: Features in RVE



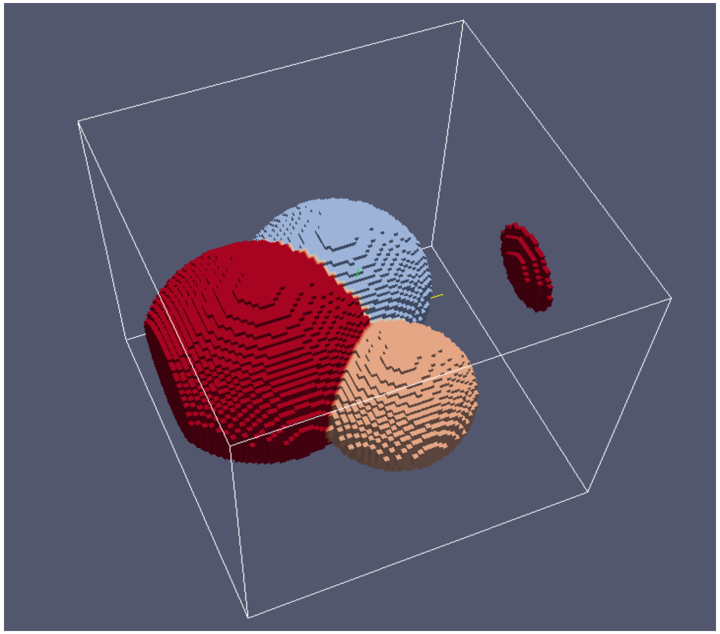
NumberFeatures in RVE : 4

FeatureIDs = 1-4

NumberFeatures belonging to Phase 1 = 2

FeatureIDs = 1 & 2

Position/Volume/Orientation of Features



Keyword	Example
FeatureID	Identifier
PhaseID	to which phase the feature belongs
Centroid	Centroid of feature
Orientation	Orientation e.g Euler Angles or Quaternions (w.r.t RVE Frame)
Volume	Volume of feature/grain
Composition	Average composition in feature
Surface	See separate slides

Note: Features may have arbitrary shapes which are described by FeatureId Field

Further Features/Fields: Defects

NumberDefectTypes
(e.g. point defects, line defects,
planar defects, 3D defects, dislocations, porosity,…)

NumberDefects(Type)

Defect(Type)_Density =
NumberDefects(Type)/Volume(RVE) (alt.: Volume(Ensemble, Feature, Field)

DefectVolume_Distribution

These keywords apply to RVE (shown here), Ensemble, Feature, or Field

Interfaces

The whole is more than the sum of its parts

…..when considering interfaces as a part of the story….

Interfaces/Surfaces/Boundaries: SurfaceElement

SurfaceElement/Face:

