From Chaos to Order:

Local Structure in Compositionally Complex Alloy $Al_8Co_{17}Cr_{17}Cu_8Fe_{17}Ni_{33}$

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Motivation: Contribution of SRO to hardness in HEA

SRO in solid solutions: deviation of local composition from statistical distribution of elements

SRO given by:

- Interatomic distance
- Debye-Waller factor

→ **EXAFS**

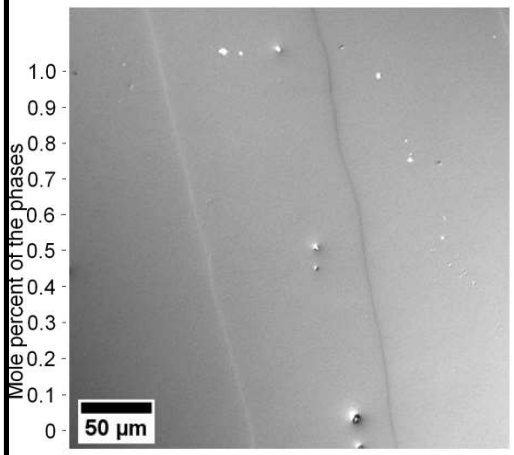
<u>Scientific aims within the project</u>

Understand:

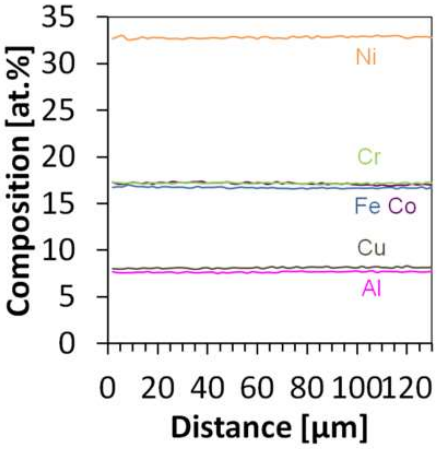
- the *influence of the* ***local structure*** *on* ***hardness and elasticity***
- the *influence of* ***temperature*** *on* ***local structure*** *and* ***hardness / elasticity***
- the *contribution* of each element to the hardness and elasticity

