Material modeling and machine learning

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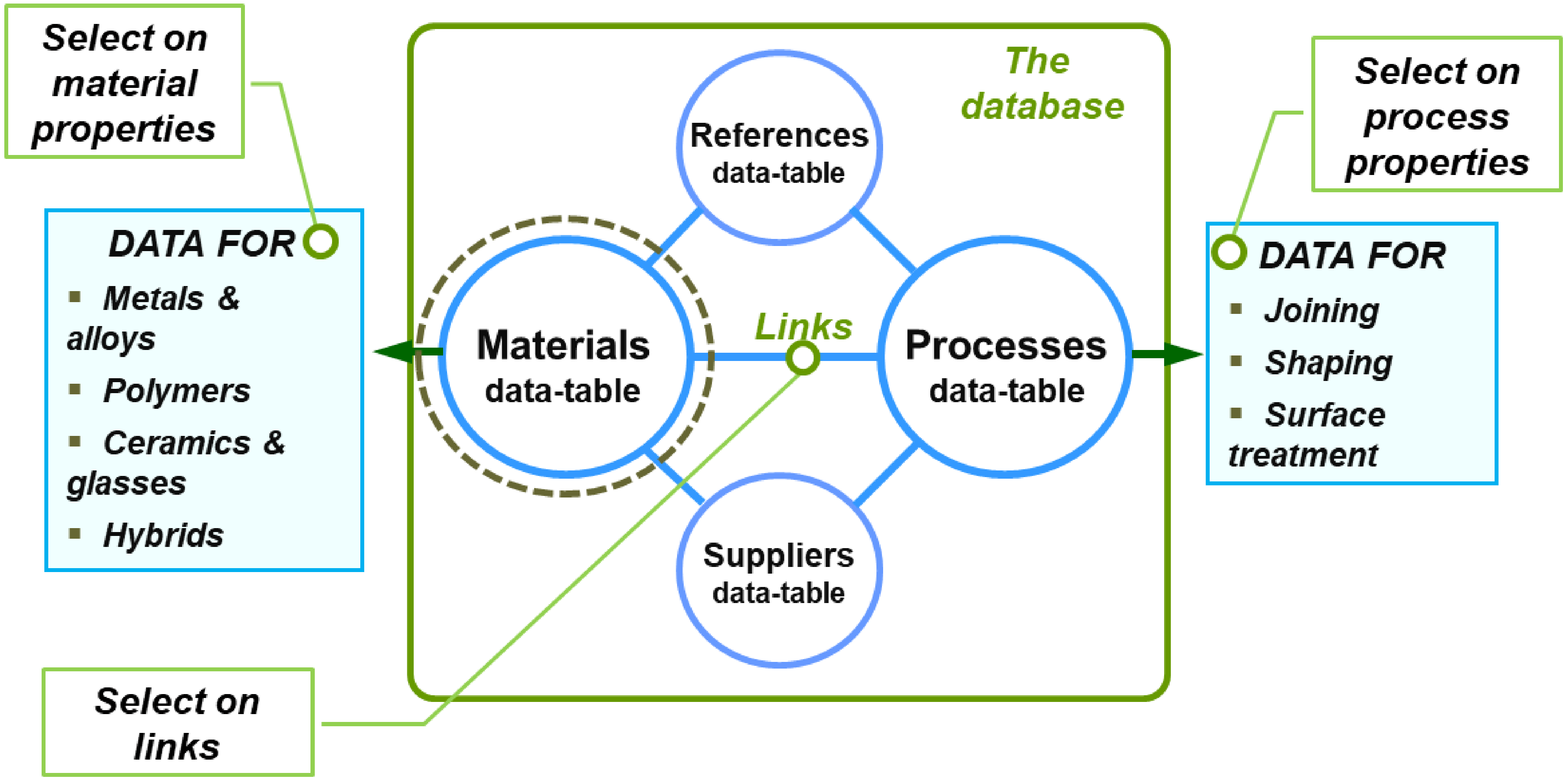
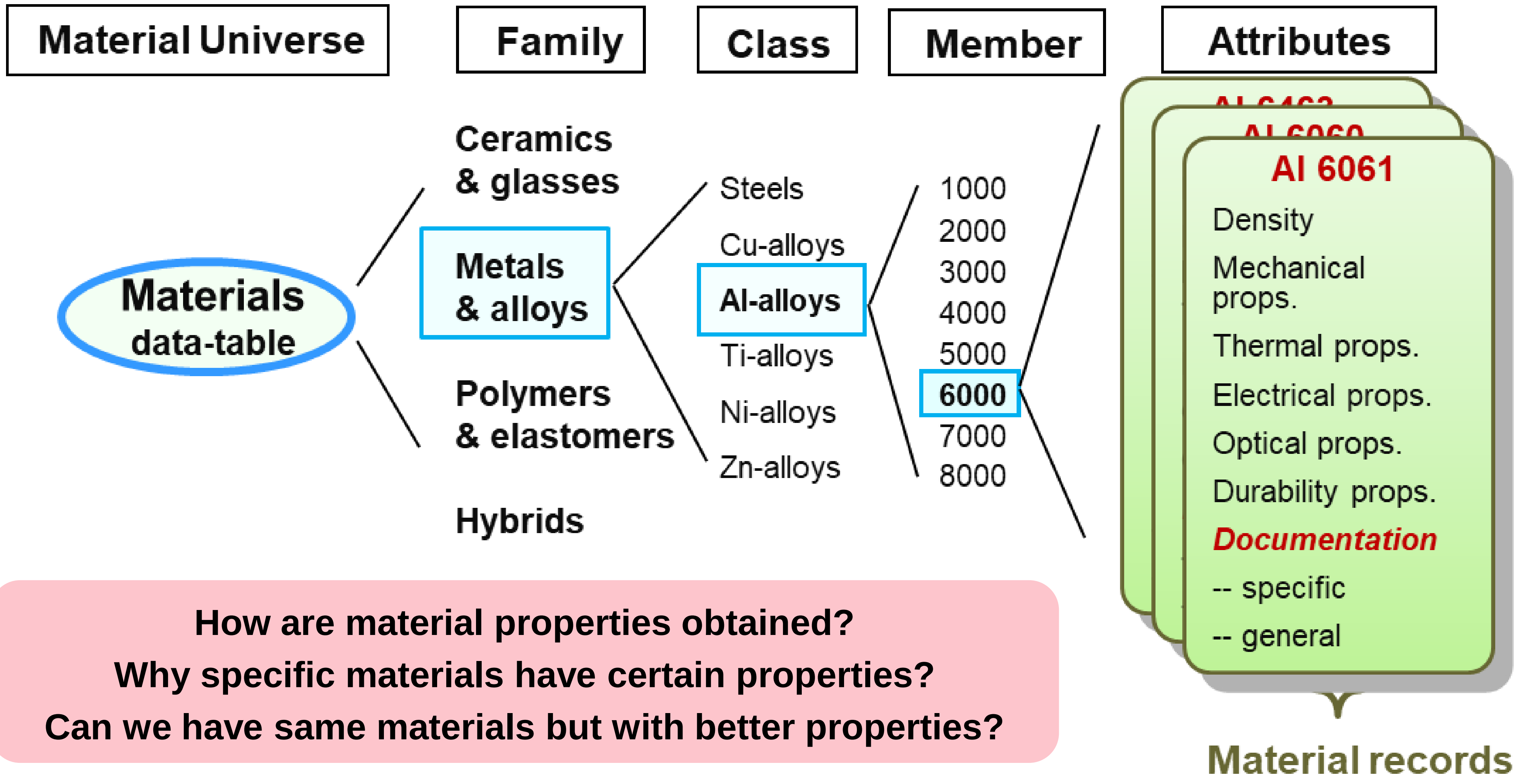
Data management for selection of engineering materials

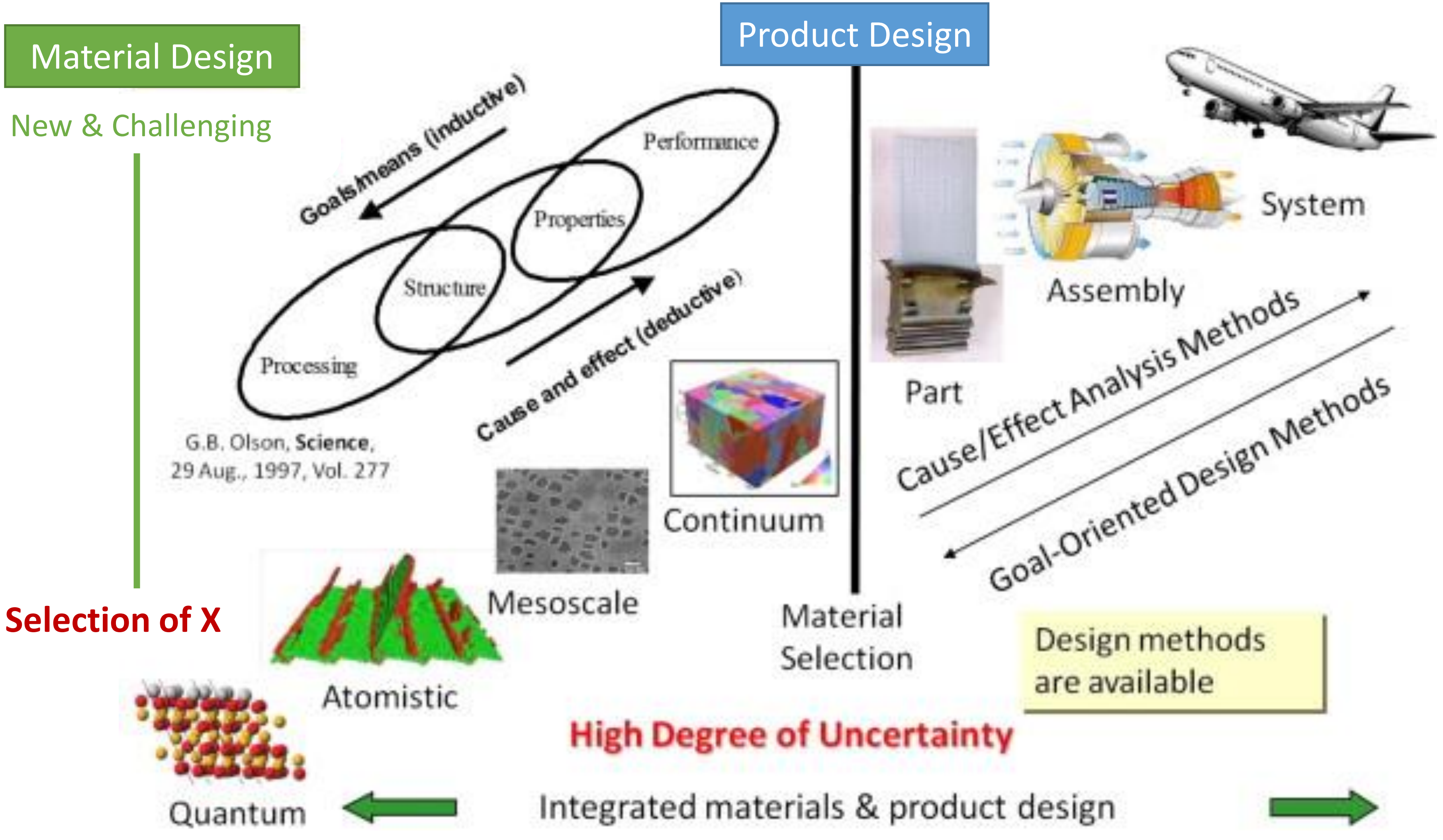


Material data management



How are material properties obtained?
Why specific materials have certain properties?
Can we have same materials but with better properties?

Beyond the selection of engineering materials



J.H. Panchal, et al., Computer-Aided Design, 2013

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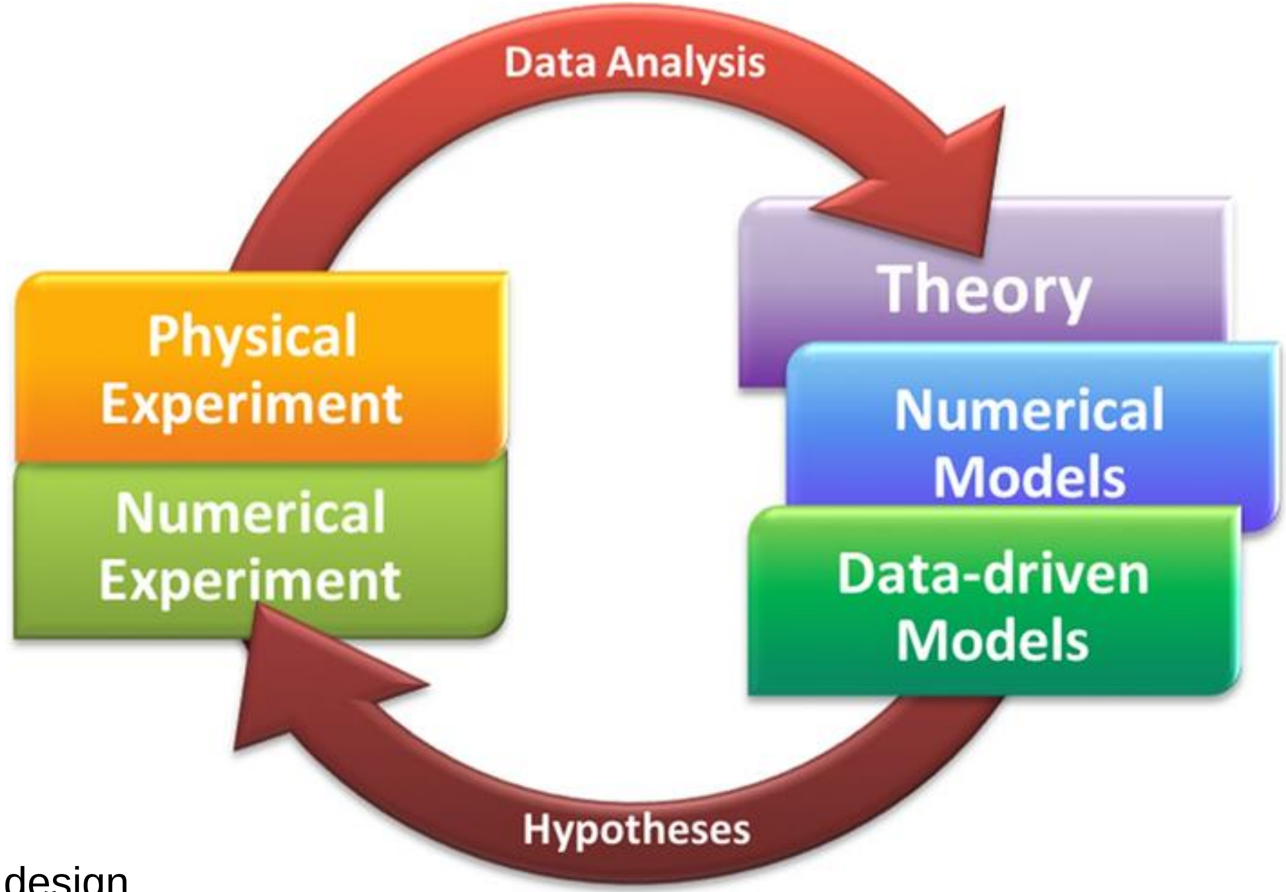
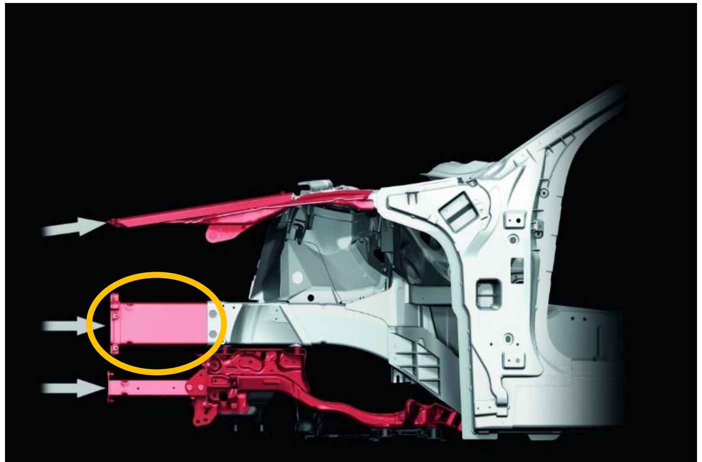


https://doi.org/10.1007/s10894-020-00258-1

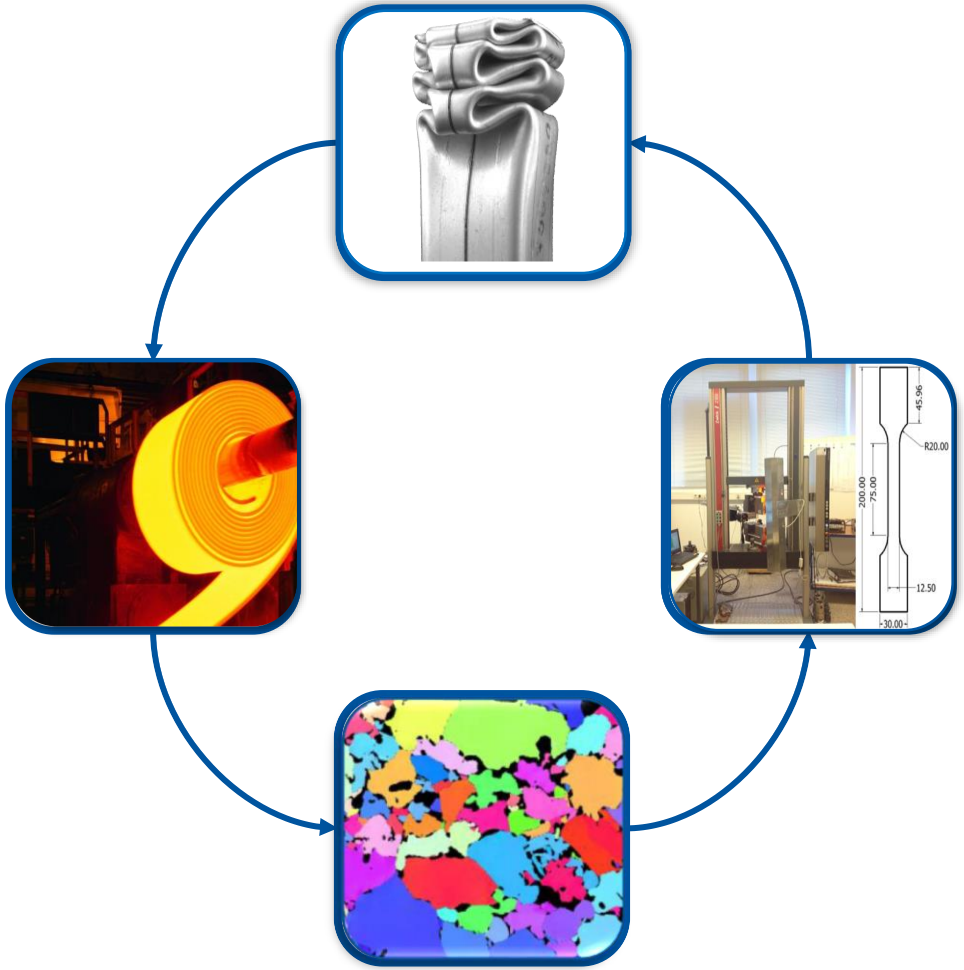
Motivation & Scope

Conventional material design

- Microstructure - Property
- Qualitative design
- Empirical based approach
- “Trial and Error”



