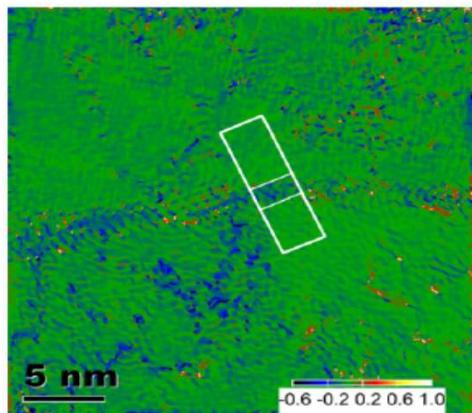


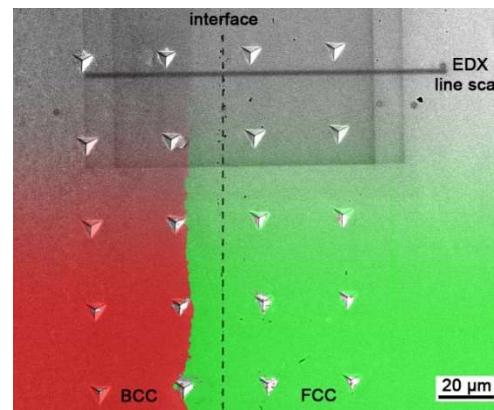
Thermomechanical properties and microstructure of fcc and bcc high-entropy alloys

G. Wilde, H. Rösner
WWU Münster
Institute of Materials Physics



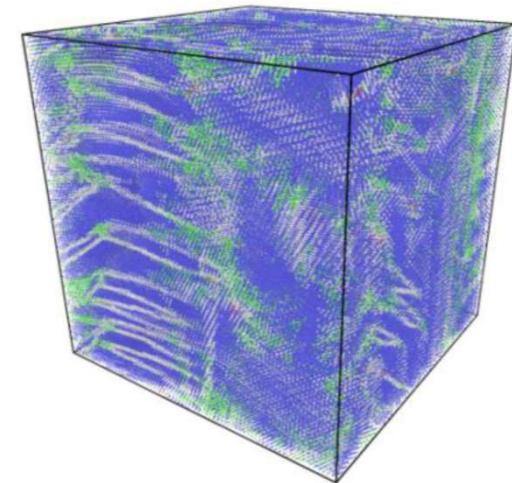
- Radiotracer diffusion
- Defect structure (TEM)

K. Durst, E. Bruder
TU Darmstadt
Physical Metallurgy



- In-situ and small scale mechanical testing
- Deformation mechanism

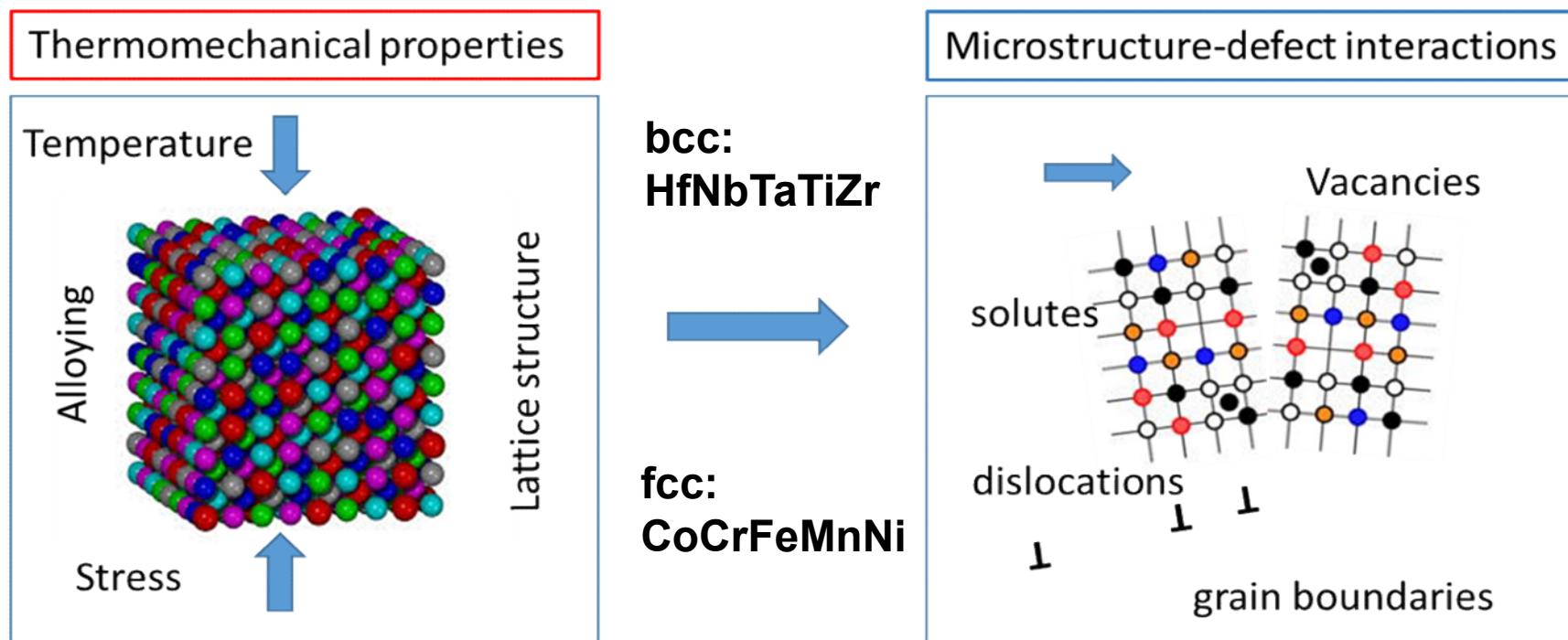
A. Stukowski, K. Albe
TU Darmstadt
Materials Modelling



