Microstructural properties of Al-containing refractory high entropy alloys for high temperature applications

Peculiarities of ordering in Ta-Nb-Mo-Cr-Ti-Al

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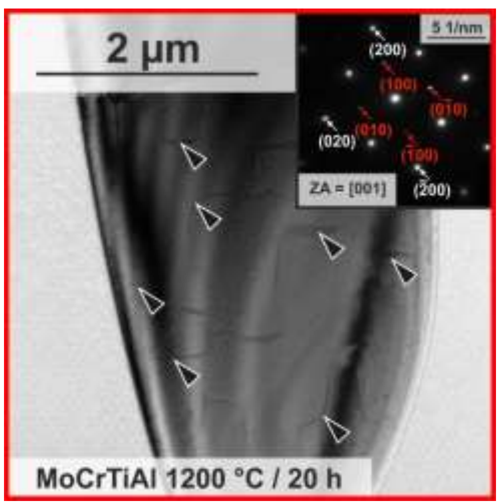
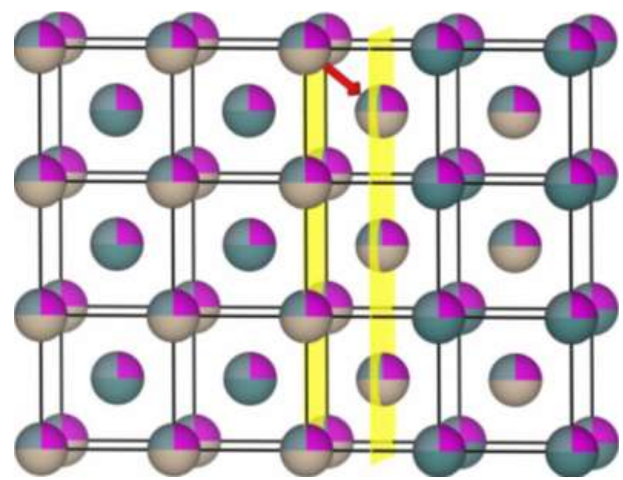




Introduction

- Alloy development → for high temperature applications

passivating

Ta-Nb-Mo-Cr-Ti-Al

high melting point

low density

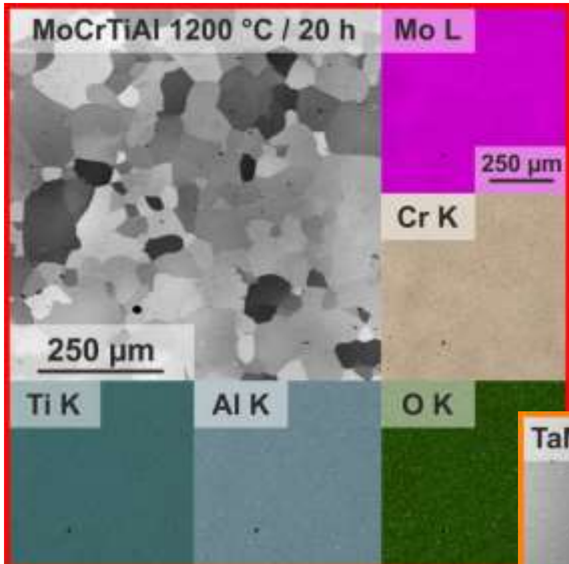
- Lack of ductility on macroscopic scale between room temperature and 400 °C[1,2] → characterization of mechanical properties difficult

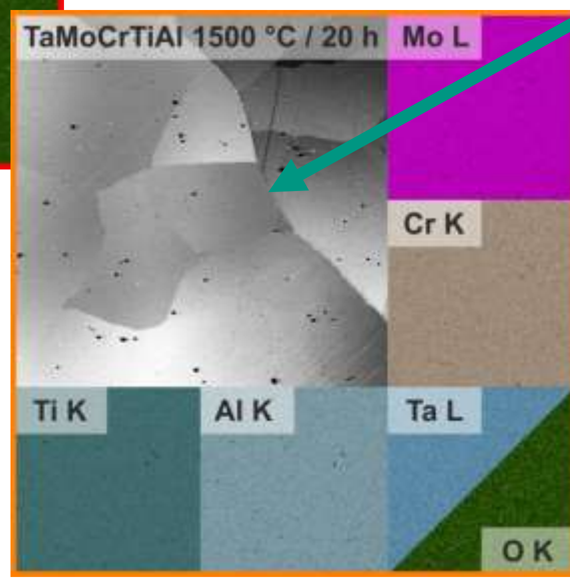
- Microstructural characterization to understand intrinsic brittleness