FaceID

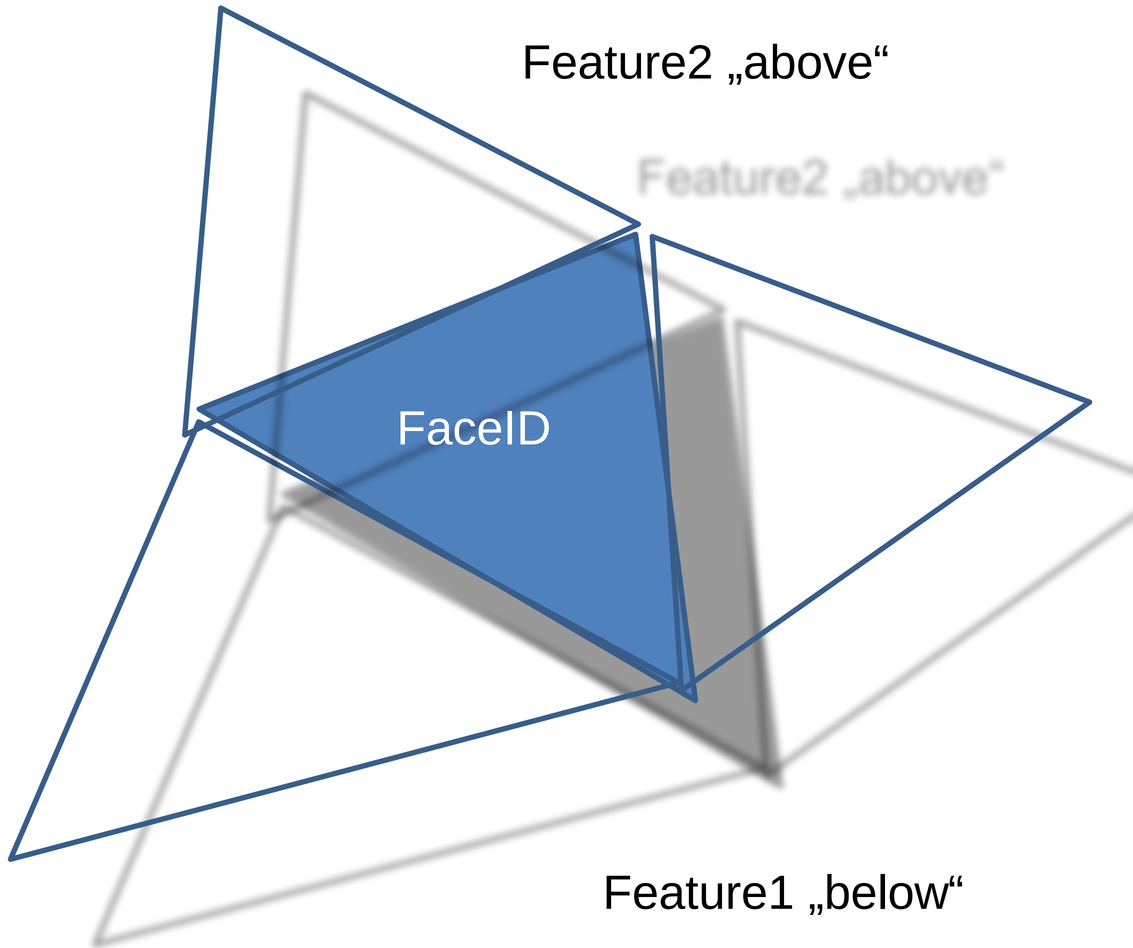
FaceLabel (FaceID,Feature1,Feature2)

Area

Orientation (of face normal)