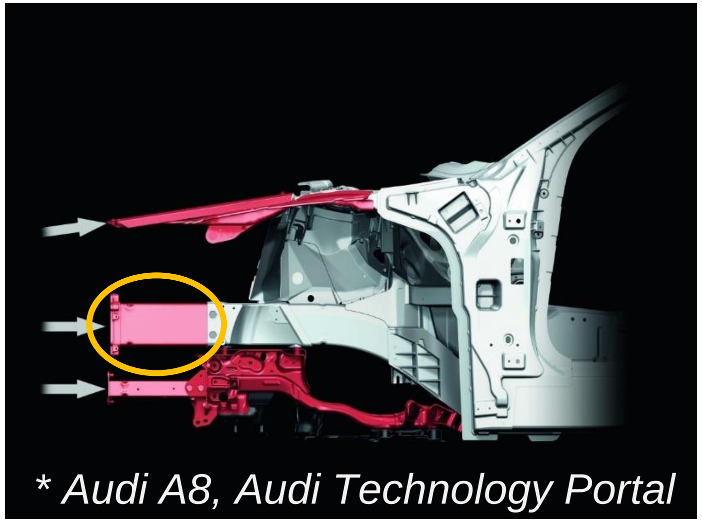
** Audi A8, Audi Technology Portal*

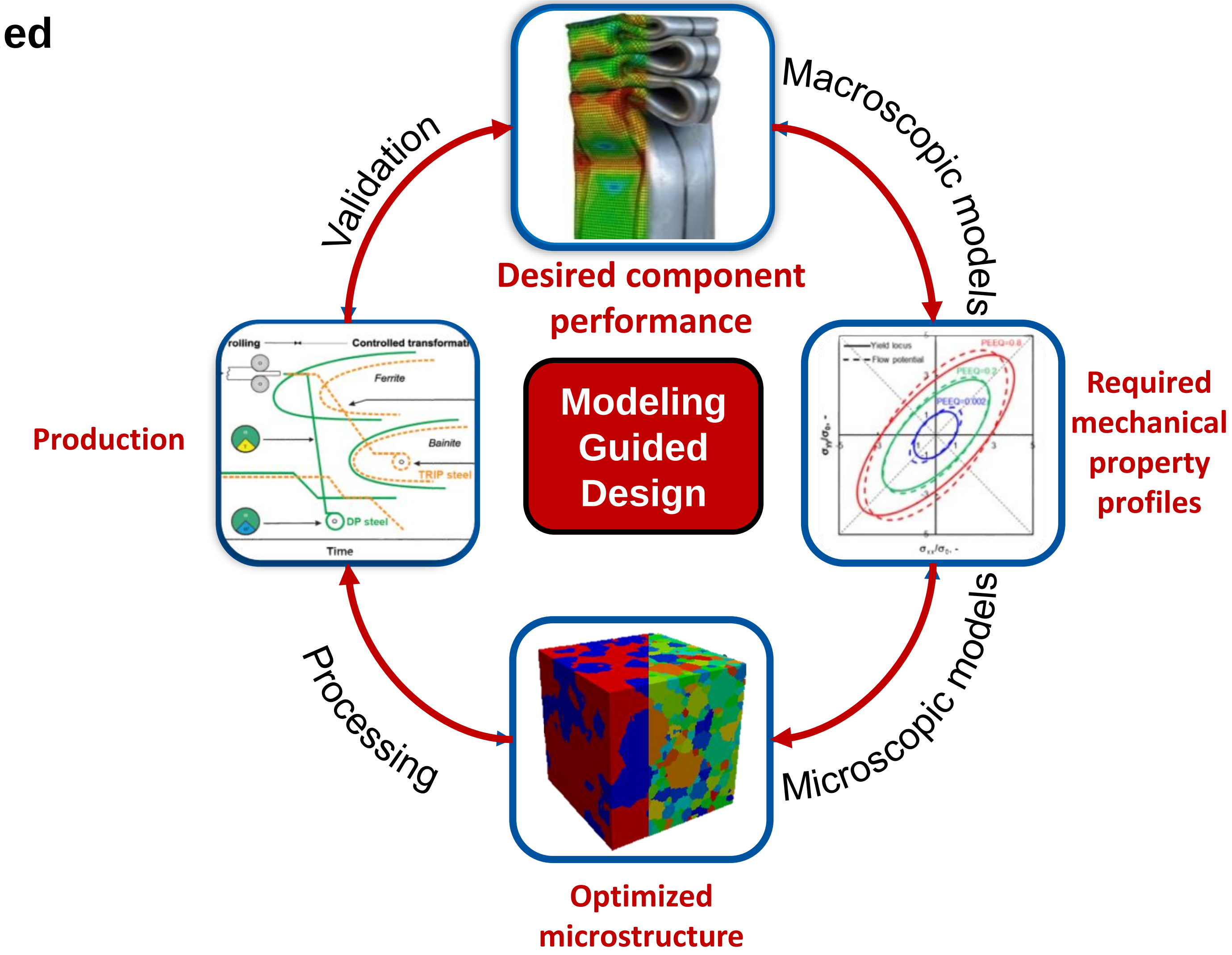


Motivation & Scope

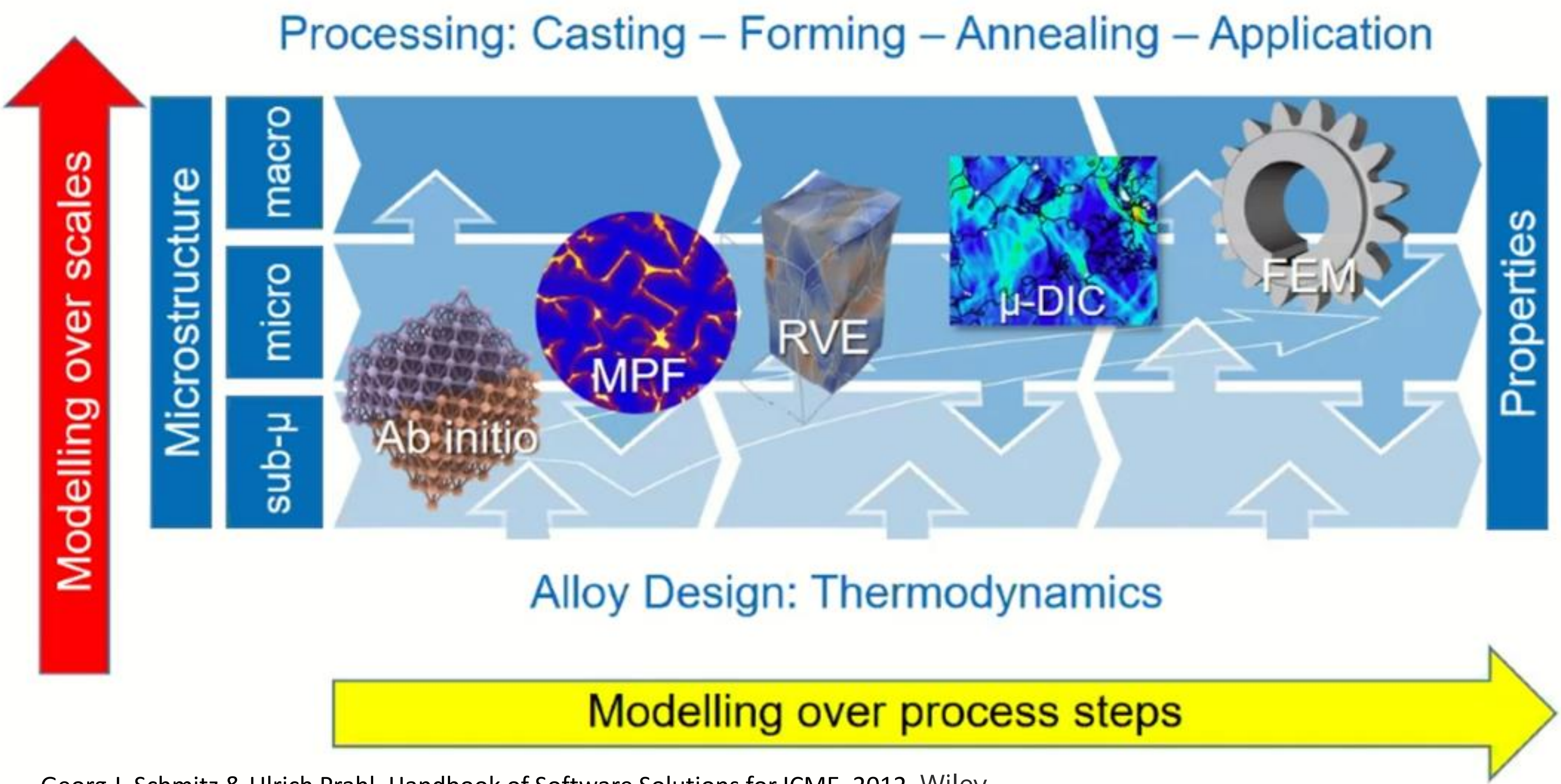
To establish a **multiscale modeling guided** design strategy for desired performance

- ✓ Structure performance - Microstructure
- ✓ Customized & quantitative design
- ✓ Knowledge based approach
- ✓ “Fast” & “Cheap”





Integrated Computational Materials Engineering – ICME



Georg J. Schmitz & Ulrich Prahl, Handbook of Software Solutions for ICME, 2012, Wiley

Software & Tools for ICME

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Possible/in reach

- Determination of phase fractions
- Prediction of onset of precipitate formation
- Determination of temperatures for phase transitions
- Estimation of solidification behaviour
- Determination of thermodynamic data
- Information on kinetics
- Information on microstructure

- Information about materials properties
- Information about properties of component
- Life cycle modelling

- Interoperability
- Automated workflows
- Physics informed Neural Networks
- Integration with experiments

Thermo-Calc Software

FactSage™

micress®

HOMAT

SIMULIA

ABAQUS

DAMASK
Düsseldorf Advanced Material Simulation Kit

EMMO

AIXVIPMAP

Georg J. Schmitz & Ulrich Prahl, Handbook of Software Solutions for ICME, 2012, Wiley

Macroscopic material modeling – Crashworthiness

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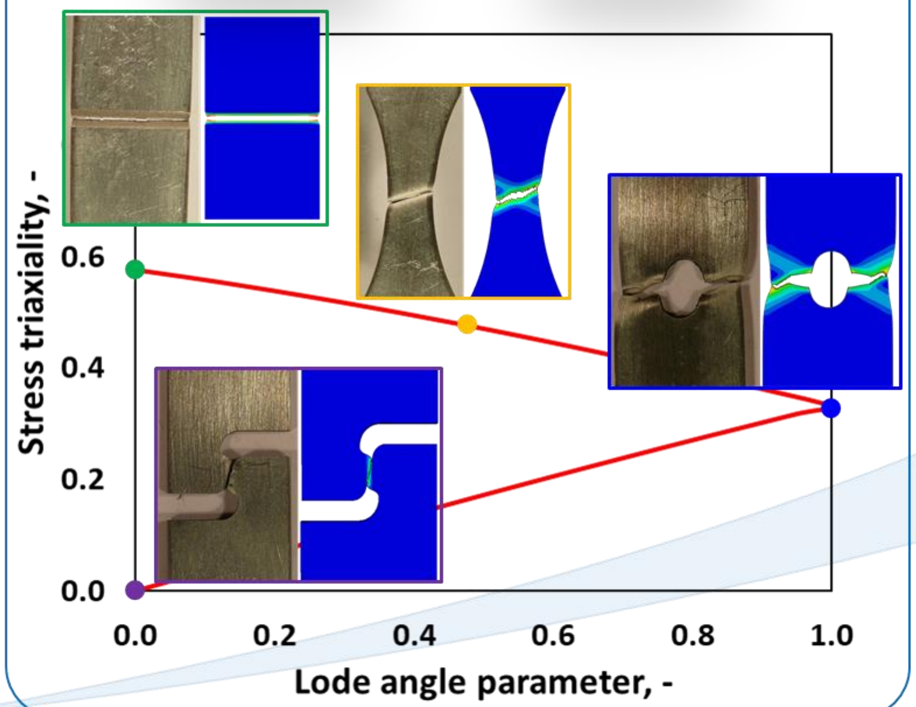
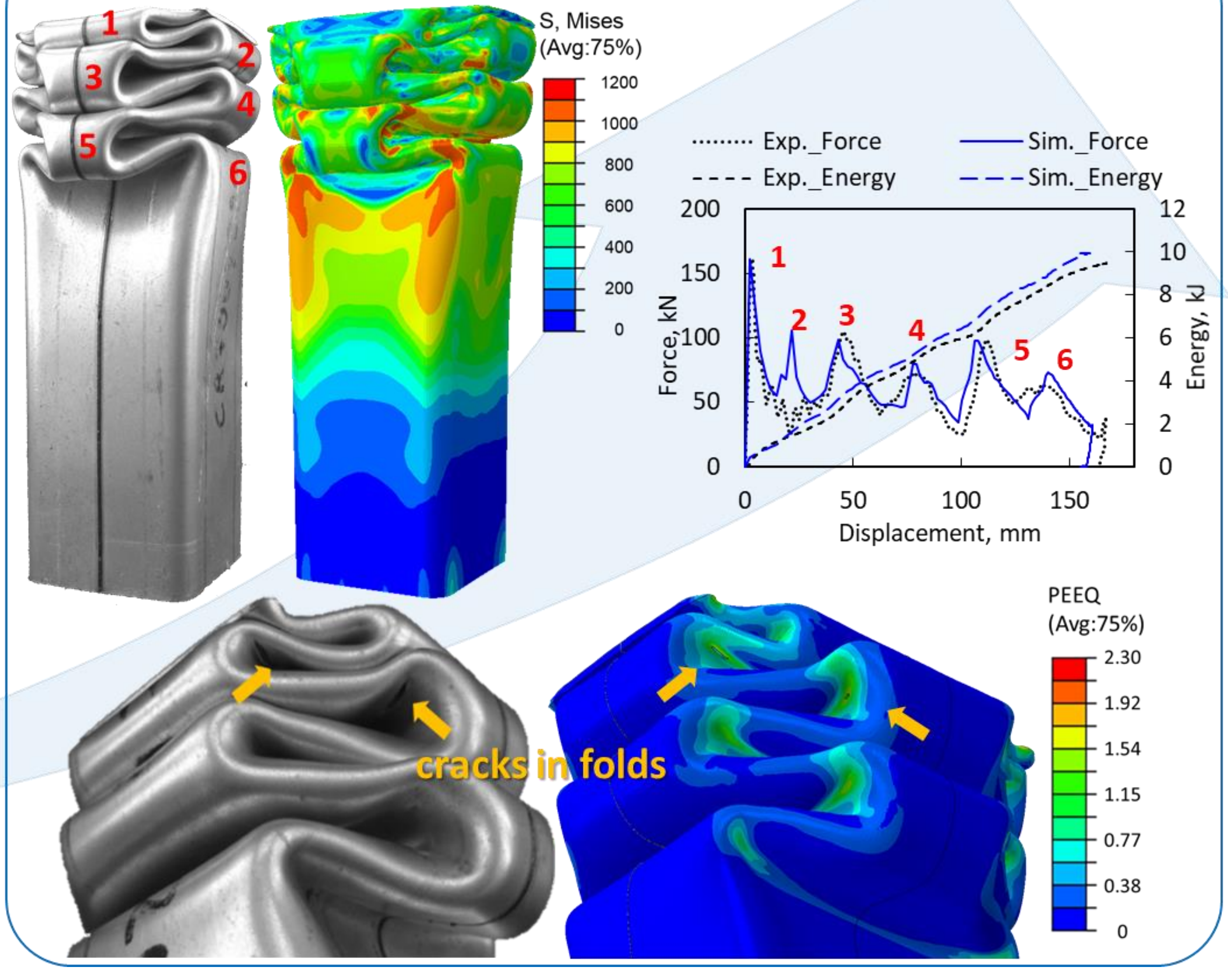
- Lab-level fracture tests