[1] H. Chen et al., Microstructure and mechanical properties at elevated temperatures of a new Al-containing refractory high entropy alloy Nb-Mo-Cr-Ti-Al, Journal of Alloys and Compounds 661 (2016) 206-215.
[2] H. Chen et al., Contribution of lattice distortion to solid solution strengthening in a series of refractory high entropy alloys, Metallurgical and Materials Transactions A 49 (2018) 772-781.

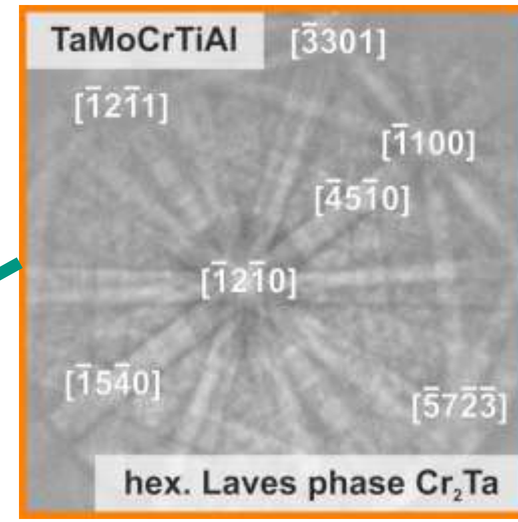
Microstructure

- Arc melting → Homogenization





- Suppression of competing phases

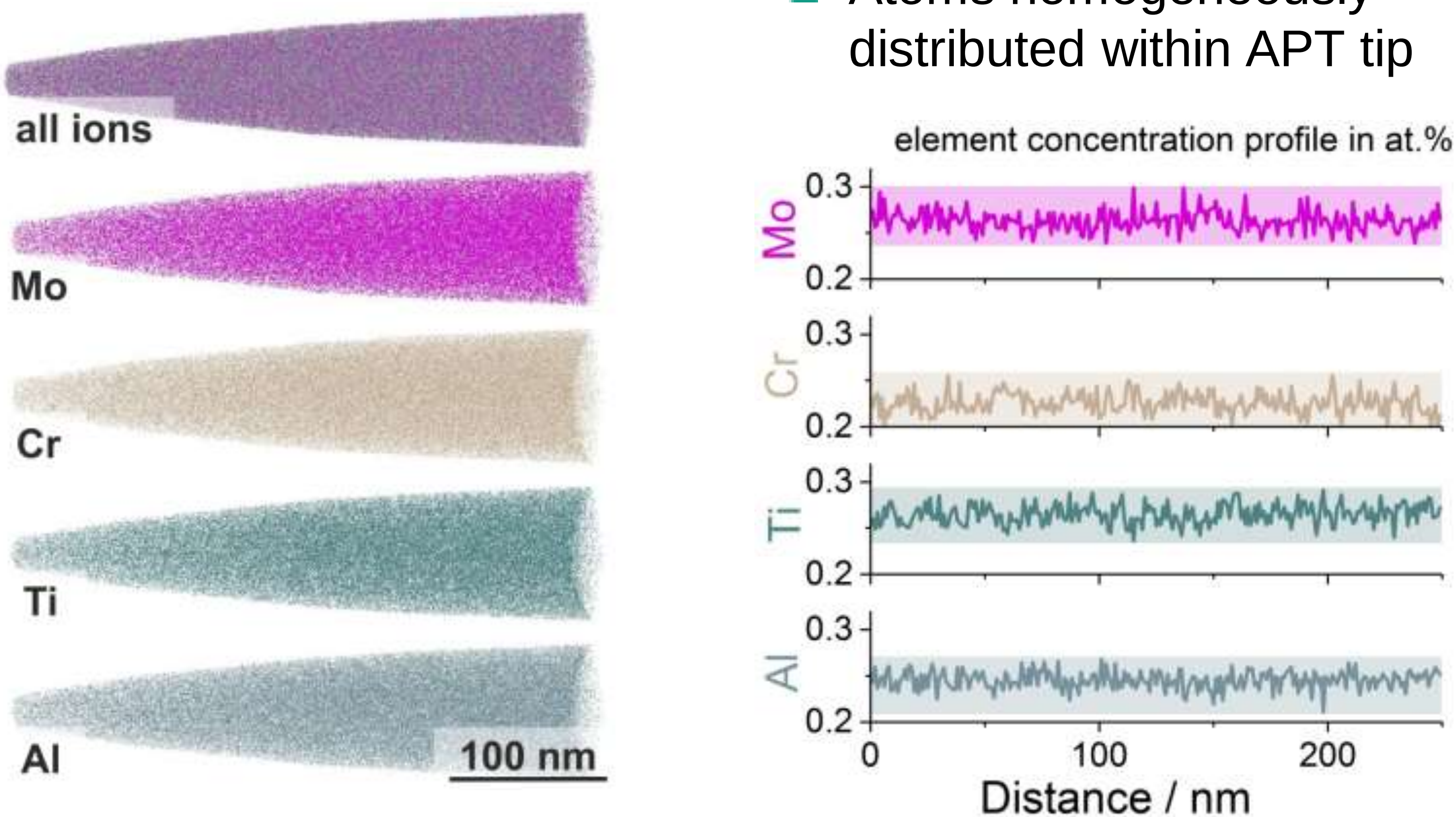


Cr_2Ta
Cr_2Nb
$Al(Mo,Nb)_3$
$Ti(Al,Cr)_3$

Atom probe tomography (APT)