Centroid

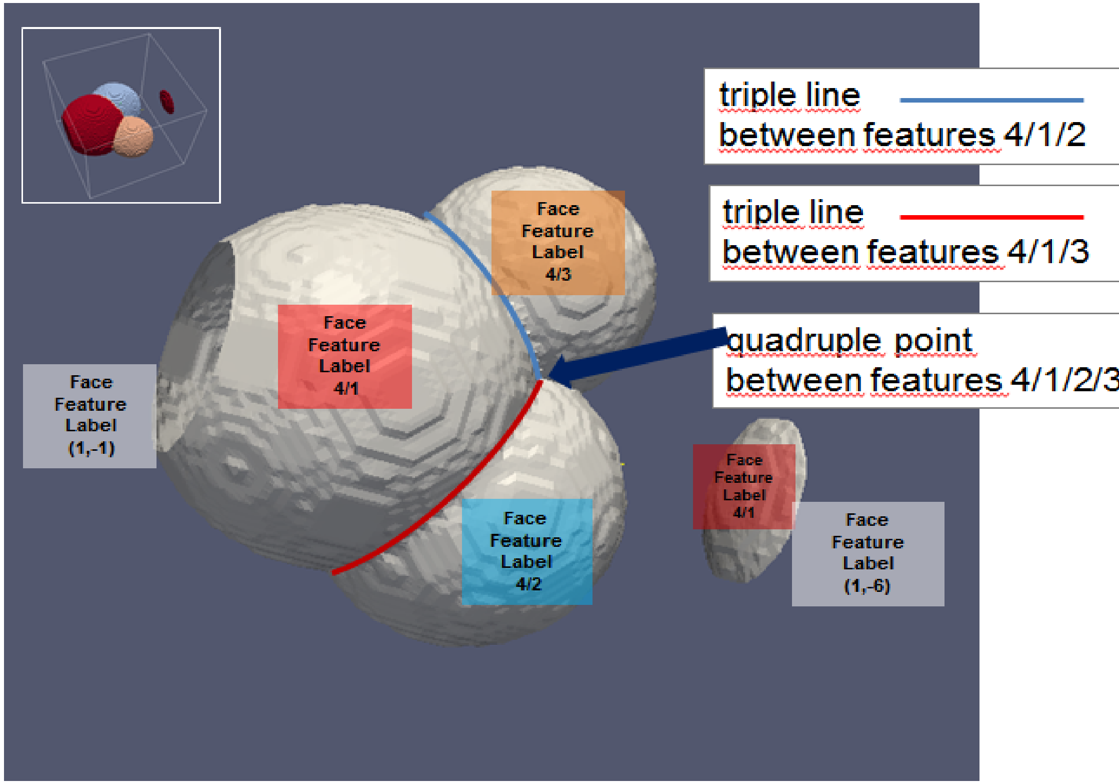
Curvature



FaceFeature

FaceFeatureLabel (FeatureID1,FeatureID2)