- Component-level square tube crushing tests



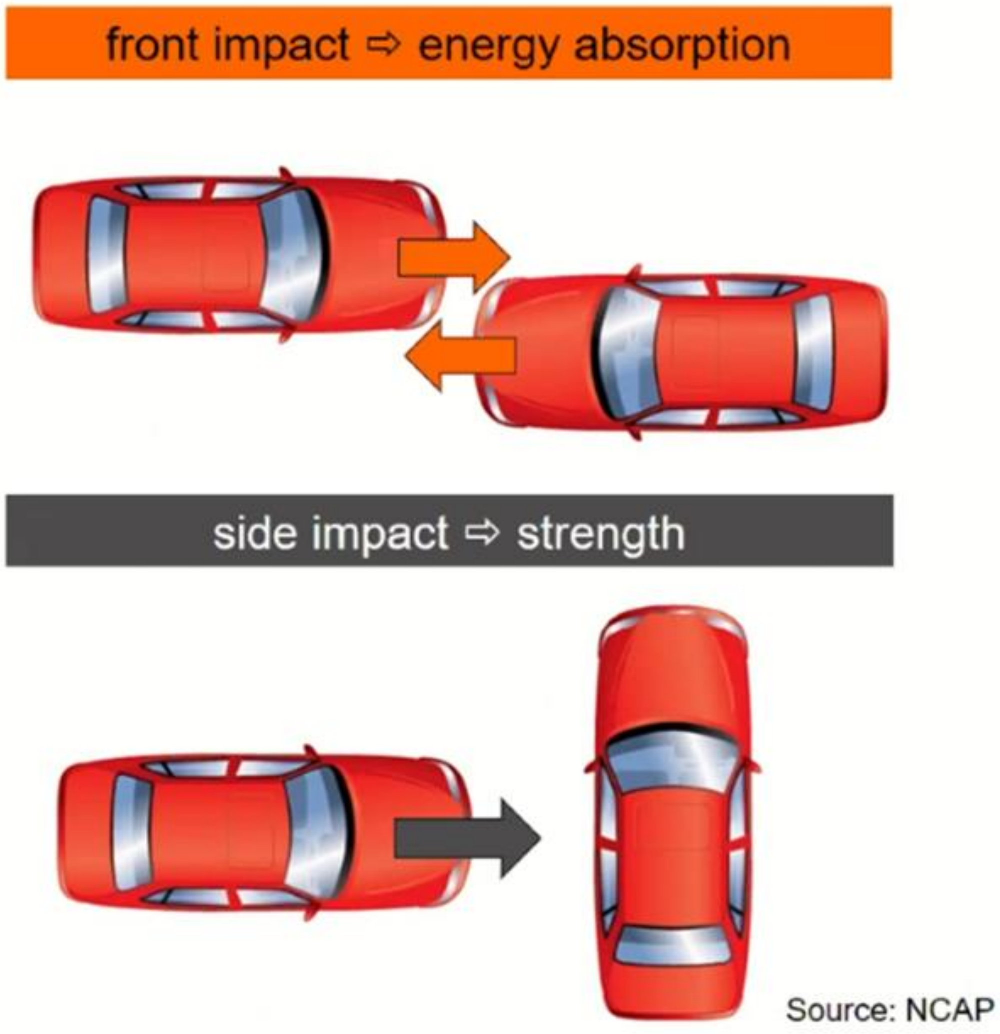
Liu, Lian, et al., Prediction of crack formation in the progressive folding of square tubes during dynamic axial crushing, IJMS, 2020

Background on crashworthiness

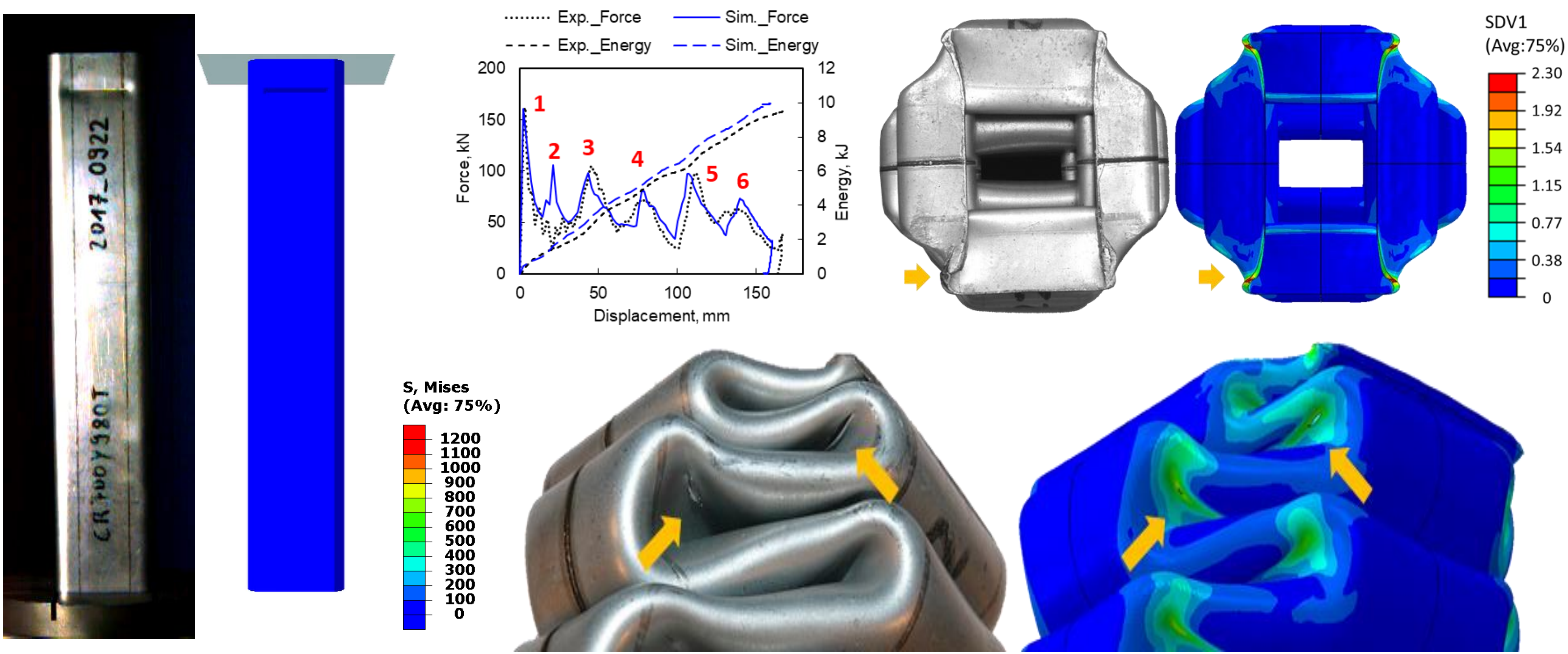








Crashworthiness prediction



**Supported by TKSE*

[Liu, Lian, et al., Prediction of crack formation in the progressive folding of square tubes during dynamic axial crushing, IJMS, 2020](#)

A hybrid damage mechanics model

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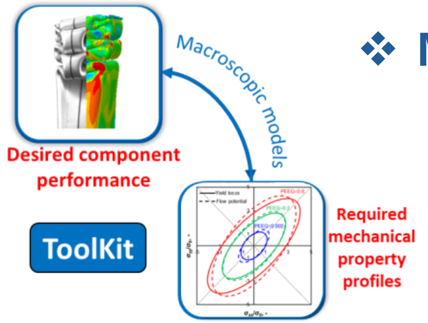
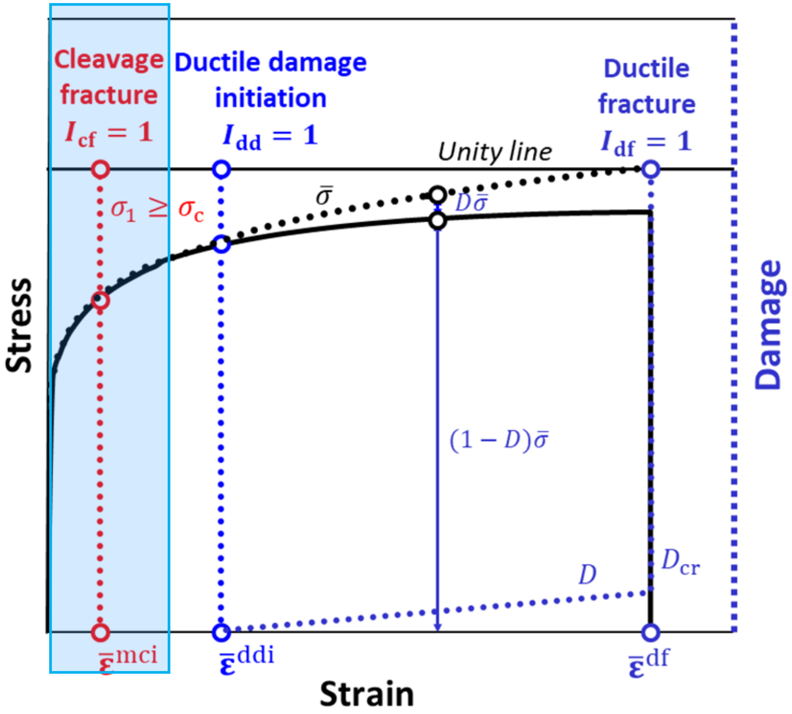
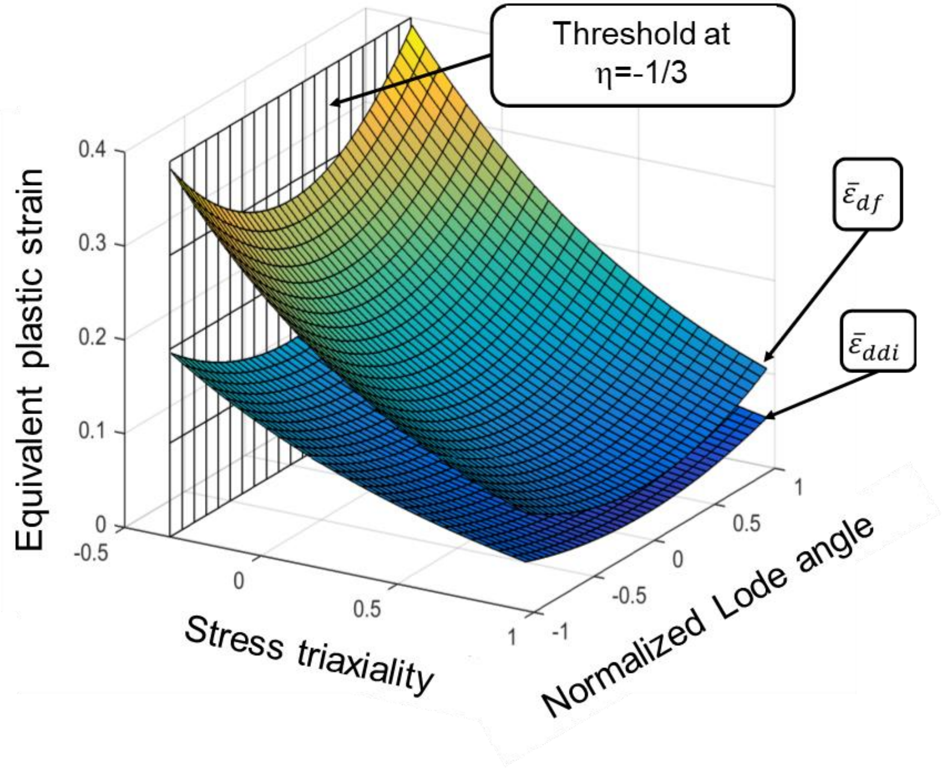


❖ Model development for component failure

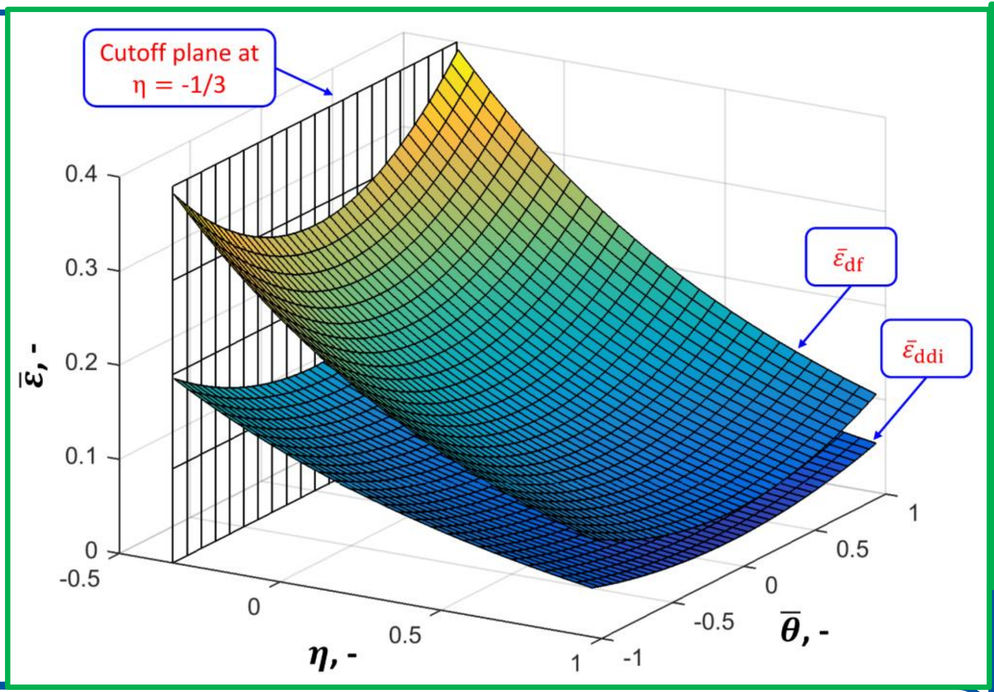
- Plasticity ($\dot{\bar{\varepsilon}}$, T, $\bar{\theta}$, α)
- Cleavage & ductile damage initiation (η, $\bar{\theta}$, α)
- Damage evolution (η, $\bar{\theta}$, $\dot{\bar{\varepsilon}}$)
- Final ductile fracture (η, $\bar{\theta}$, α)

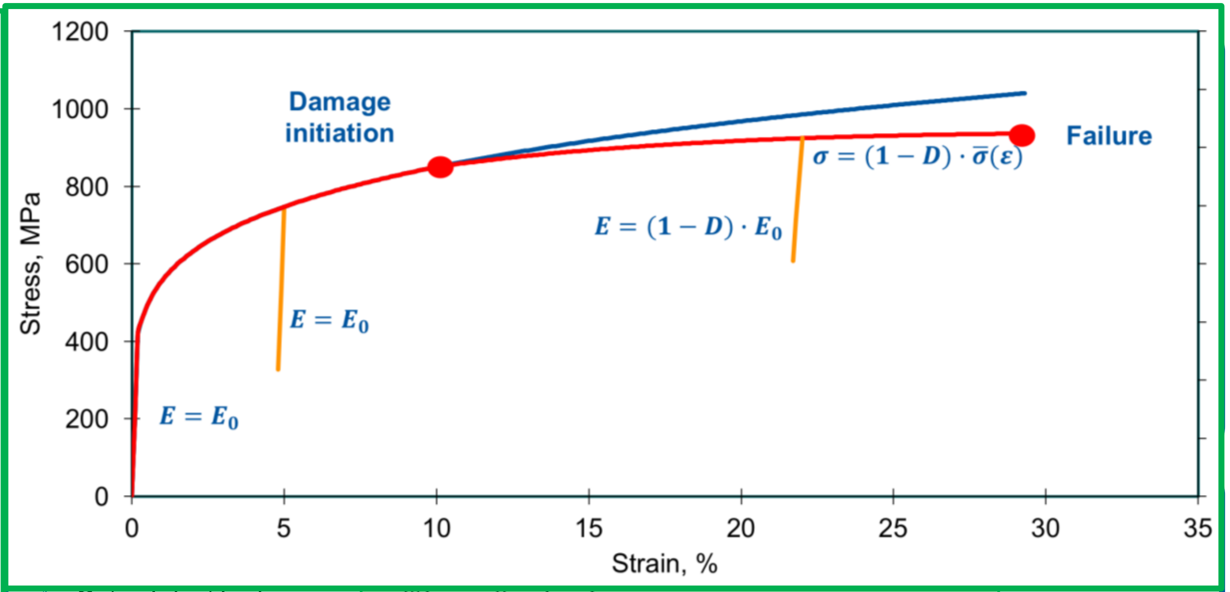
- Plasticity and fracture (η, $\bar{\theta}$, D)
  - ** Lian et al., IJDM, 2013 & 2015*
- Non-proportional loadings
  - ** Wu et al., FFEMS, 2017*
- Cleavage & ductile fracture (η, $\bar{\theta}$)
  - ** He et al., EFM, 2017*
- Anisotropic hardening (α)
  - ** Lian et al., IJSS, 2018*





Constitutive equations





- Critical ductile damage accumulation function: $\varepsilon^{\rm df}(\eta_{\rm avg}, \theta_{\rm avg}) = \{ h(\eta_{\rm avg}, \bar{\theta}_{\rm avg}) \quad \text{for } \eta > \eta_c$

$$h(\eta_{\rm avg}, \bar{\theta}_{\rm avg}) = [F_1 e^{-F_2\eta} - F_3 e^{-F_4\eta}]\bar{\theta}^2 + F_3 e^{-F_4\eta}$$