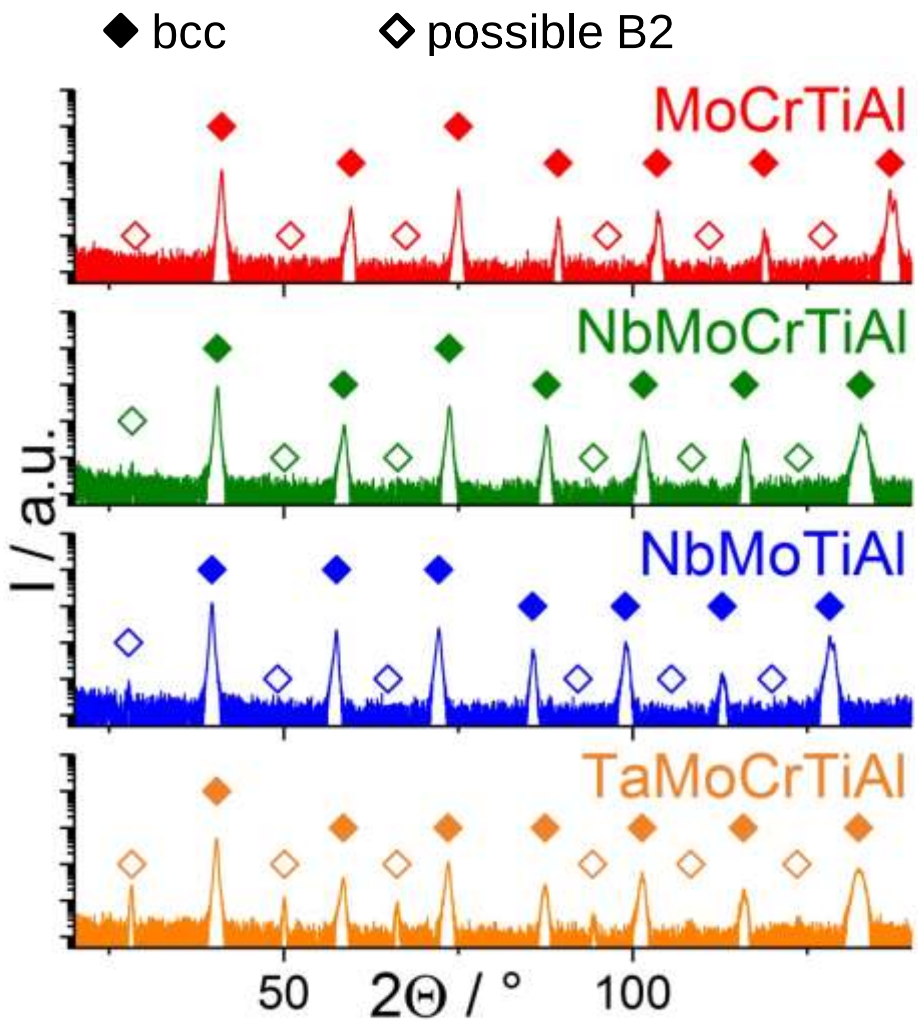
MoCrTiAl

- Atoms homogeneously distributed within APT tip



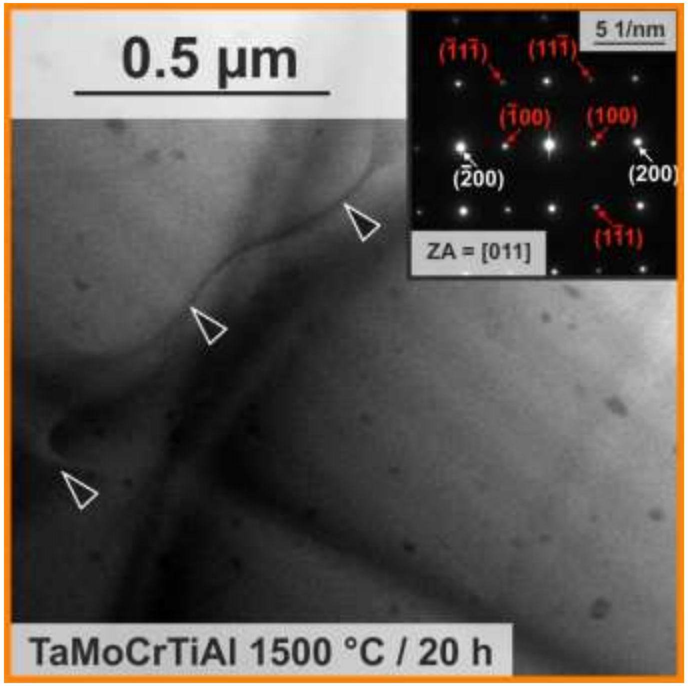
➡ Homogeneous microstructure down to nm scale