Ensemble of Faces shared
between two Features
e.g 3 and Feature1



Area (FaceFeatureLabel)

InterfaceArea consisting of all faces shared
between FeatureID1 and FeatureID2

Centroid

Orientation

Curvature

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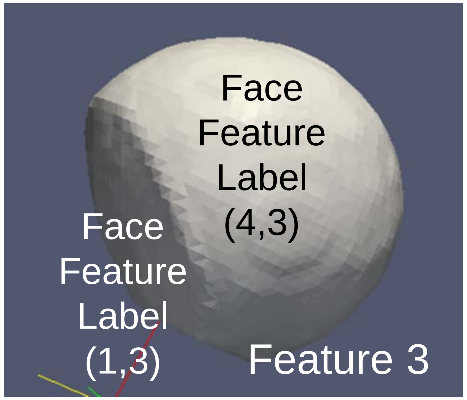
FaceFeatureEnsembles



FaceFeatureEnsemble:

e.g:

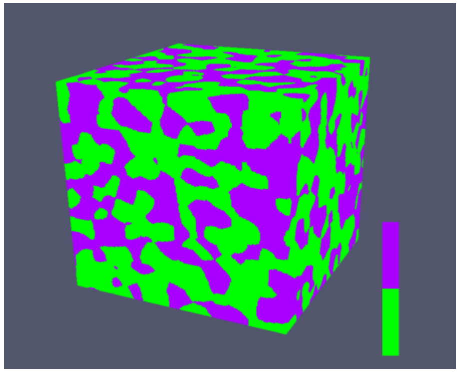
Surface(FeatureID)

SurfaceRVE

InterfacesRVE

PhaseBoundary(PhaseID1,PhaseID2)

GrainBoundary(PhaseID1,PhaseID1)



Canonical set of keywords?

- Is there a hierarchical and canonical base of keywords being sufficient to describe any type of material resp. microstructure?

- Can all further required keywords be derived by suitable schemes?

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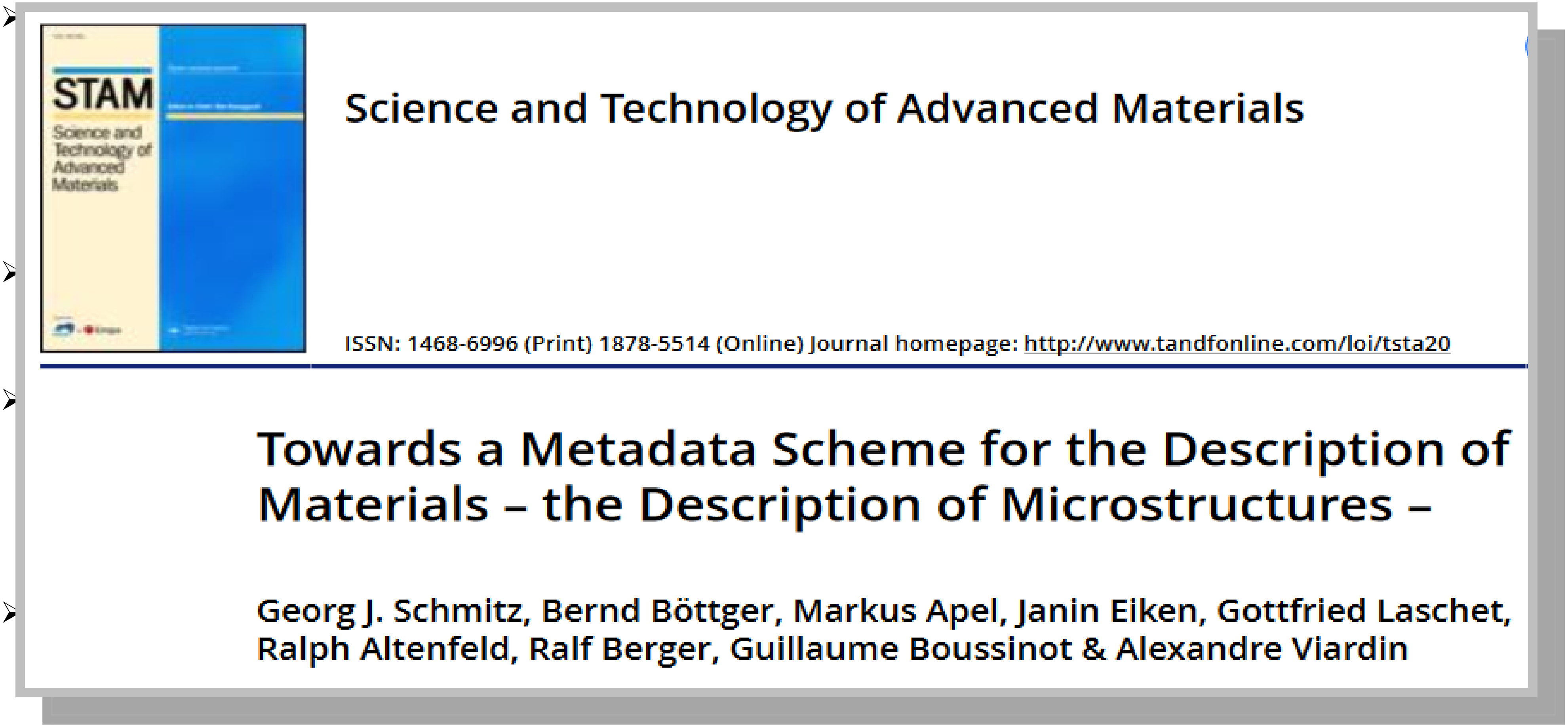
Canonical keywords (Volumetric)