- Atomistic modelling
- Defect interactions

Project goal

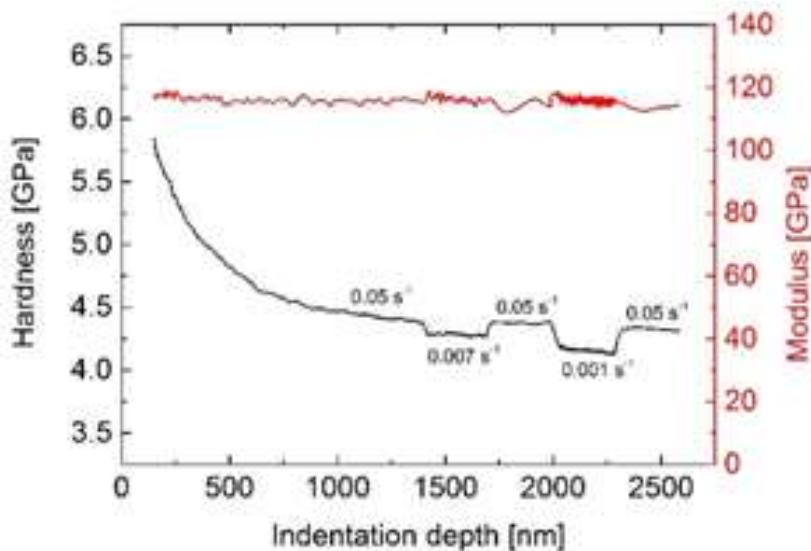
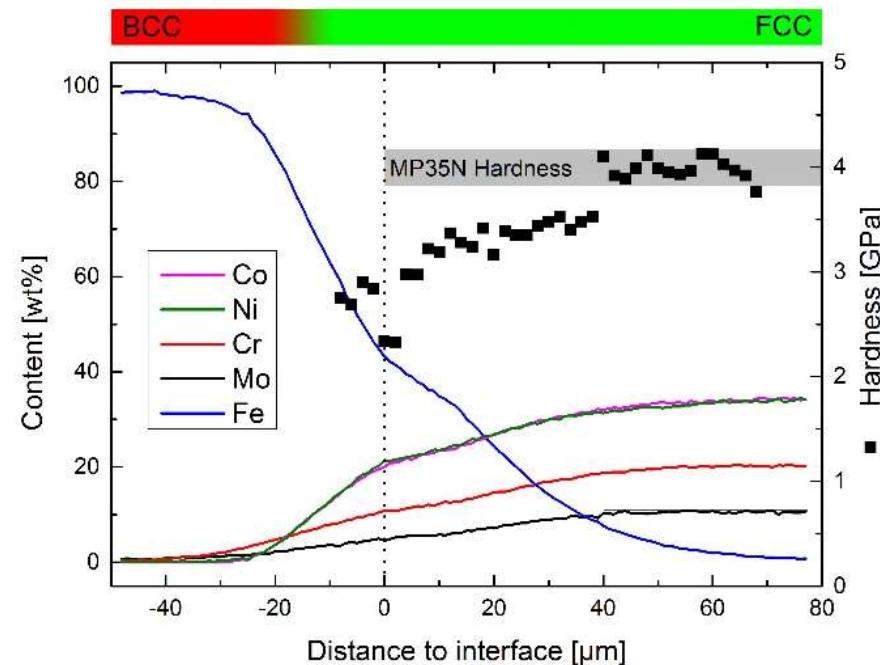
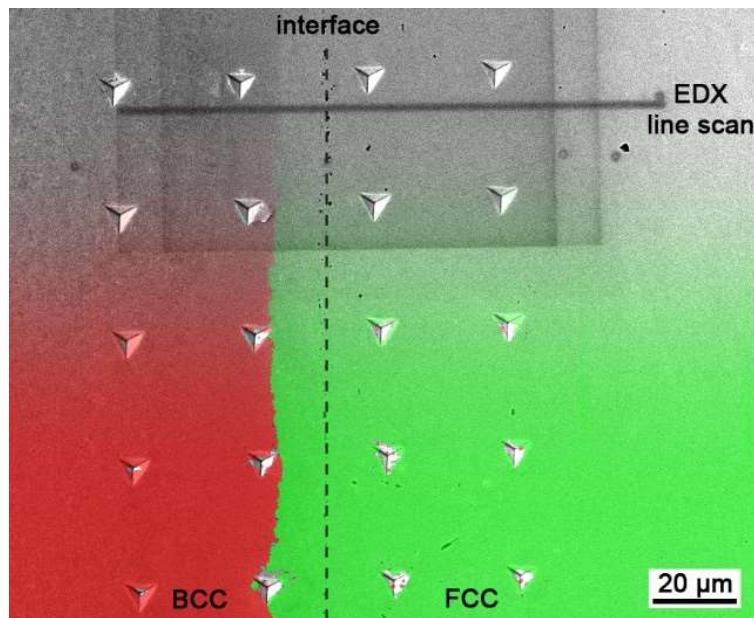
Understanding the influence of lattice structure and microstructure on the *thermomechanical properties of single-phase HEAs*