Preliminary results

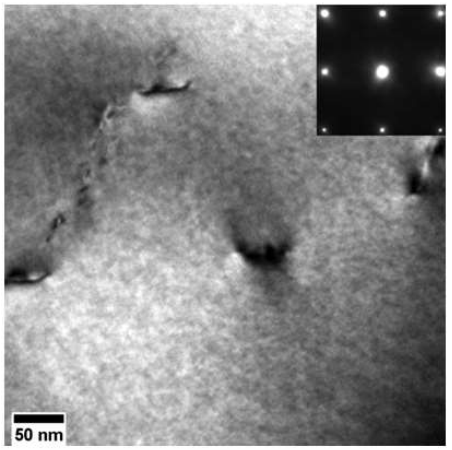
OM



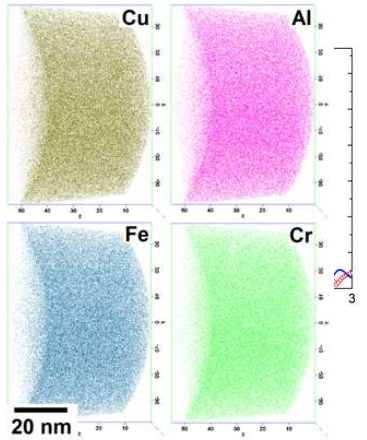
EPMA



TEM

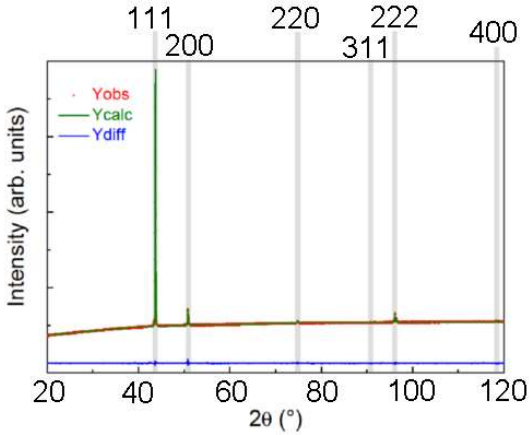


APT



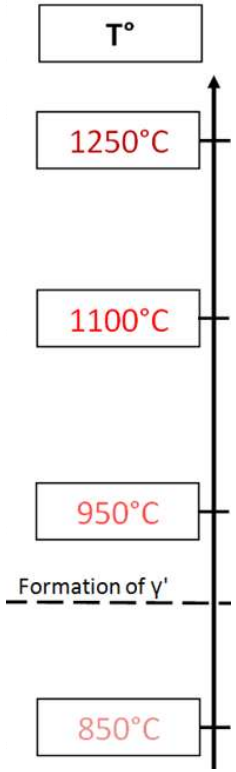
10 mm | 100 µm | 1 µm | 10 nm | 1 Å

XRD



Work program / methods

- WP1: Alloy and sample preparation
- WP2: Pre-characterization and selection of samples
- WP3: Local chemical composition
- WP4: Determination of the local structure (SRO)
- WP5: Mechanical testing and correlation with the local structure



Scientific aims / benefit for the Priority Program

Expected results:

- Different **bond lengths** for different absorbing elements in EXAFS
- Debye Waller factor **higher** than in corresponding pure metals
- Debye Waller factor different for **different absorbing elements**
- **T-dependence** of all SRO parameters
- **Correlation between SRO and hardness / elasticity**

Benefit for the priority program:

- Basic understanding of SRO – hardness/elasticity correlation for other CCA/HEA consisting mainly of TM elements
- Establish a link between the single phase high temperature region („HEA“) and the two phase γ- γ' CCA at low temperatures

→ Enhancing the understanding of the two families HEA-CCA

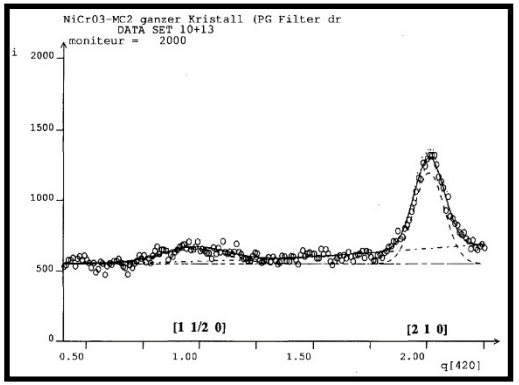
Thank you!

Motivation: Contribution of SRO to hardness in HEA

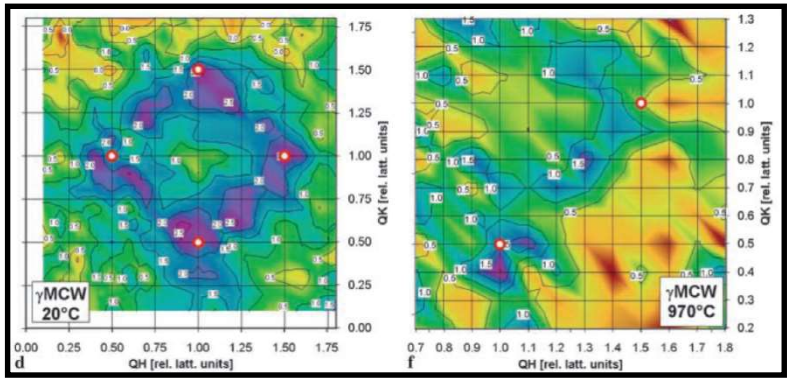
SRO in solid solutions**:** deviation of local composition from statistical distribution of elements

SRO given by**:** Warren-Cowley SRO Parameter
Interatomic distance
Debye-Waller factor
Number of nearest neighbors

Example:
Superalloy matrix phase



MC-2, RT,
(*Glas et al., Acta Mater 1996*)



MCW at 20°C, 970°C
(*Prem et al., Appl. Phys. 2002*)