RVE	Phase	Feature	Field at Cell
NumberElements	NumberElements	NumberElements	NumberElements
NumberAtoms	NumberAtoms	NumberAtoms	NumberAtoms
NumberPhases			
	PhaseID	PhaseID	
NumberFeatures	NumberFeatures		
		FeatureID	FeatureID
NumberDefects	NumberDefects	NumberDefects	NumberDefects
Composition	Composition	Composition	Composition
Volume	Volume	Volume	Volume
Centroid	Centroid	Centroid	Centroid
Orientation	Orientation	Orientation	Orientation
Crystallinity	Crystallinity	Crystallinity	Crystallinity

Summary: Canonical keywords (2Dimensional)

Surface	Interfaces/ surfaces	FaceFeature	Face
Centroid	Centroid	Centroid	Centroid
Area	Area	Area	Area
Composition	Composition	Composition	Composition
Curvature	Curvature	Curvature	Curvature
Orientation	Orientation	Orientation	Orientation
Area/Volume	Area/Volume	Area/Volume	Area/Volume

metadata description of a static microstructure


STAM Science and Technology of Advanced Materials

Science and Technology of Advanced Materials

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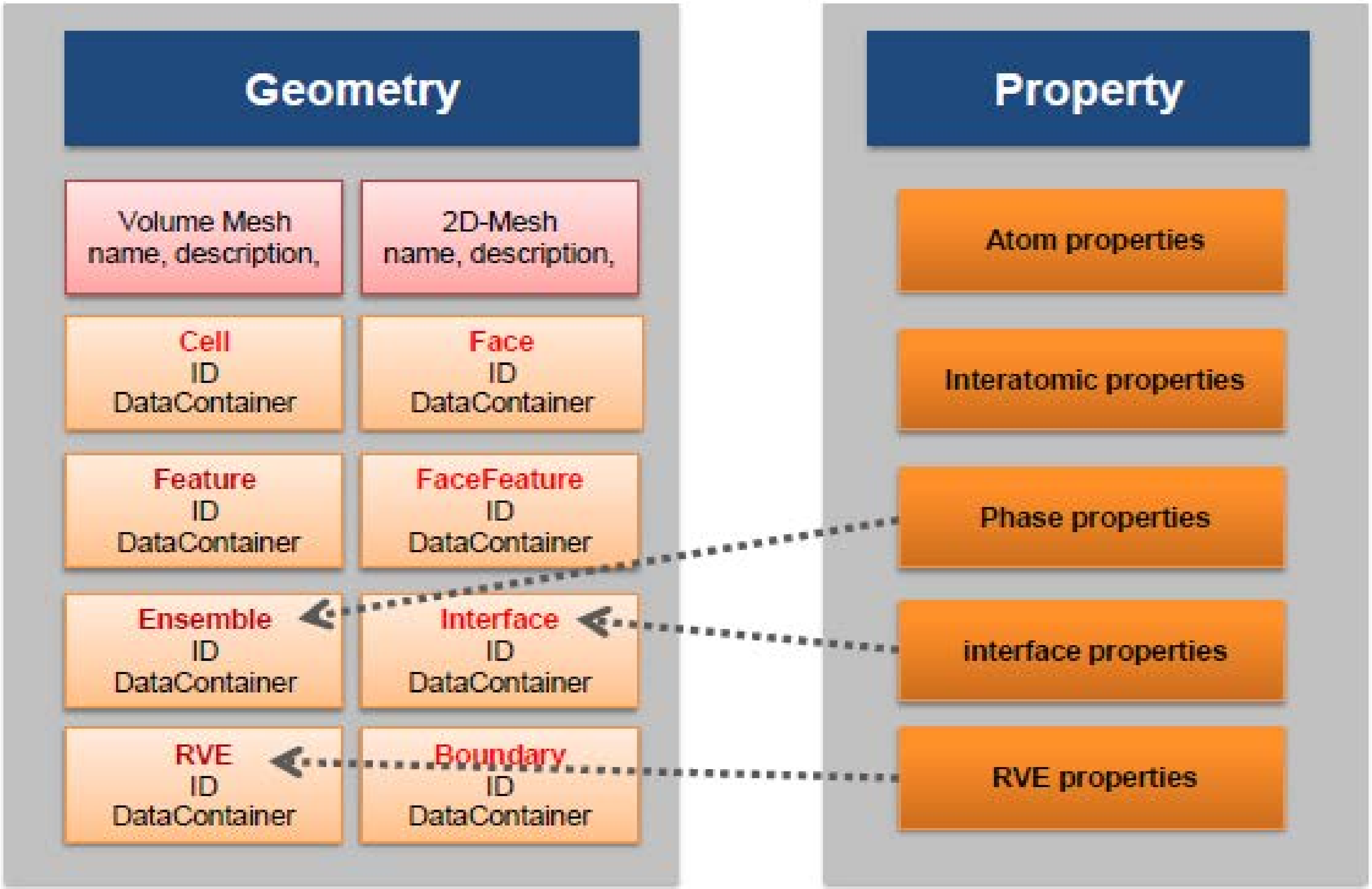
Towards a Metadata Scheme for the Description of Materials – the Description of Microstructures –

Georg J. Schmitz, Bernd Böttger, Markus Apel, Janin Eiken, Gottfried Laschet, Ralph Altenfeld, Ralf Berger, Guillaume Boussinot & Alexandre Viardin

- **The proposed metadata keyword structure may even be applicable to e/a/m models**
  - ***to be verified….***