- Influence of short-range order
- Self diffusion
- Dislocation mobility
- Phase stability: HEA → CCA

- Solute vs GB strengthening
- GB segregation
- Microstructural stability

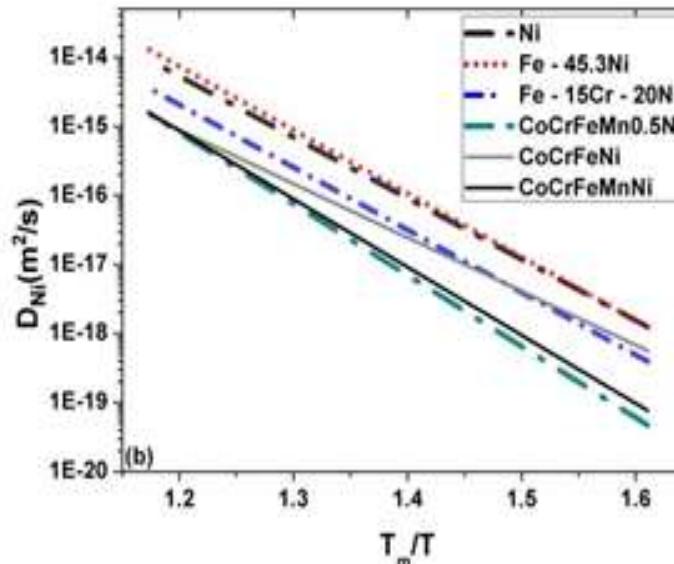
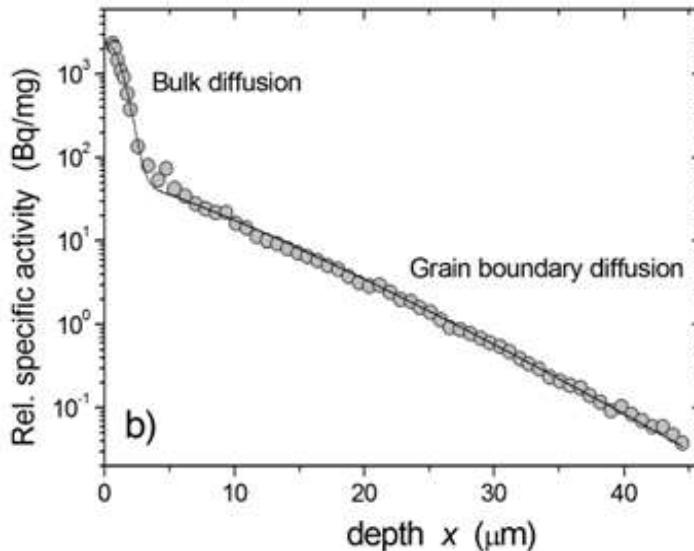
Diffusion couples and nanoindentation