- Ductile fracture indicator: $I_{\rm df} = \int_{\bar{\varepsilon}^{\rm ddi}}^{\bar{\varepsilon}^{\rm p}} \frac{d\varepsilon^{\rm p}}{\bar{\varepsilon}^{\rm df}(\eta_{\rm avg}, \bar{\theta}_{\rm avg}) - \bar{\varepsilon}^{\rm ddi}(\eta_{\rm avg}, \bar{\theta}_{\rm avg})}$

Cleavage fracture initiation

- Cleavage fracture initiation: $(\cdot)_{\rm avg} = \frac{1}{\bar{\varepsilon}^{\rm p}} \int_0^{\bar{\varepsilon}^{\rm p}} (\cdot)(\varepsilon^{\rm p}) d\varepsilon^{\rm p}$

$$\bar{\varepsilon}^{\rm mci}(\eta_{\rm avg}, \bar{\theta}_{\rm avg}) = f(\eta_{\rm avg}, \bar{\theta}_{\rm avg})$$

$$f(\eta_{\rm avg}, \bar{\theta}_{\rm avg}) = [C_1 e^{-C_2\eta} - C_3 e^{-C_4\eta}]\bar{\theta}^2 + C_3 e^{-C_4\eta}$$

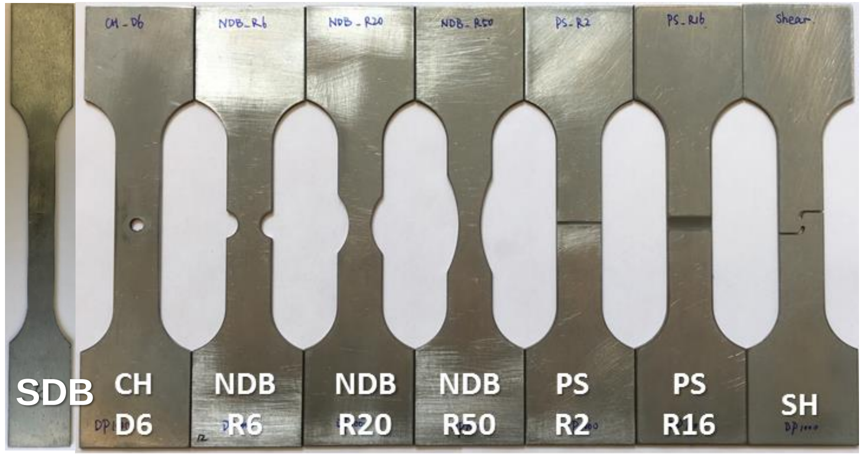
- Cleavage fracture initiation indicator: $I_{\rm cf} = \int_0^{\bar{\varepsilon}^{\rm p}} \frac{d\bar{\varepsilon}^{\rm p}}{\bar{\varepsilon}^{\rm mci}(\eta_{\rm avg}, \bar{\theta}_{\rm avg})}$

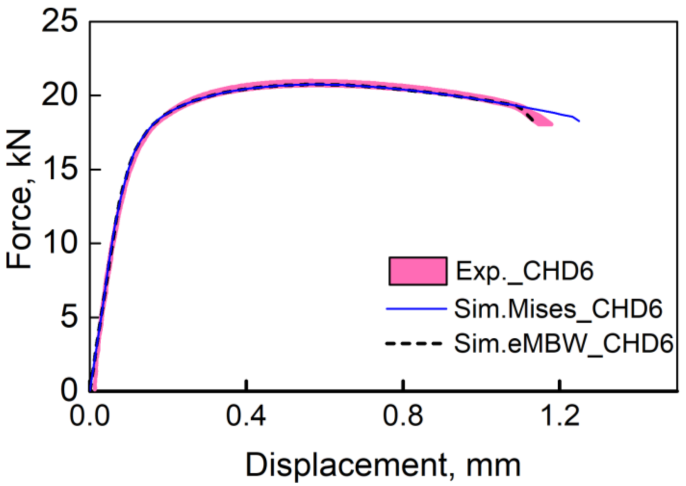
Ductile & cleavage interaction

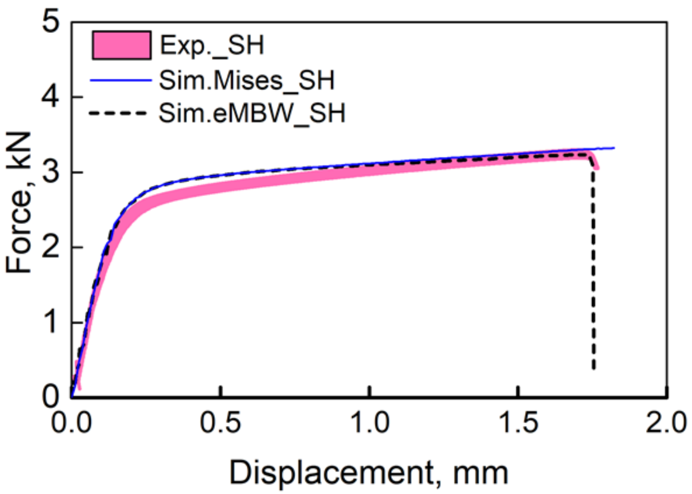
- Cleavage and ductile damage:

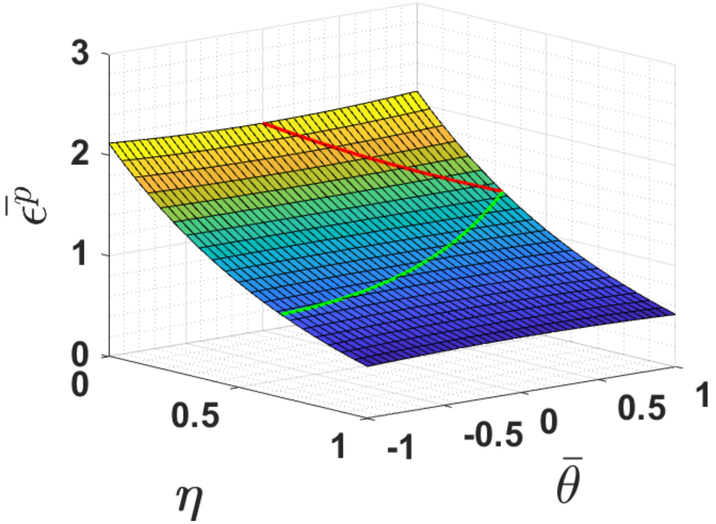
$$D = \begin{cases} 0 & \text{for } I_{\rm cf} < 1 \wedge I_{\rm dd} < 1 \\ 0 & \text{for } I_{\rm cf} \geq 1 \wedge \sigma_1 < \sigma_c \wedge I_{\rm dd} < 1 \\ 1 & \text{for } I_{\rm cf} \geq 1 \wedge \sigma_1 \geq \sigma_c \wedge I_{\rm dd} < 1 \\ I_{\rm df} \cdot \frac{\sigma_c^{\rm ddi}}{G_f}(\bar{\varepsilon}^{\rm df} - \bar{\varepsilon}^{\rm ddi}) & \text{for } I_{\rm dd} \geq 1 \wedge I_{\rm df} \leq 1 \\ 1 & \text{for } I_{\rm dd} \geq 1 \wedge I_{\rm df} > 1 \end{cases}$$

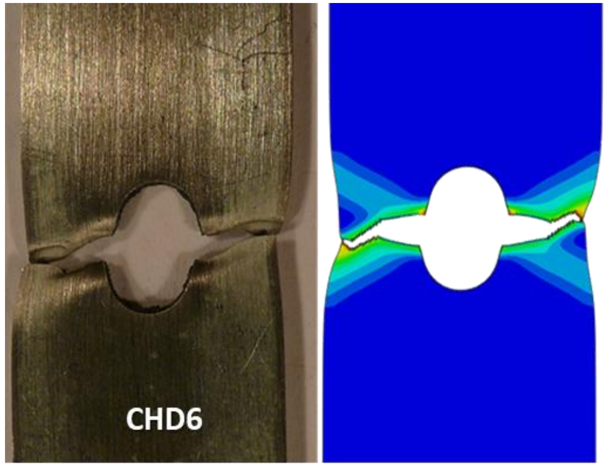
Damage & fracture parameter calibration

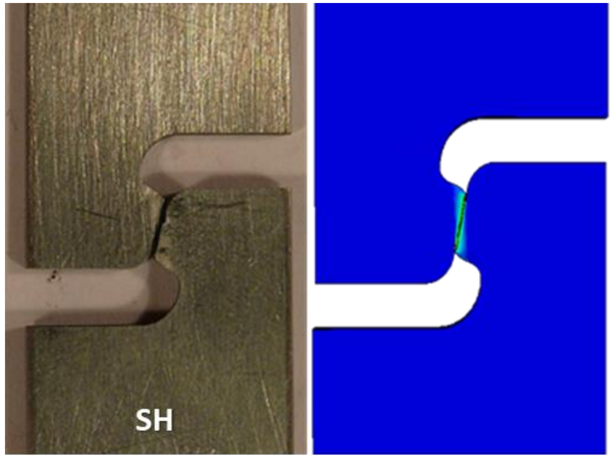






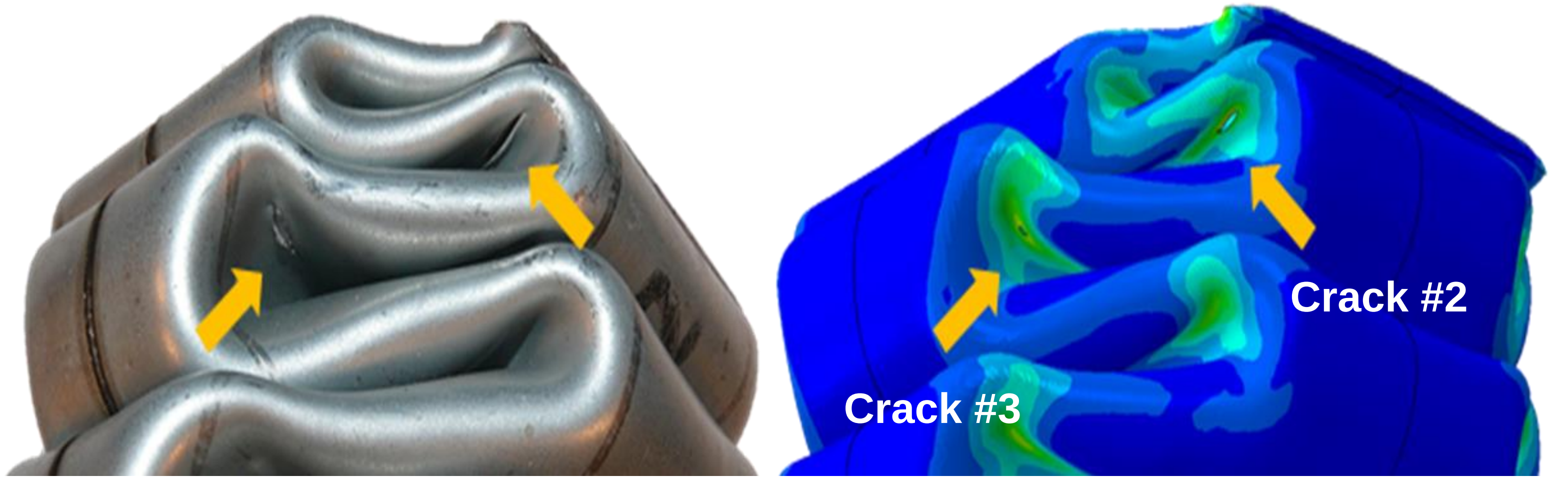


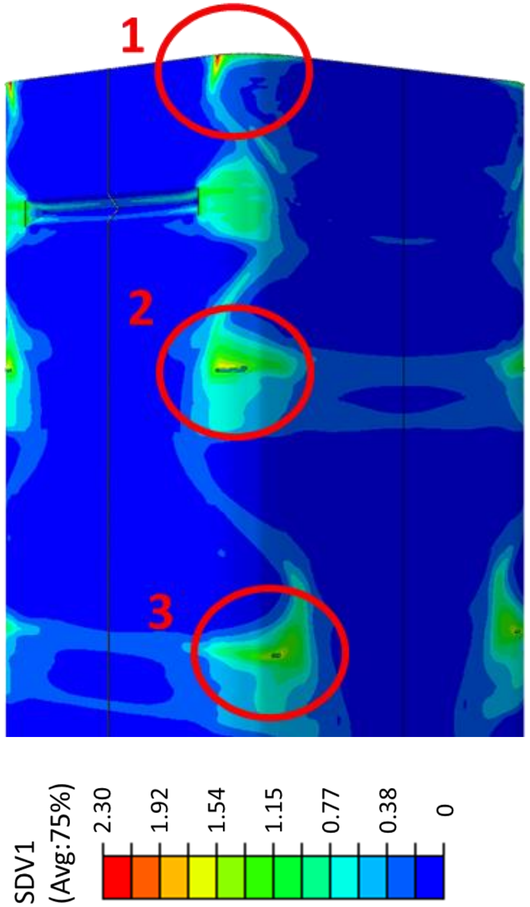


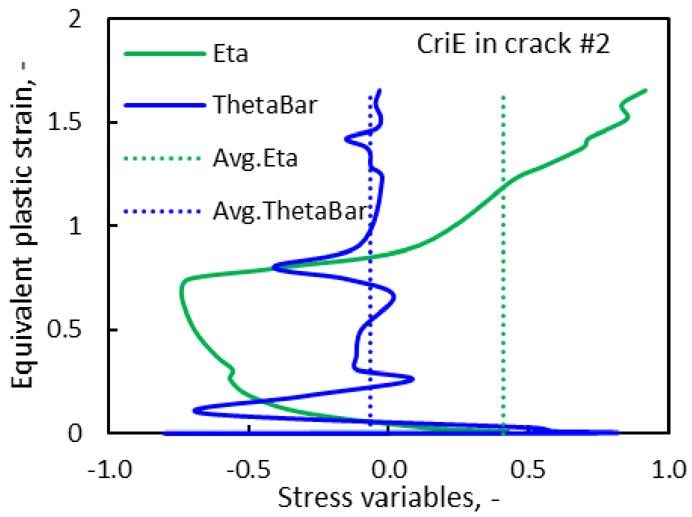


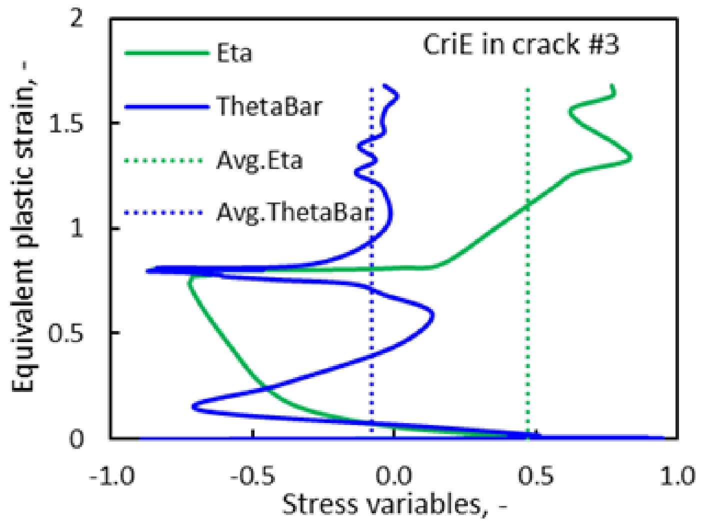
[Liu, Lian, et al., Prediction of crack formation in the progressive folding of square tubes during dynamic axial crushing, IJMS, 2020]