Metadata for properties to complement



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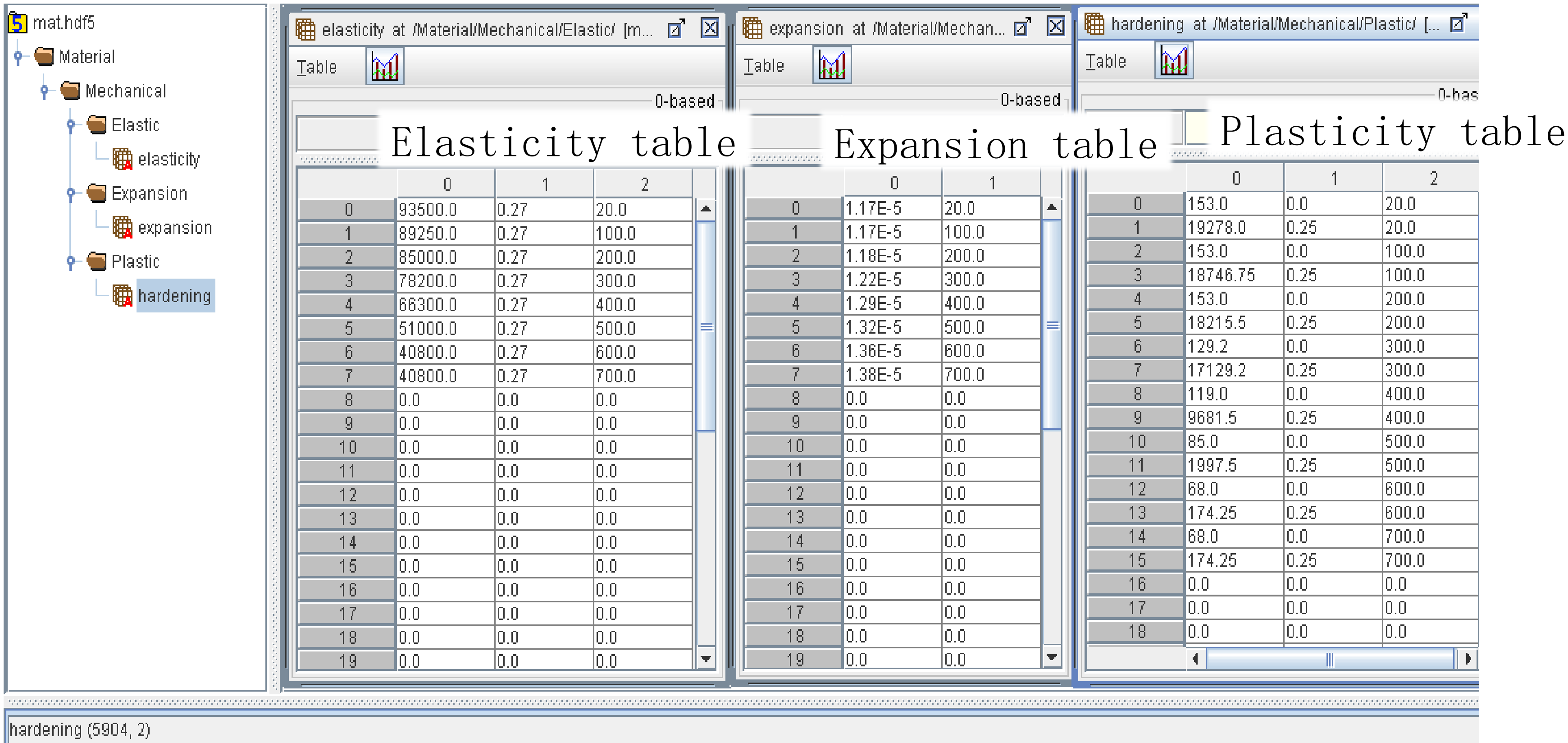
first keywords for properties

An HDF5 file generated based on keywords for mechanical properties from Abaqus-Python, showing Material Elasticity, Plasticity and Expansion, tables.



Elasticity table

	0	1	2
0	93500.0	0.27	20.0
1	89250.0	0.27	100.0
2	85000.0	0.27	200.0
3	78200.0	0.27	300.0
4	66300.0	0.27	400.0
5	51000.0	0.27	500.0
6	40800.0	0.27	600.0
7	40800.0	0.27	700.0
8	0.0	0.0	0.0
9	0.0	0.0	0.0
10	0.0	0.0	0.0
11	0.0	0.0	0.0
12	0.0	0.0	0.0
13	0.0	0.0	0.0
14	0.0	0.0	0.0
15	0.0	0.0	0.0
16	0.0	0.0	0.0
17	0.0	0.0	0.0
18	0.0	0.0	0.0
19	0.0	0.0	0.0

Expansion table

	0	1
0	1.17E-5	20.0
1	1.17E-5	100.0
2	1.18E-5	200.0
3	1.22E-5	300.0
4	1.29E-5	400.0
5	1.32E-5	500.0
6	1.36E-5	600.0
7	1.38E-5	700.0
8	0.0	0.0
9	0.0	0.0
10	0.0	0.0
11	0.0	0.0
12	0.0	0.0
13	0.0	0.0
14	0.0	0.0
15	0.0	0.0
16	0.0	0.0
17	0.0	0.0
18	0.0	0.0
19	0.0	0.0

Plasticity table

	0	1	2
0	153.0	0.0	20.0
1	19278.0	0.25	20.0
2	153.0	0.0	100.0
3	18746.75	0.25	100.0
4	153.0	0.0	200.0
5	18215.5	0.25	200.0
6	129.2	0.0	300.0
7	17129.2	0.25	300.0
8	119.0	0.0	400.0
9	9681.5	0.25	400.0
10	85.0	0.0	500.0
11	1997.5	0.25	500.0
12	68.0	0.0	600.0
13	174.25	0.25	600.0
14	68.0	0.0	700.0
15	174.25	0.25	700.0
16	0.0	0.0	0.0
17	0.0	0.0	0.0
18	0.0	0.0	0.0

Work performed by Anshuman Singh

UPC BarcelonaTech

All this also fits into a larger picture

……