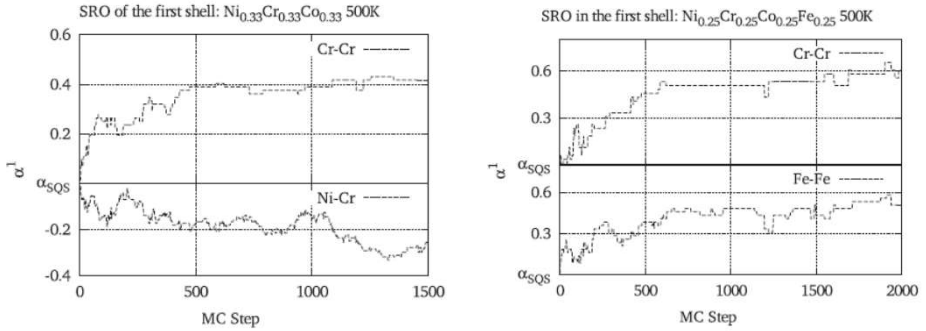
- **(1 ½ 0)** reflection not allowed in γ and γ' phase
- SRO (~ 1 nm) pronounced at **RT**
- SRO dissolves at **T > 600 °C**
- **Influence on hardness expected**
- **MC + DFT :** T-dependence of SRO in NiCrCoFe HEA HEA (Tamm, 2015)
- Change in hardness of

Motivation

High entropy alloys: supposed to be solid solutions with random distribution of elements
However: Deviations from random distribution of elements observed by MC-simulation + DFT calculations (Tamm et al., 2015) $\Rightarrow$ influence hardness/strength (Maitia et al. 2016)
Short-range order not stable at high temperatures

Warren Cowley short range order (SRO) parameter: $\alpha_{ij}^{\nu} = 1 - p_{ij}/c_j$,
p_{ij} : Probability of finding atomic spezies j around an atom of type i in shell ν
c_j : atomic concentration of element type j
$p_{ij} = c_j : \alpha_{ij}^{\nu} = 0$, random distribution of elements
$p_{ij} < c_j : \alpha_{ij}^{\nu} > 0$, Clustering of i-type elements
$p_{ij} > c_j : \alpha_{ij}^{\nu} < 0$, preferred location of j-type elements around i-type elements (SRO)

MC-Simulation + DFT calculations (Tamm et al., 2015):



Short-range order parameter of the NiCrCoFe quaternary FCC system averaged over last steps of the lattice MC simulation at three temperatures.

Pair	500 K	800 K	1200 K
Ni–Ni	0.30	0.16	0.13
Ni–Cr	−0.18	−0.21	−0.22
Ni–Co	0.14	0.10	0.12
Ni–Fe	−0.27	−0.04	−0.04
Cr–Cr	0.59	0.54	0.65
Cr–Co	−0.31	−0.18	−0.26
Cr–Fe	−0.10	−0.14	−0.17
Co–Co	0.33	0.13	0.11
Co–Fe	−0.16	−0.05	0.03
Fe–Fe	0.54	0.23	0.17

- Pronounced SRO in NiCrCoFe HEA
- T - dependence of SRO

Tamm et al., (2015)

Previous results (Koteski et al)

Previous results: EXAFS (+ DFT-LAPW) - study of Ni:M (M: Mo, Ru, Hf, Ta, W, Re):

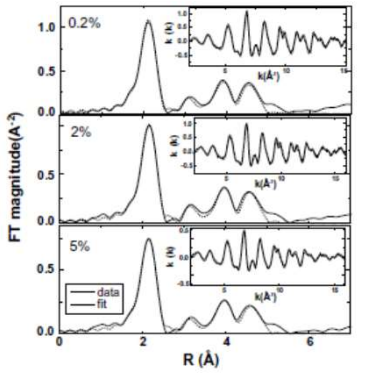
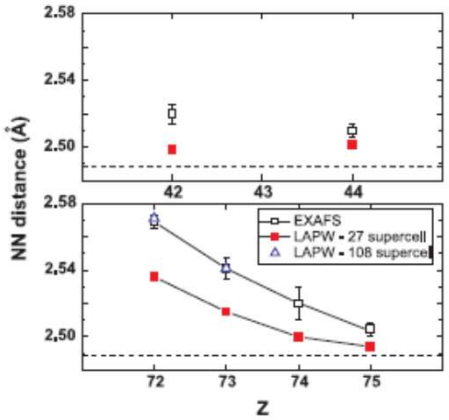


Fig. 3. Fourier-transforms of the EXAFS oscillations of the NiRu samples (solid line) and fit (dotted line). The corresponding EXAFS spectra are given in the insets.



Z - dependence of Ni-M bond length

(Koteski et al. 2008)