Crashworthiness prediction



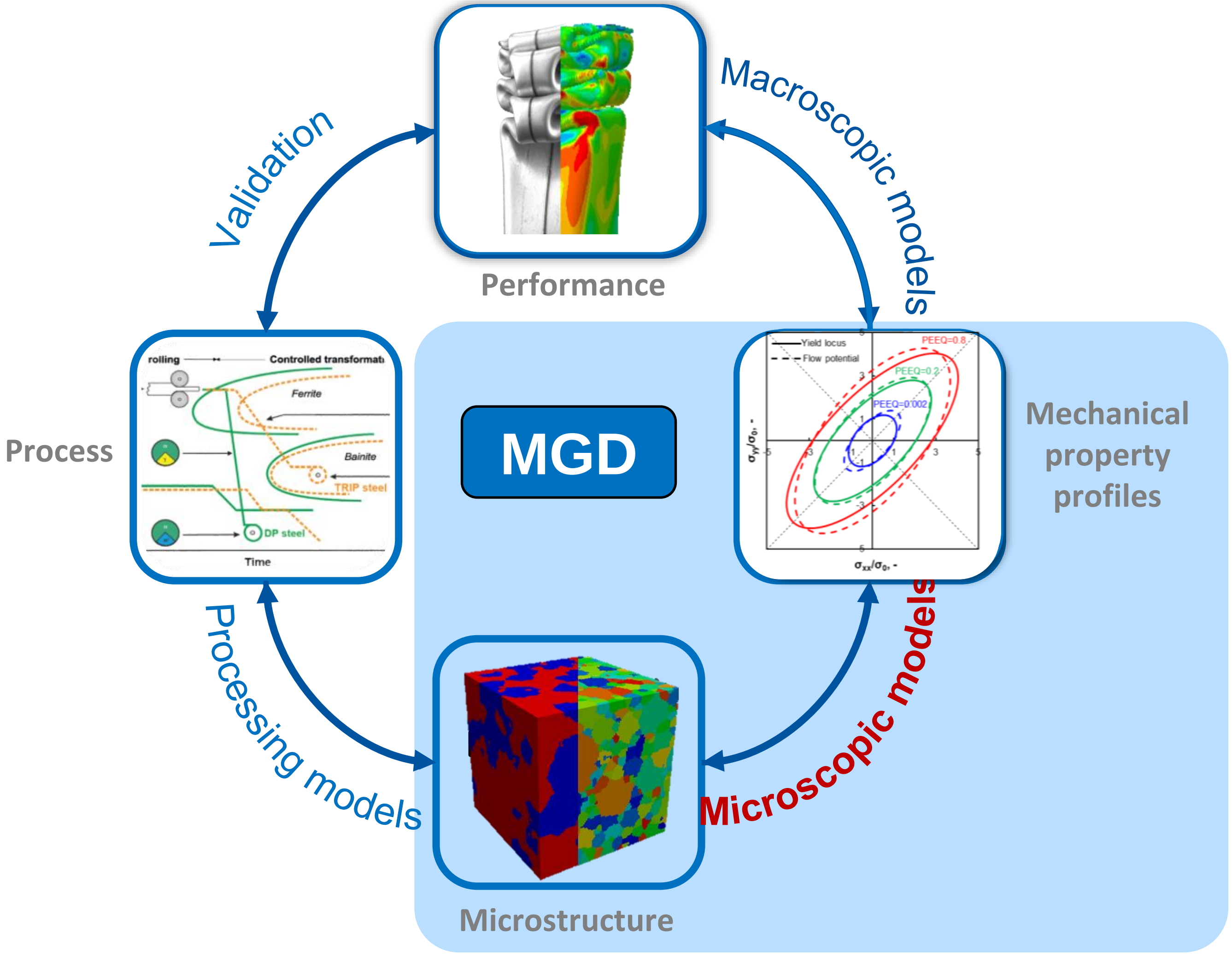






Liu, Lian, et al., Prediction of crack formation in the progressive folding of square tubes during dynamic axial crushing, IJMS, 2020

Microscopic material modeling – Strength & Anisotropy



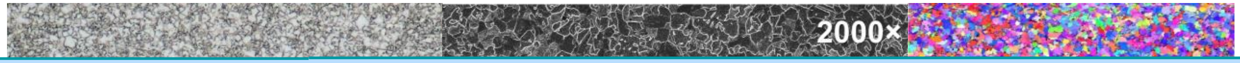
- Micromechanical model development and validation
  - Crystal plasticity modeling
  - Artificial microstructure model for dual-phase structure
  - Parameter calibration
  - Flow behavior and anisotropy prediction

Mechanical property profile → Microstructure

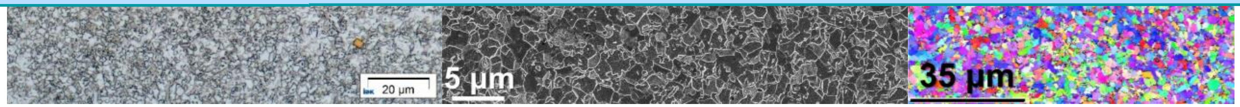
RVE generation

Microstructure characterization

- **Phase level**
  - Phase fraction f
- **Grain level**
  - Grain size d
  - Grain shape asp
  - Grain orientation t
  - …



Material	Phase	Fraction	Grain size	Grain shape factor	Texture index
DP1000	Ferrite	55%	< 2 µm	RD:TD:ND=1:0.48:0.47	1.08
	Martensite	45%	< 0.5 µm	RD:TD:ND=1:0.49:0.48	1.05

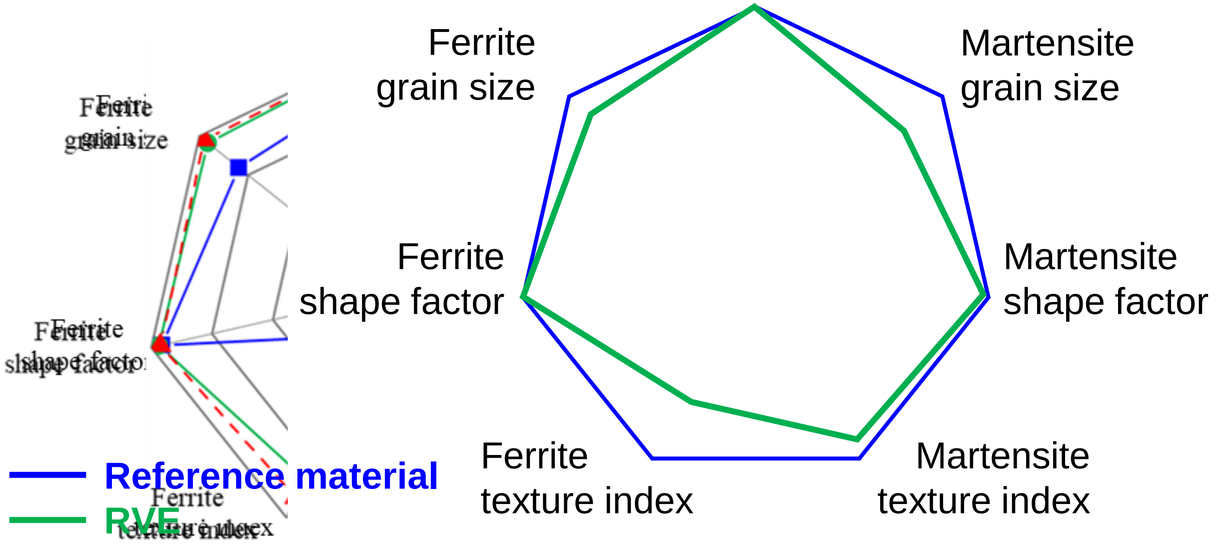


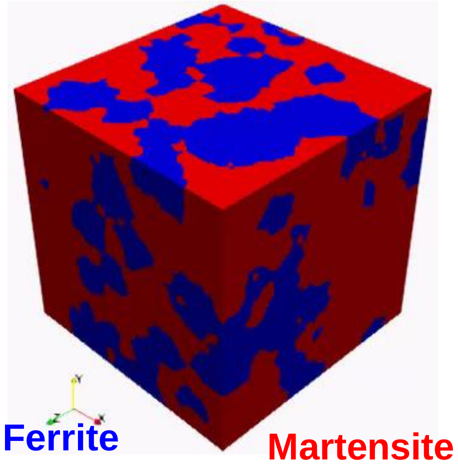
- Mesh si
- Element number
- Phase fraction

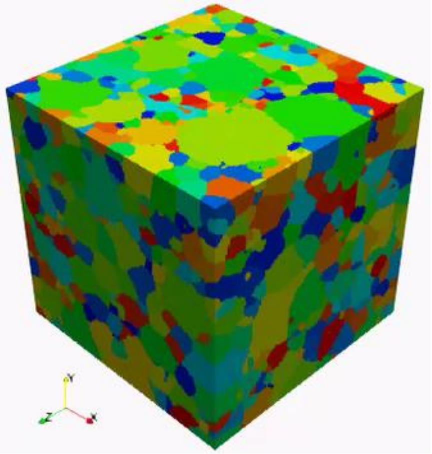
$Deviation$: $\Delta f, \Delta d, \Delta asp, \Delta t$

$\Rightarrow Overall\ deviation$:

$\Delta = avg(\Delta f, \Delta d, \Delta asp, \Delta t)$







[Liu, Lian et al., A strategy for synthetic microstructure generation and crystal plasticity parameter calibration of fine-grain-structured dual-phase steel, IJP, 2020]

Mechanical property profile → Microstructure

Representativeness assessment

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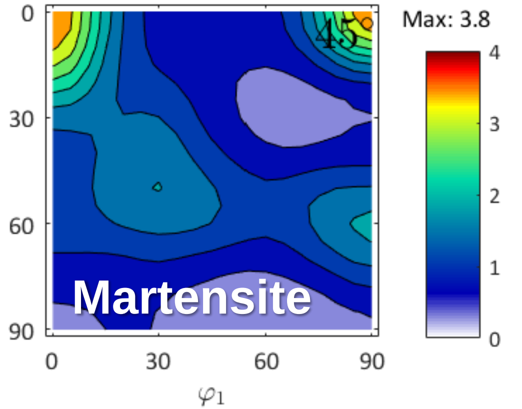
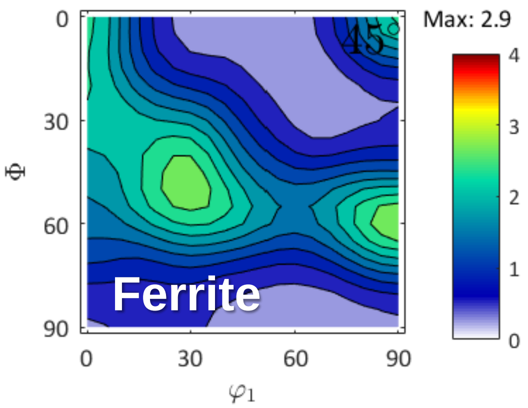
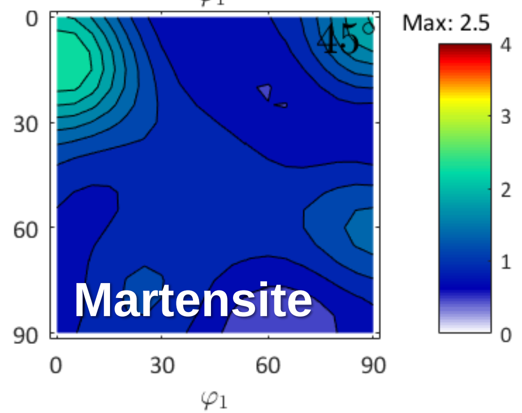
Mesh size, nm	RVE size, μm
200×200×200	8×8×8
Ferrite grain number	**Martensite grain number**
51	1040

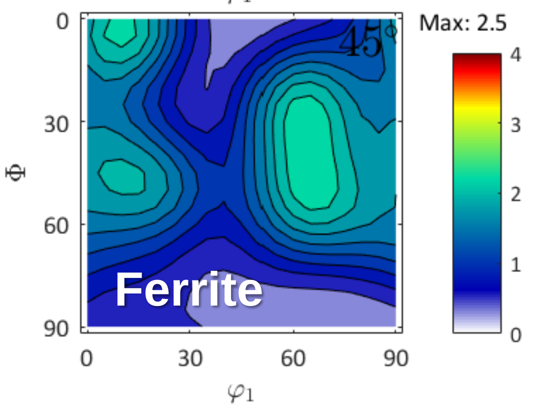
Input

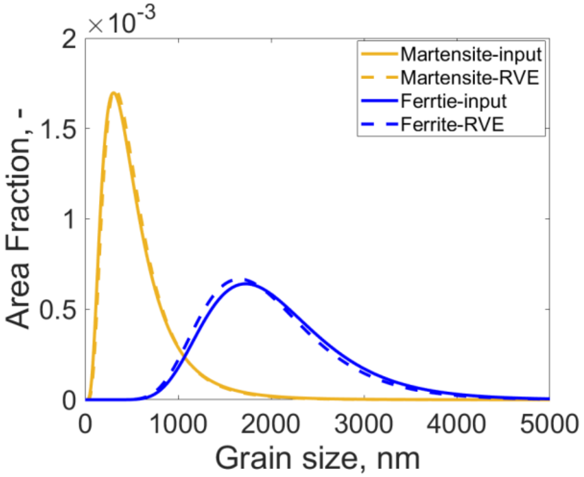


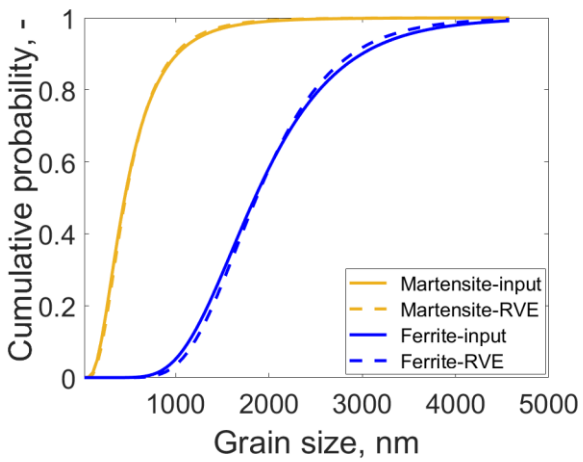


RVE

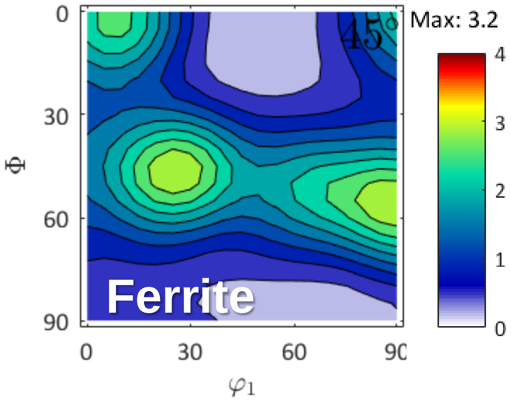








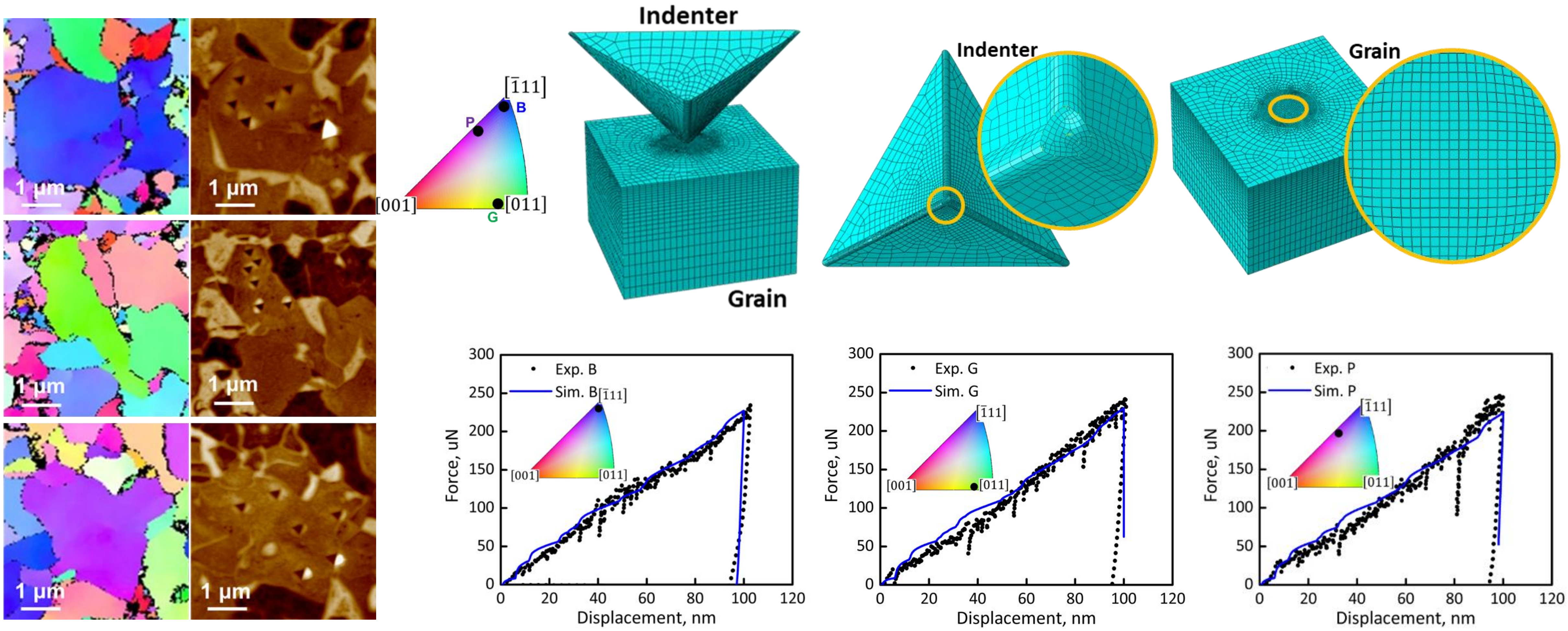
Optimized



	Phase fraction	Ferrite	Martensite
	f	*asp*	*asp*
I	0.45	1:0.48:0.47	1:0.49:0.48
R	0.45	1:0.49:0.45	1:0.51:0.47

Liu, Lian et al., A strategy for synthetic microstructure generation and crystal plasticity parameter calibration of fine-grain-structured dual-phase steel, IJP, 2020

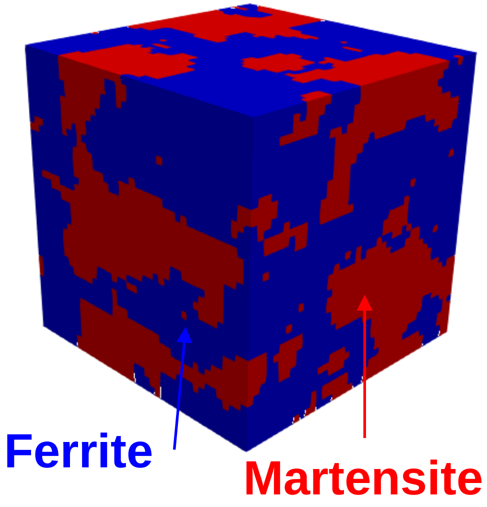
Crystal plasticity parameter calibration