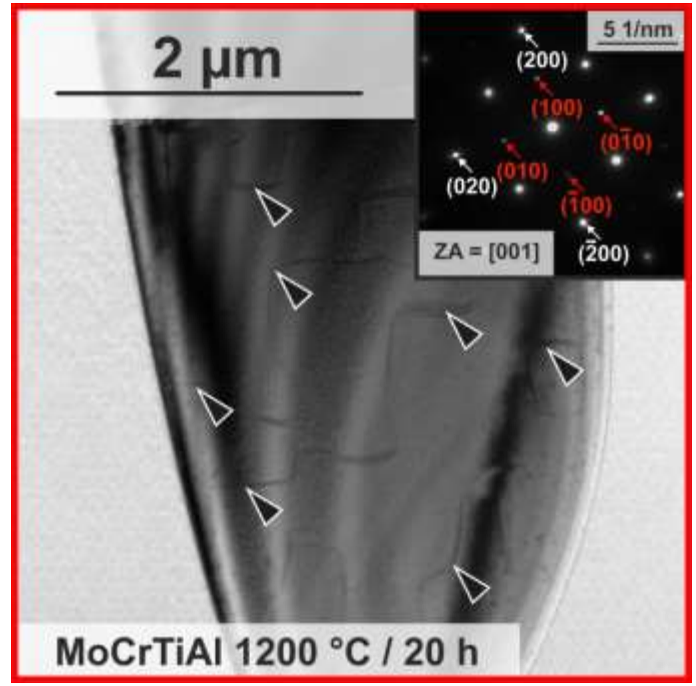
Indications of ordering



- XRD: gentle indications of B2 superstructure in Nb-Mo-Cr-Ti-Al
- TaMoCrTiAl exhibits significant superlattice peaks
- Morphology of B2 ordered phase? → TEM