- Thermodynamic and structural stability
- Solid solution strengthening
- Strain rate sensitivity

Self-diffusion and microstructure

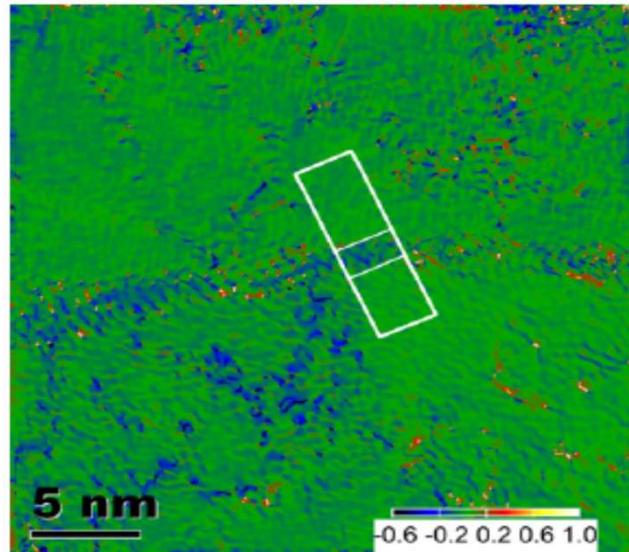
^{63}Ni tracer diffusion in CoCrFeMnNi @1173 K



First results:

- no sluggish diffusion
- indication for fast GB diff.

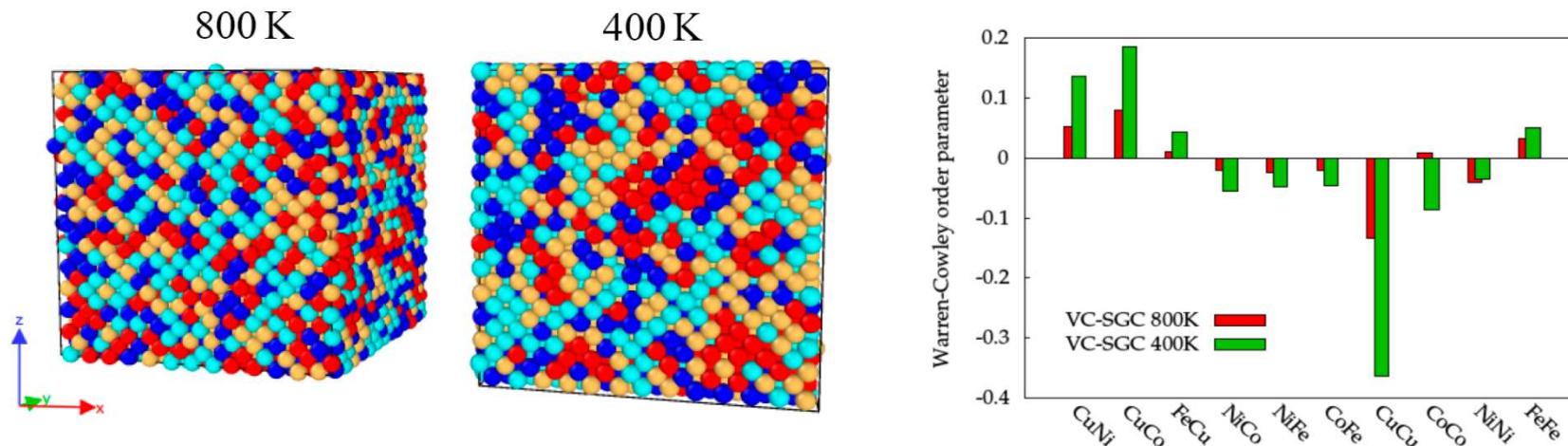
Strain distribution
at a GB after
severe deformation