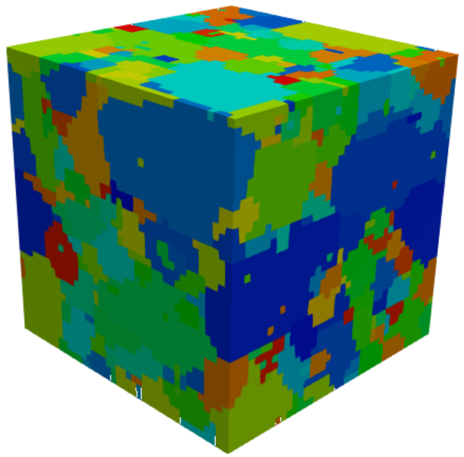


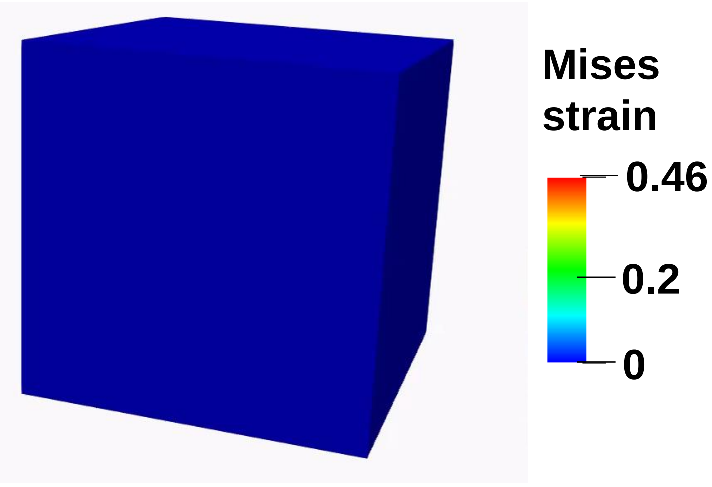
Liu, Lian et al., A strategy for synthetic microstructure generation and crystal plasticity parameter calibration of fine-grain-structured dual-phase steel, IJP, 2020

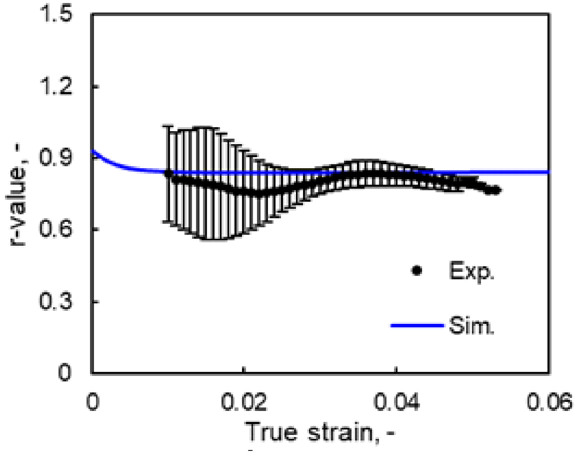
Crystal plasticity parameter validation

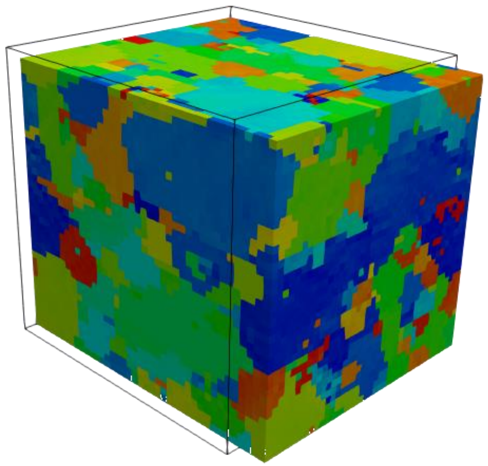
❑ Parameter calibration of martensite

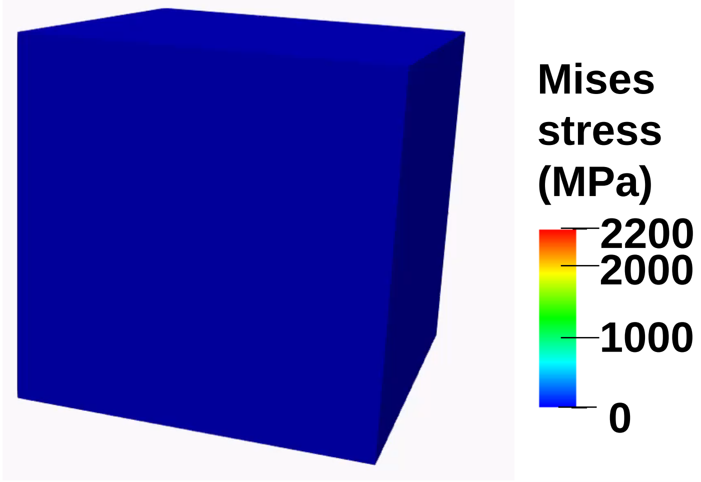




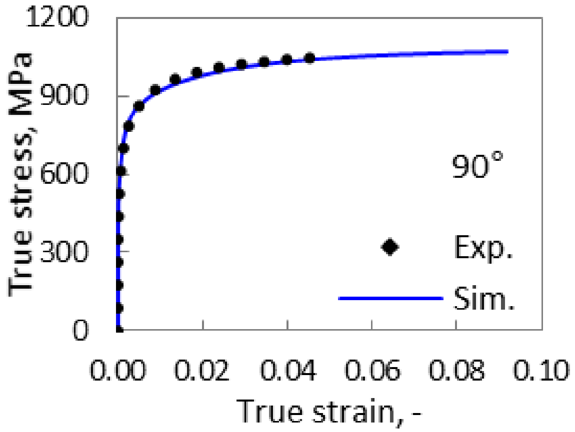


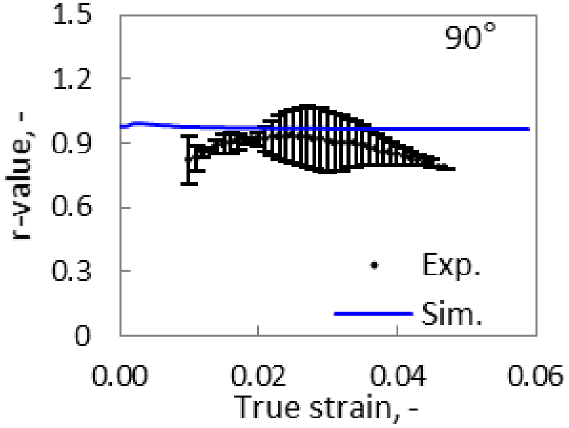






❑ Prediction





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Conclusions & Next steps

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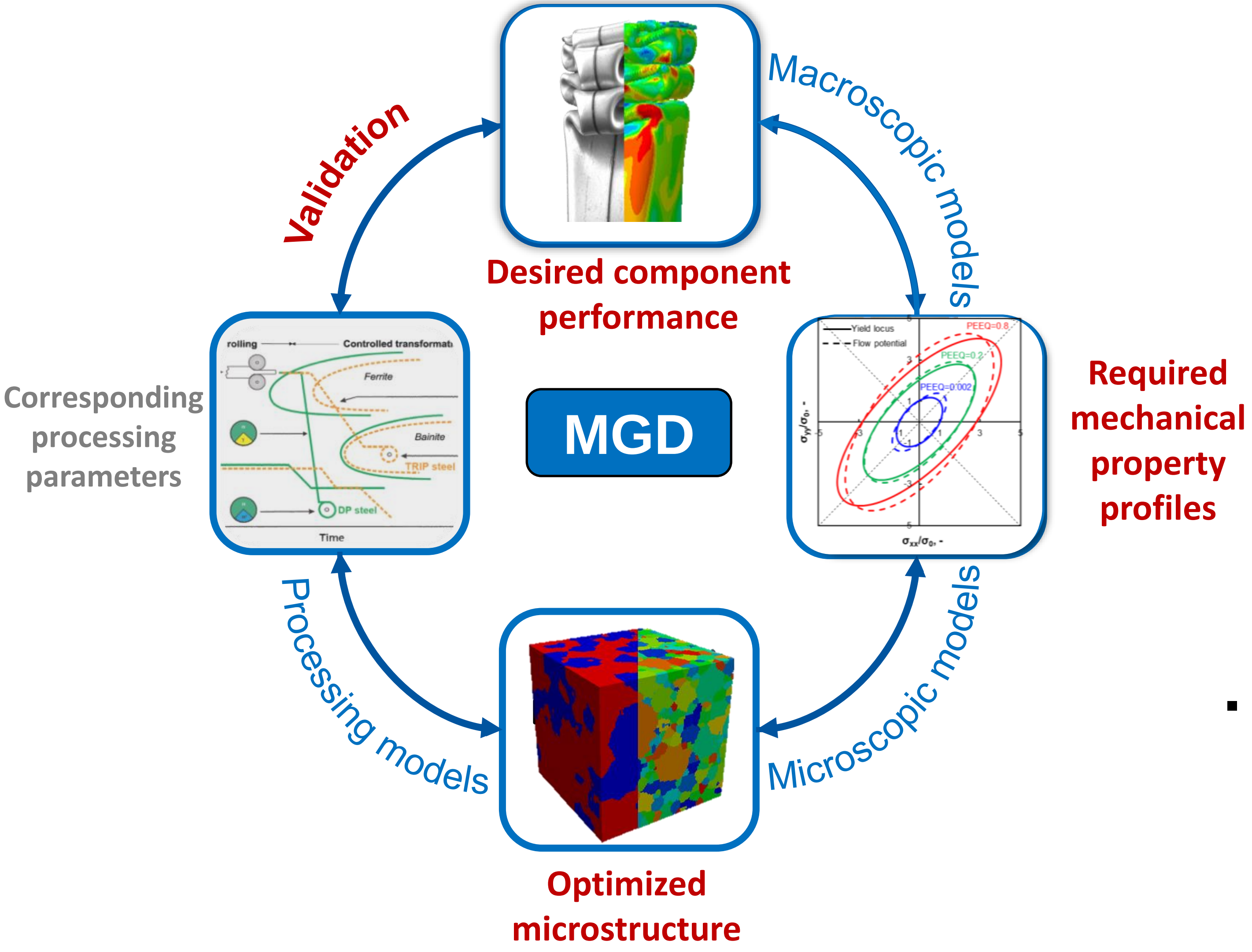
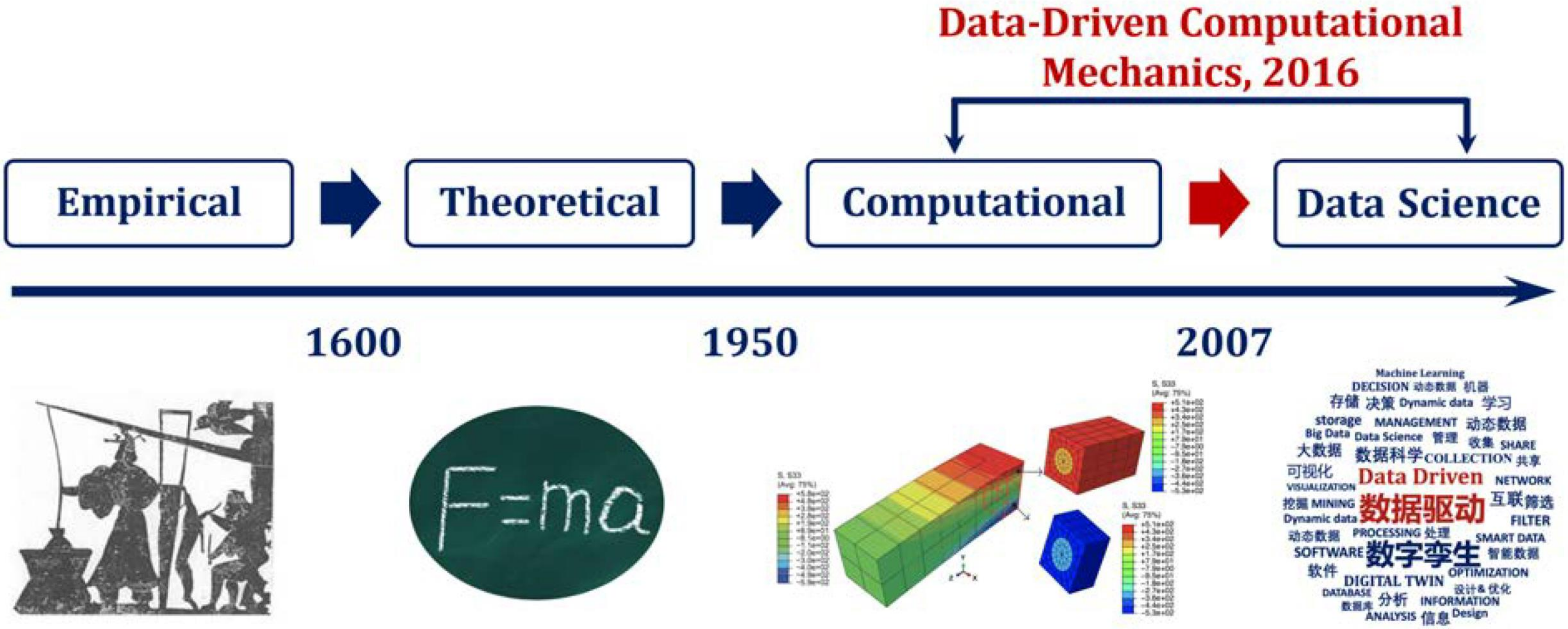


- Tailoring microstructure by modeling and validation
  - Design mechanical properties for desired performance
  - Microstructure design for required properties
  - Validation by experiments

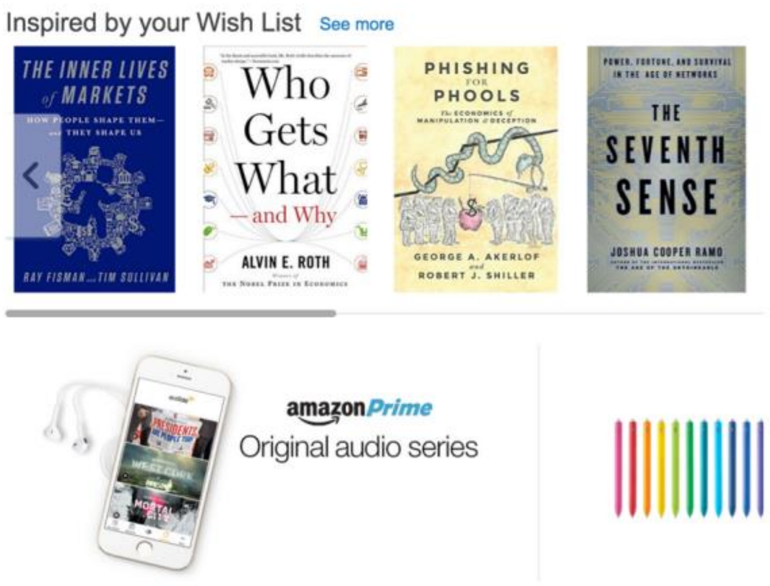
Machine learning based modeling

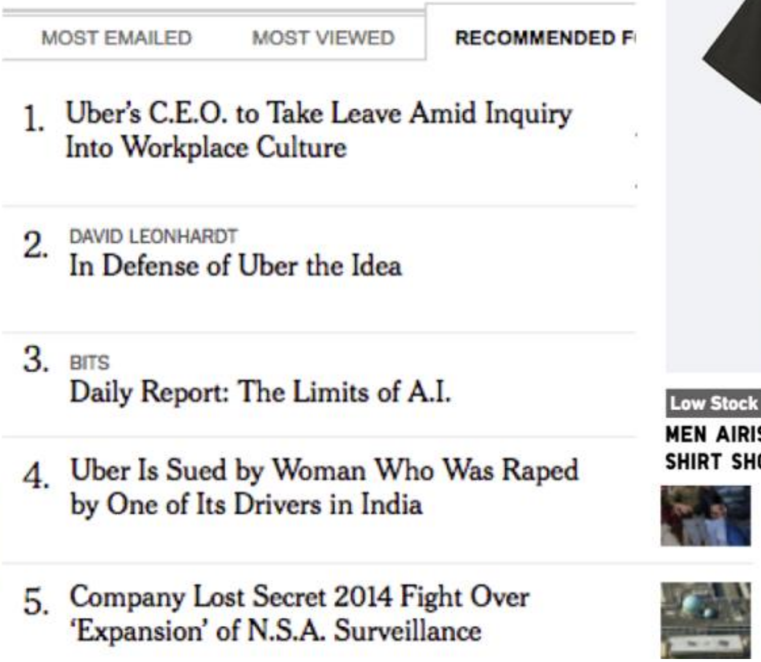


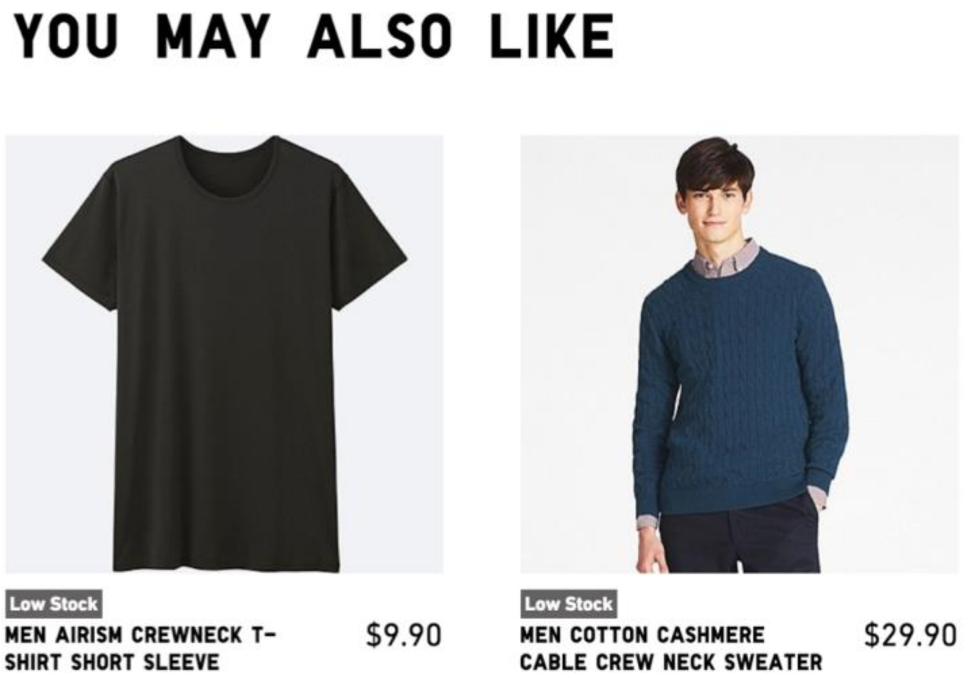
Rui Xu, 2020, PhD thesis, Multiscale modeling of heterogeneous materials: application to Shape Memory Alloys

What is Machine Learning?