Peculiarities of ordering





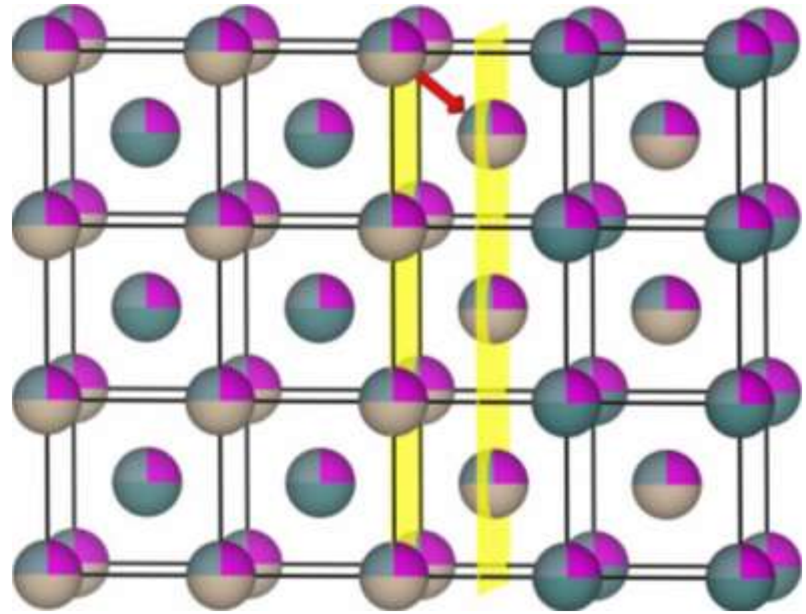
- TEM-SAD: Superlattice spots observable in all investigated alloys
- TEM-BF: Antiphase domain boundaries (APBs) reveal disorder-order phase transformation during cooling

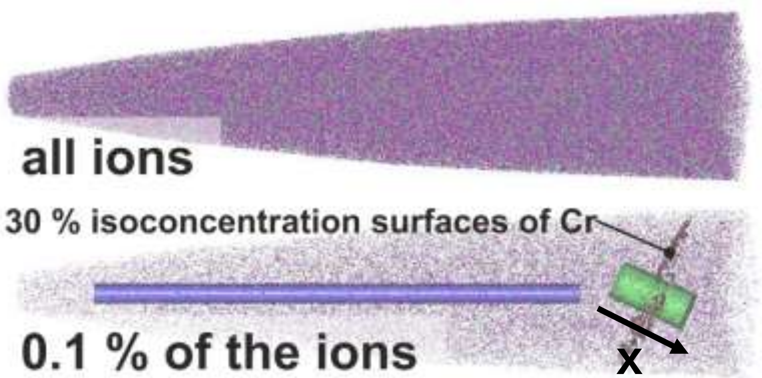
➡ Homogeneously ordered B2 crystal structure in all alloys

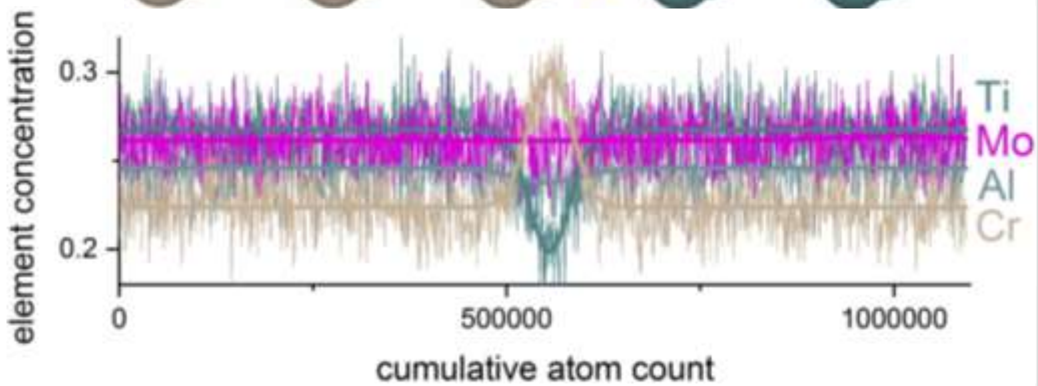
Properties of ordering

- Lattice shift at APB→ chemical inhomogeneity
- APBs reveals site occupation
  Cr: site 1 Ti: site 2
  Mo, Al: evenly distributed
- **MoCrTiAl**

