From Chaos to Order:
Local Structure in Compositionally Complex
Alloy Al$_8$Co$_{17}$Cr$_{17}$Cu$_8$Fe$_{17}$Ni$_{33}$

Anna Manzoni$^1$, Tobias Scherb$^1$, Gerhard Schumacher$^1$, John Banhart$^{1,2}$

$^1$Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Germany
$^2$Technische Universität Berlin, Germany
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

Scientific aims within the project

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

**EXAFS**
- Interatomic distance increases with increasing Z (Z: ordering number)
- Local disorder decreases with increasing Z

**Alloy development**
- After heat treatment at 1250°C-1h: single phase is confirmed at all scales (OM, EPMA, TEM, APT)

**ThermoCalc**
- Single phase is expected above 900°C
- γ' phase at lower temperatures
- Many phases at low temperature
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

$T^\circ$

- 1250°C
- 1100°C
- 950°C (Formation of γ')
- 850°C
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

- (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

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

**MCW** at 20°C, 970°C
(Prem et al., Appl. Phys. 2002)
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) ⇒ influence hardness/strength (Maitia et al. 2016)
Short-range order not stable at high temperatures

Warren Cowley short range order (SRO) parameter: $\alpha_{ij}^\nu = 1 – p_{ij}/c_j^\nu$, $p_{ij}$ : Probability of finding atomic spezies j around an atom of type i in shell $\nu$
$c_j$ : 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):

- 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):

Z - dependence of Ni-M bond length

(Koteski et al. 2008)