- Data-driven algorithms to discern patterns and make predictions on big, high-dimensional data
- Clustering, classification, regression, generation



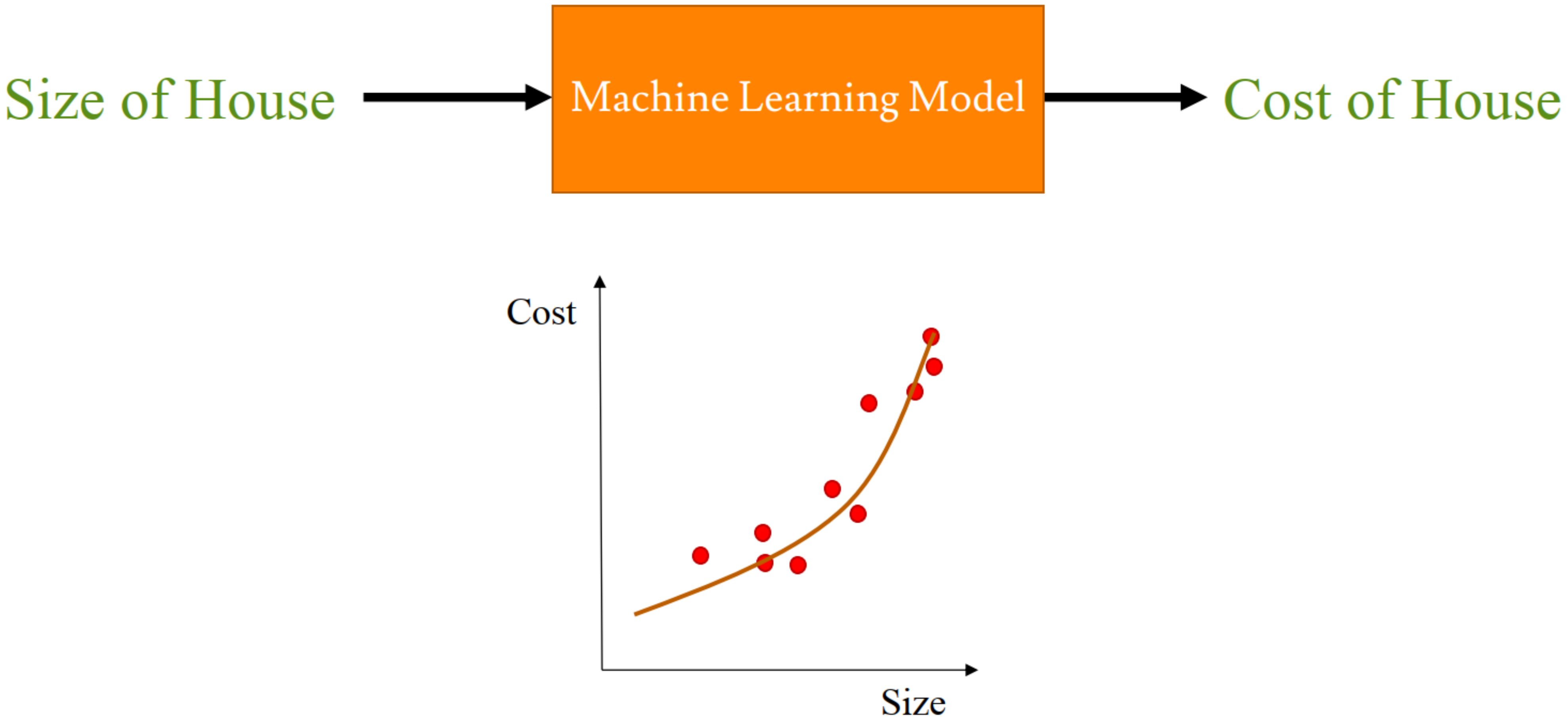




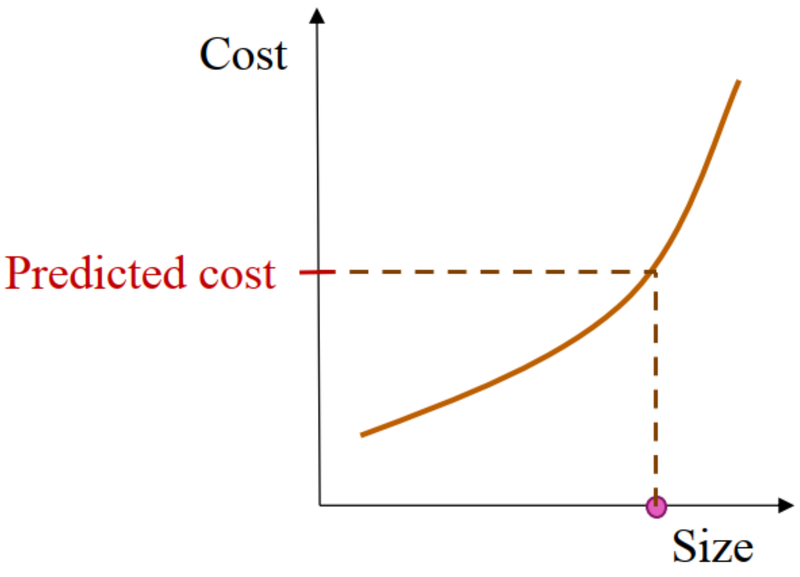
Machine Learning

- The **machine learning model** is just a mapping between **inputs** and **outputs**
- Unlike typical functions y = f(x), the mapping is often too complex to write in a compact form

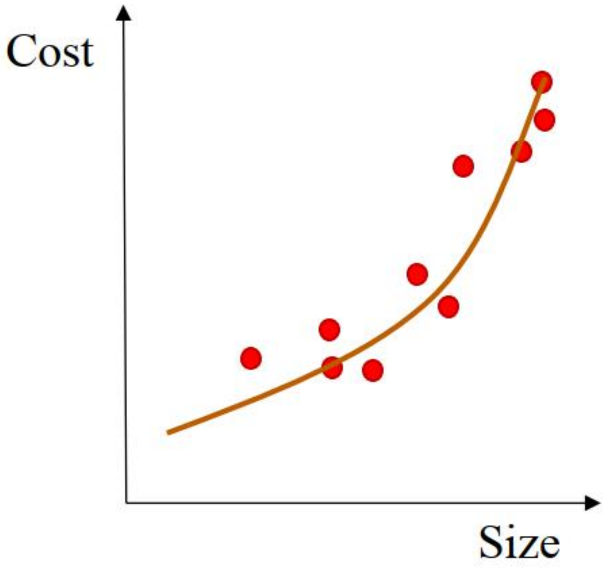
Housing example: Training



Housing example: Prediction



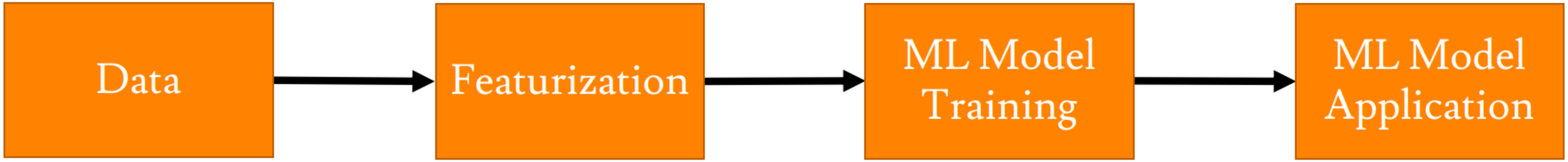
Real housing example



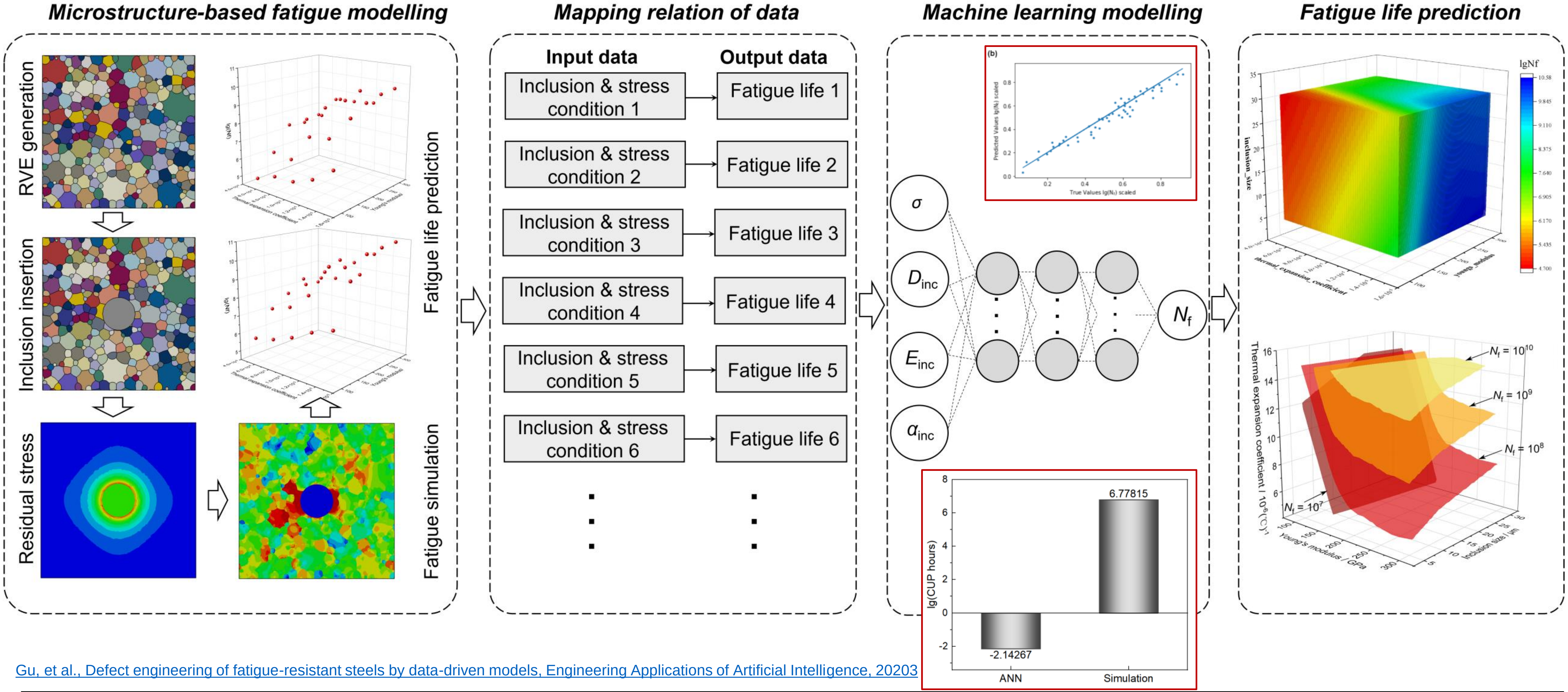
- Why do we need machine learning?
- What if cost is a function of size, neighborhood, yard, number of stories, schools, building material, age of structure, previous owner maintenance, color of paint
- Machine learning lets us make sense of high-dimensional data sets

Machine learning jargon & workflow

- **Input:** Degrees of freedom for a problem that could have an impact on the output
- **Output:** Quantity (can be a real number or a category) to be predicted with a machine learning model
- **Machine learning model:** A mapping between the inputs and output(s)
- **Model training:** A process that uses a set of data where inputs and outputs are known to create a machine learning model.
- **Model prediction:** A process that uses a trained machine learning model to generate predicted output(s) corresponding to a complete set of inputs



Cases study in material science:
Defect engineering of fatigue-resistant steels by data-driven models



[Gu, et al., Defect engineering of fatigue-resistant steels by data-driven models, Engineering Applications of Artificial Intelligence, 20203](#)

Cases study in material science:
Defect engineering of fatigue-resistant steels by data-driven models

Published to a top engineering journal as research assistant work of Sayoojya during summer!

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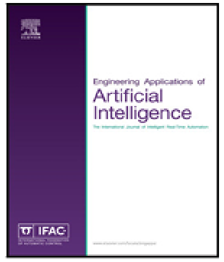

Sayoojya Prasad

Defect engineering of fatigue-resistant steels by data-driven models

Check for updates

Chao Gu [a], Yanping Bao [a], Sayoojya Prasad [b], Ziyu Lyu [a], Junhe Lian [b,*]

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ARTICLE INFO

Keywords:
Machine learning
Microstructure-sensitive modeling
Inclusion
Young's modulus
Thermal expansion coefficient

ABSTRACT

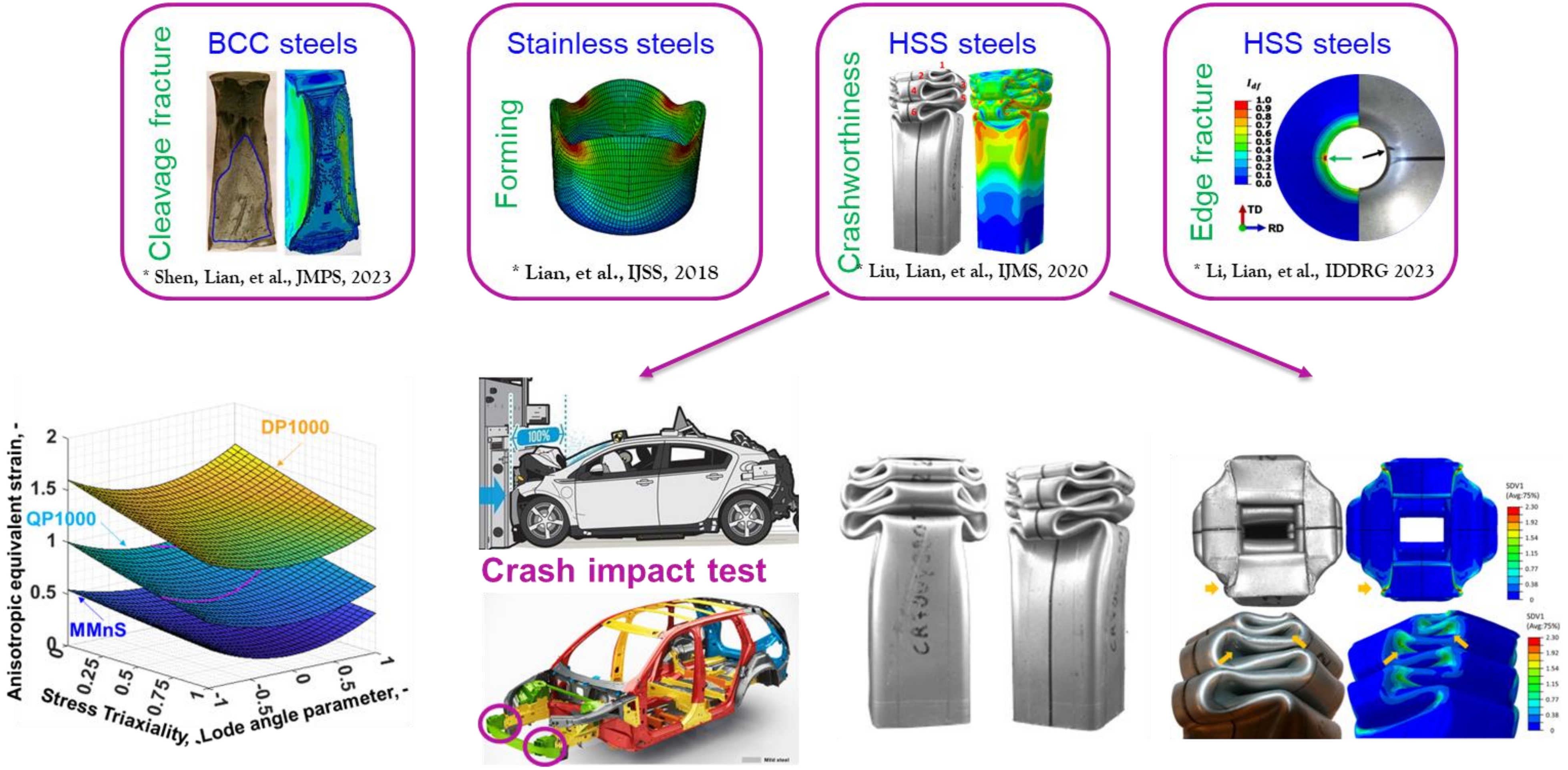
As inclusions are inevitable from the material-producing processes, an engineering concept regarding multiple features of them is needed for material design. In this study, a unique approach integrating physical-meaningful microstructure-sensitive models with the machine-learning-based data-driven model is proposed to reveal the complex relationship between the fatigue life of materials with intrinsic features of inclusions including size, stiffness, thermal properties, and extrinsic stress amplitudes. This high-fidelity presentation of the relation of these variables enables a detailed and systematic analysis of the effects of inclusions on fatigue life. The data-based phase map provides a designing envelope of inclusion features for fatigue-resistant steels.