(100) ½ [111] APB







- APBs enriched in Cr (occupies lattice site 1) and depleted in Ti (site 2)

Summary

- Ta-Nb-Mo-Cr-Ti-Al: Uniform element distribution after homogenization treatment
- B2 type ordered crystal structure forms during cooling
- Approach to reveal site occupation by APT on APBs
- Contribution of ordering to lack of ductility → project outlook

decrease DBTT

passivating

Ta-Nb-Mo-Re-Cr-Ti-Al

high melting point

suppress Laves phase

low density

Thank you for your kind attention.

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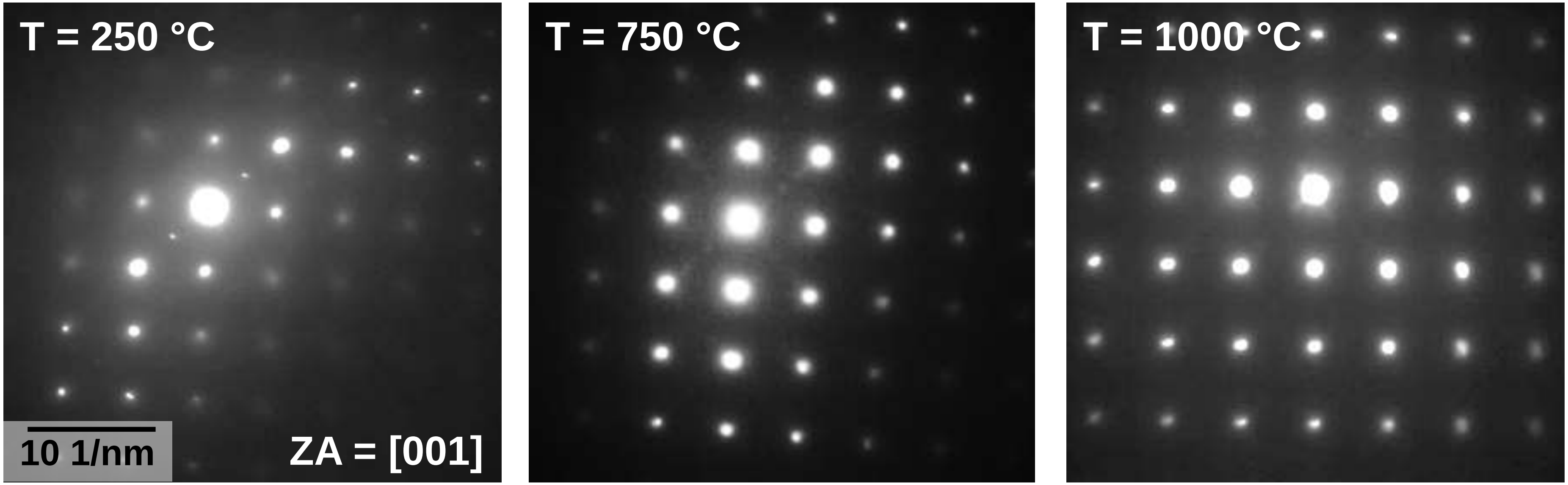
Karlsruhe Nano Micro Facility (KNMF)