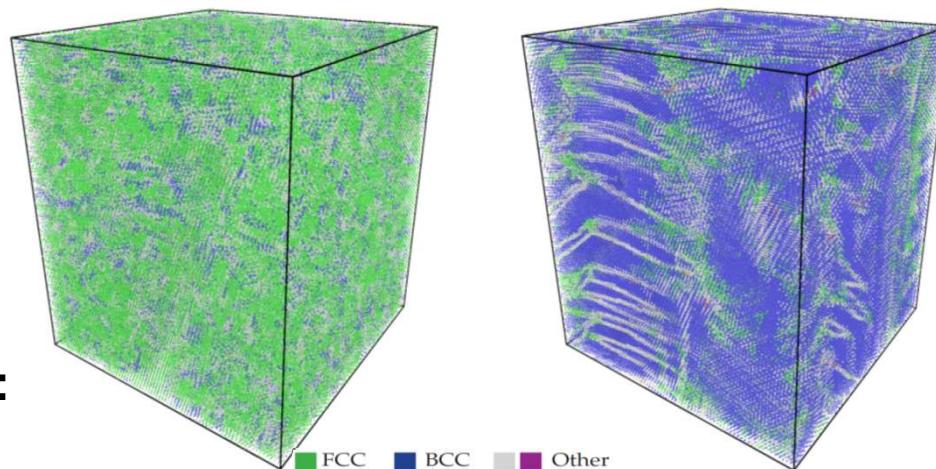
- Self-diffusion rates
- Lattice distortion
- GB structure & segregation

Variance-constrained MD/MC simulations

Ordering effects in CuNiFeCr:



MD simulation of
temperature induced
fcc-bcc transition in equi-
molar AlCrFeCoNiCu (500 K):



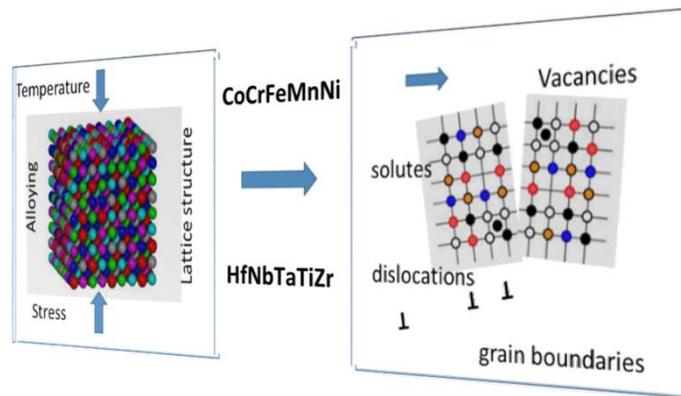
Work packages and deliverables

Radiotracer diffusion
In- & ex-situ (HR)TEM
Calorimetry (1.9-1700 K)
Wilde, Rösner

Massive parallel MD
Hybrid MD/MC
Dislocation Analysis
Stukowski, Albe

Uniaxial testing
Indentation testing
Severe plastic deformation
Durst, Bruder

Migration barriers
Correlation coefficients
Thermodynamics
Stability



SFE
Activation volume
Dislocation glide paths
Defect densities

Generic HEA properties

Lattice Distortion & stability
HEA / CCA demarcation
Diffusion rates
Configurational entropy

Mechanical properties

Mechanical prop. ($\dot{\varepsilon}$, T, D)
Dislocation storage & strengthening
GB structure

Structure & role of GBs

Segregation at GBs
GB-med. plasticity
Grain size dependence
Dislocation-GB interaction

Contributions to goals and collaborations

Verification of HEA characteristics

„Transition“ from CCA to HEA?
Volume & grain boundary self-diff.
Strain distribution
Mechanical properties
Defect interactions

Impact of microstructure

fcc
&
bcc

Role & structure of GBs
Segregation
Short-range order
Deformation mechanisms
Dislocation mobility