Topic theme #1: Material Mechanics & Modeling

Aalto University

- 1-2 open topics for research and/or thesis on experimental & numerical work
- Collaboration with institutes in Sweden and Germany, industry in Finland, France and Austria

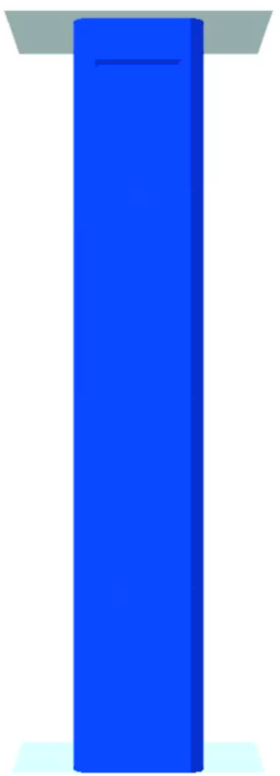
Zinan Li



Formability

Crash boxes

Crashworthiness



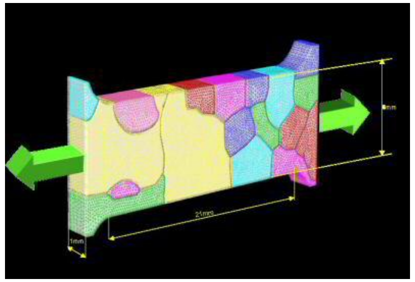
Topic theme #2: Microstructure Characterization and Modeling

Aalto University

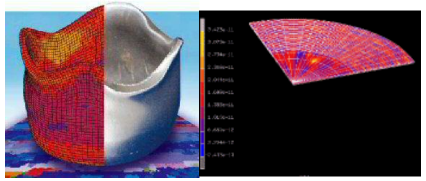
Rongfei Juan

- Advanced microstructure modeling: The Crystal Plasticity Finite Element Simulation Method
- Describing and understanding the micromechanical behavior of crystalline materials

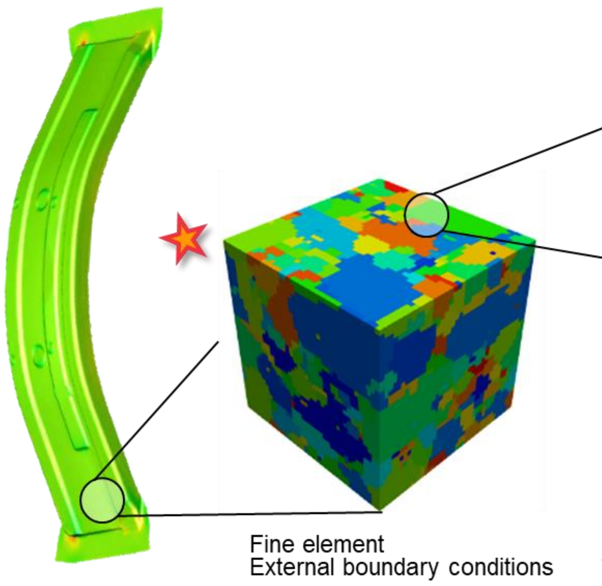
- 1-2 open topics for research and/or thesis
- Collaboration with institutes in Spain and Germany industry in France and Austria

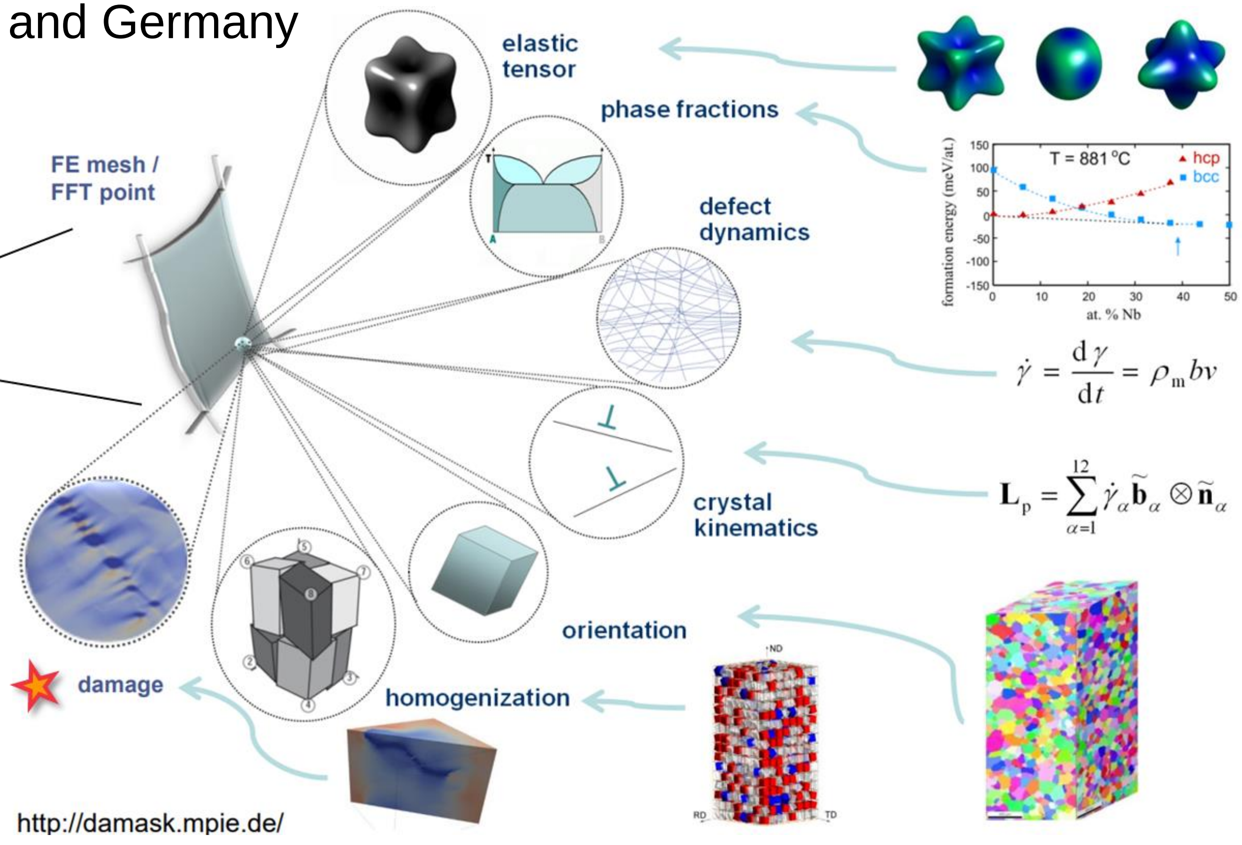


Tension test: view in microscale



Anisotropic elastic-plastic deformation in crystals and their interplay

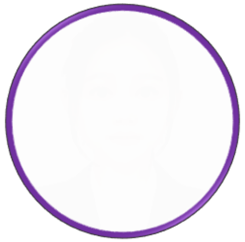




Multi-Physics Crystal Plasticity Simulation application

* http://www.dierk-raabe.com/crystal-plasticity-finite-element-method/

Topic theme #3: Materials & Modeling for Hydrogen Ecosystem

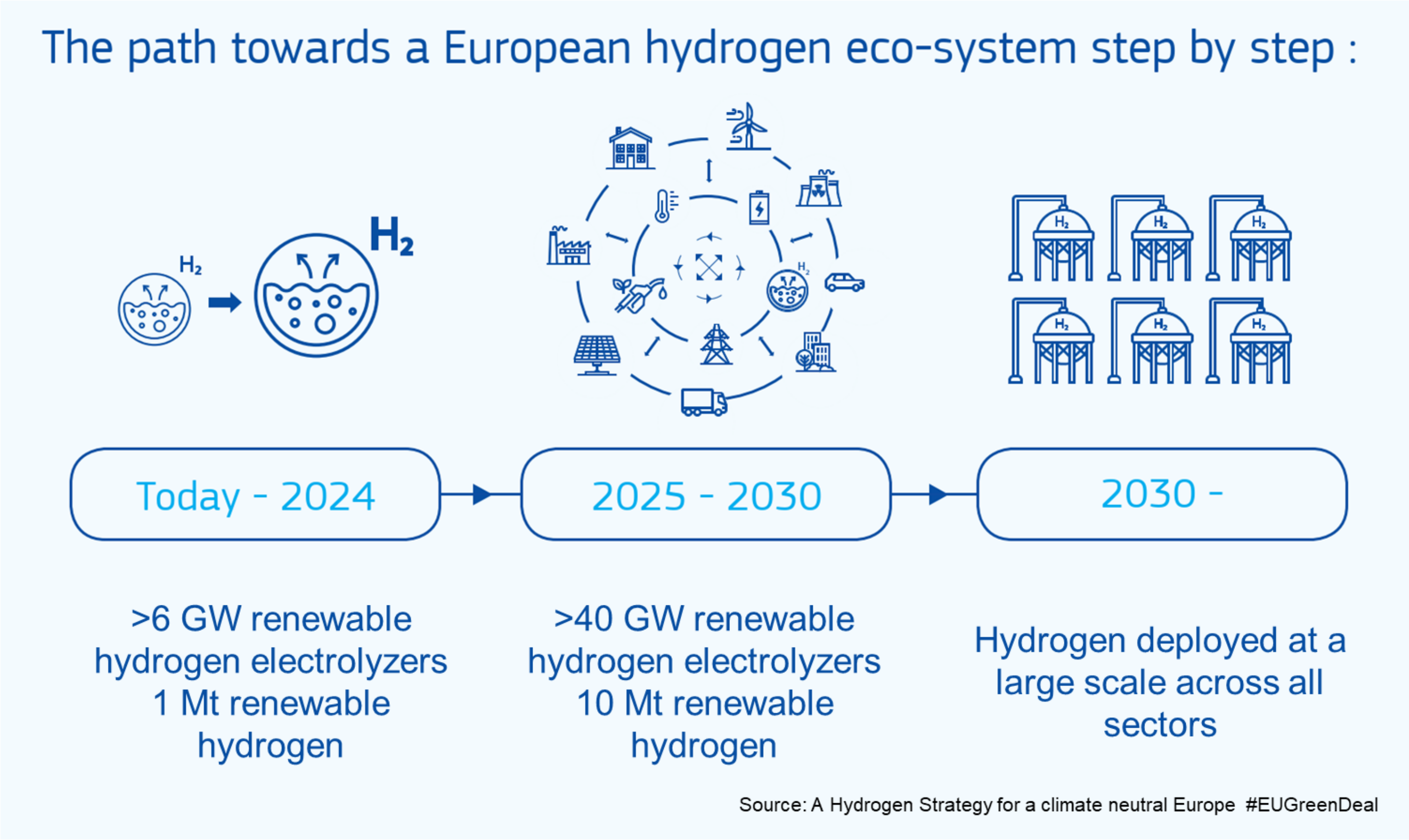


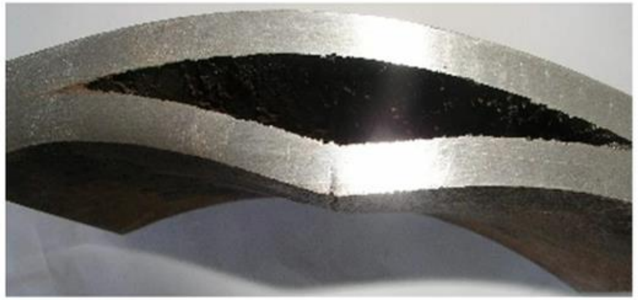
Shengzhao Yang

Zinan Li

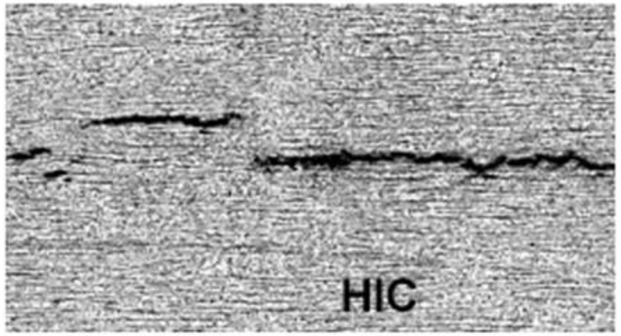
- Characterizing hydrogen diffusion and embrittlement of hydrogen storage/transport materials
- Multiphysics chemo-mechanical multiscale modeling

- 1 open topic for research and/or thesis
- Collaboration with 20+ institutes and leading industries across Europe





Fatal failure in the cross-section



Topic theme #4: Data Science and Data-driven Approaches

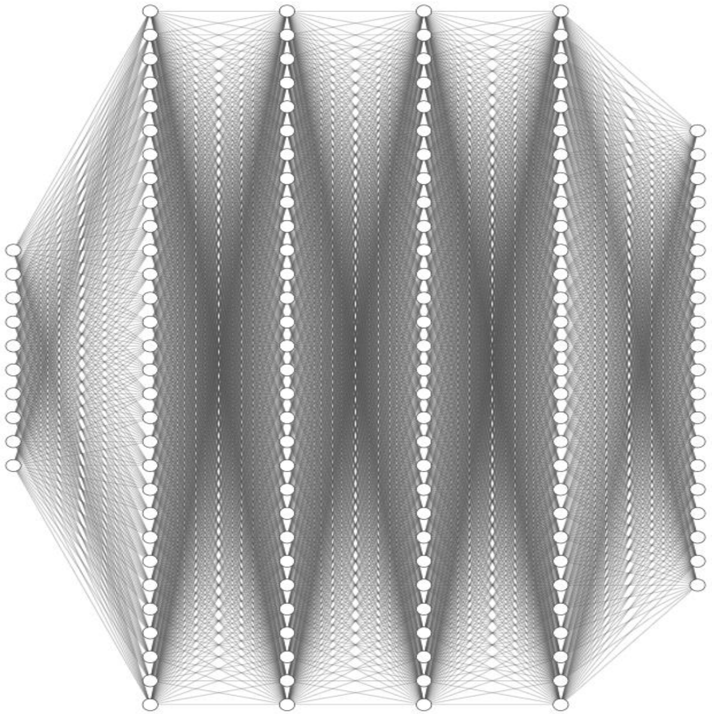
Aalto University

Sayoojya Prasad

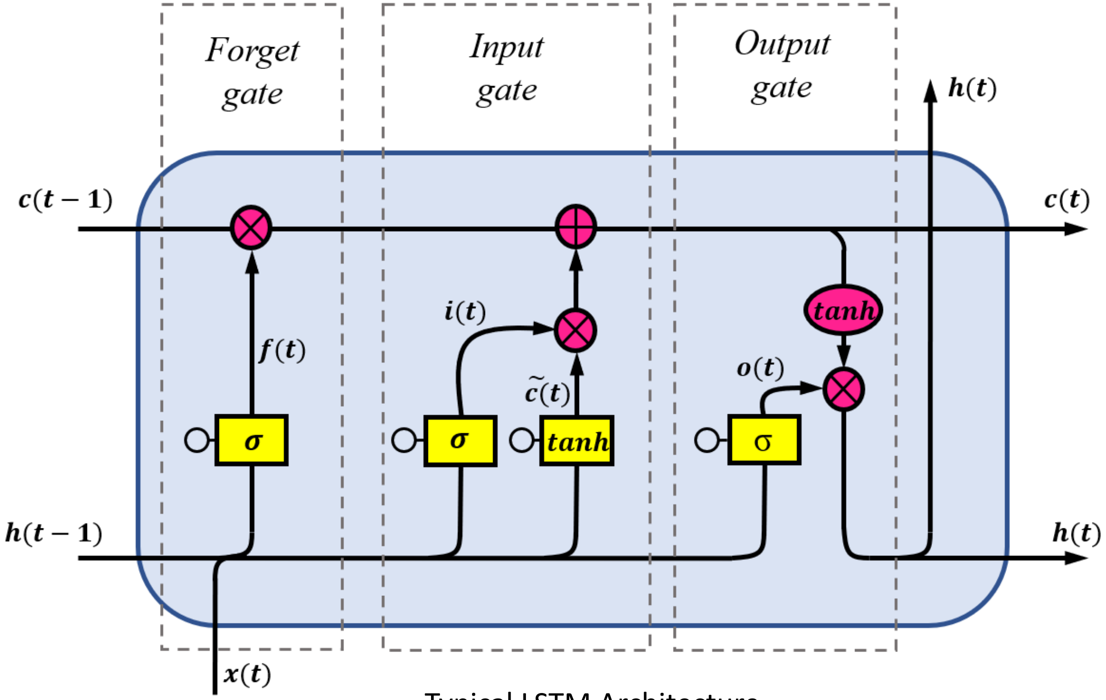
Binh Nguyen

- Machine-learning-based models for parameter optimization and material modeling
- Data-based alloy discovery and material design
- 1-2 open topic for research and/or thesis
- Collaboration with experienced experts and researchers at School of Science

Fully-connected Neural Networks



Long Short Term Memory and RNN



Typical LSTM Architecture

Aalto University

Thank you!

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Email: junhe.lian@aalto.fi

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