Carl Zeiss Stiftung

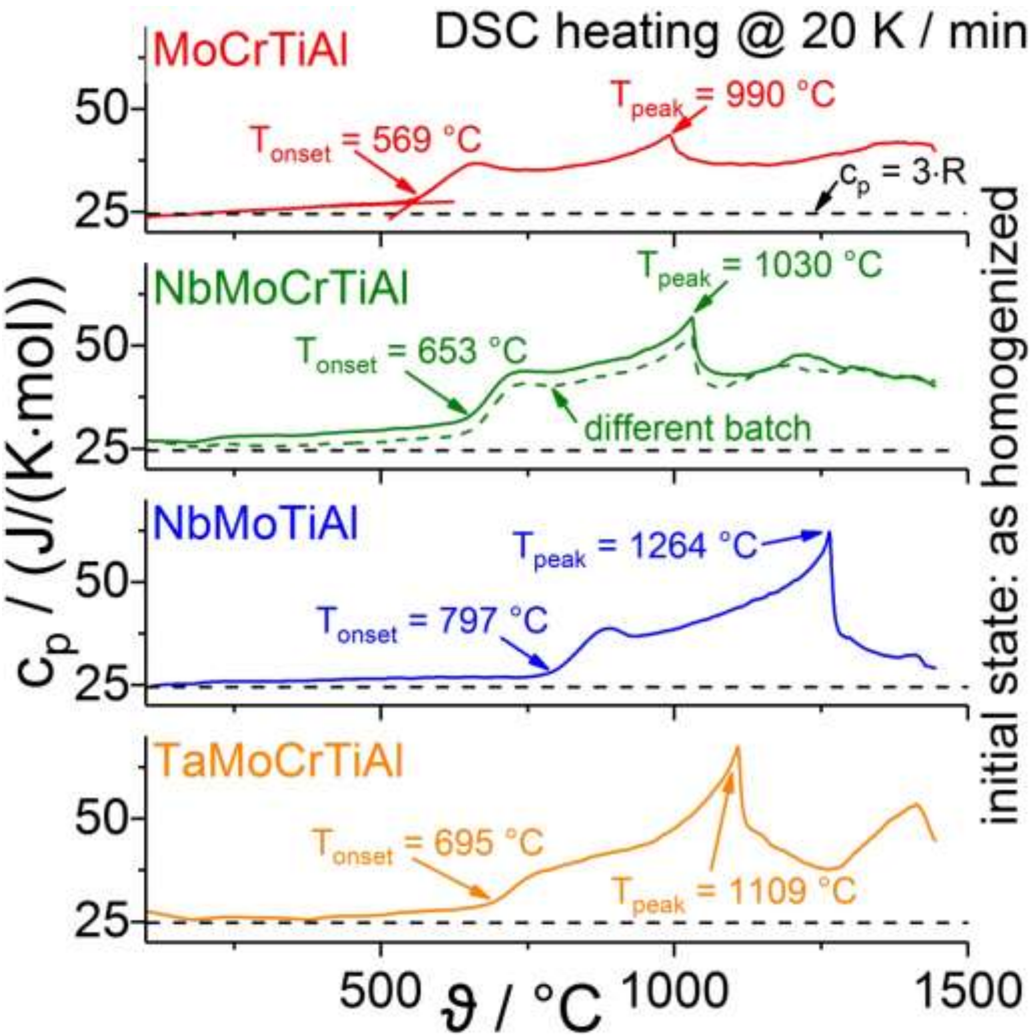
Thermal stability of ordering

MoCrTiAl, as homogenized



- At which temperature does bcc-B2-transformation occur?
  → TEM heating experiment
- TEM-SAD: Super lattice spots completely vanish at 1000 °C

Disorder-order phase transformation



- λ-shaped peaks reveal second order phase transformation at T_{peak}
- Observable in all alloys
- DSC at varying heating rates → T_{onset} does not seem to be related to disorder-order phase transformation

Solid solution strengthening of HEAs

- Atomic size difference δ ↔ mechanical properties

$$\boxed{\delta = \sqrt{\sum_i x_i \left(1 - \frac{r_i}{\bar{r}}\right)^2}}$$

x_i: Concentration of element i
r_i: Atomic radius of element i
$\bar{r}$: Mean atomic radius

- Bcc alloys: T dependent mechanical properties

- Influence of thermally activated processes on strengthening of bcc high entropy alloys

δ ↔ alloy composition

NbMoTiAl

$NbMoCr_{0.25}TiAl$

$NbMoCr_{0.5}TiAl$

$NbMoCr_{0.75}TiAl$

Suppression of Cr_2Nb and $Al(Mo,Nb)_3$

Cr reduction ← **NbMoCrTiAl** → Nb reduction

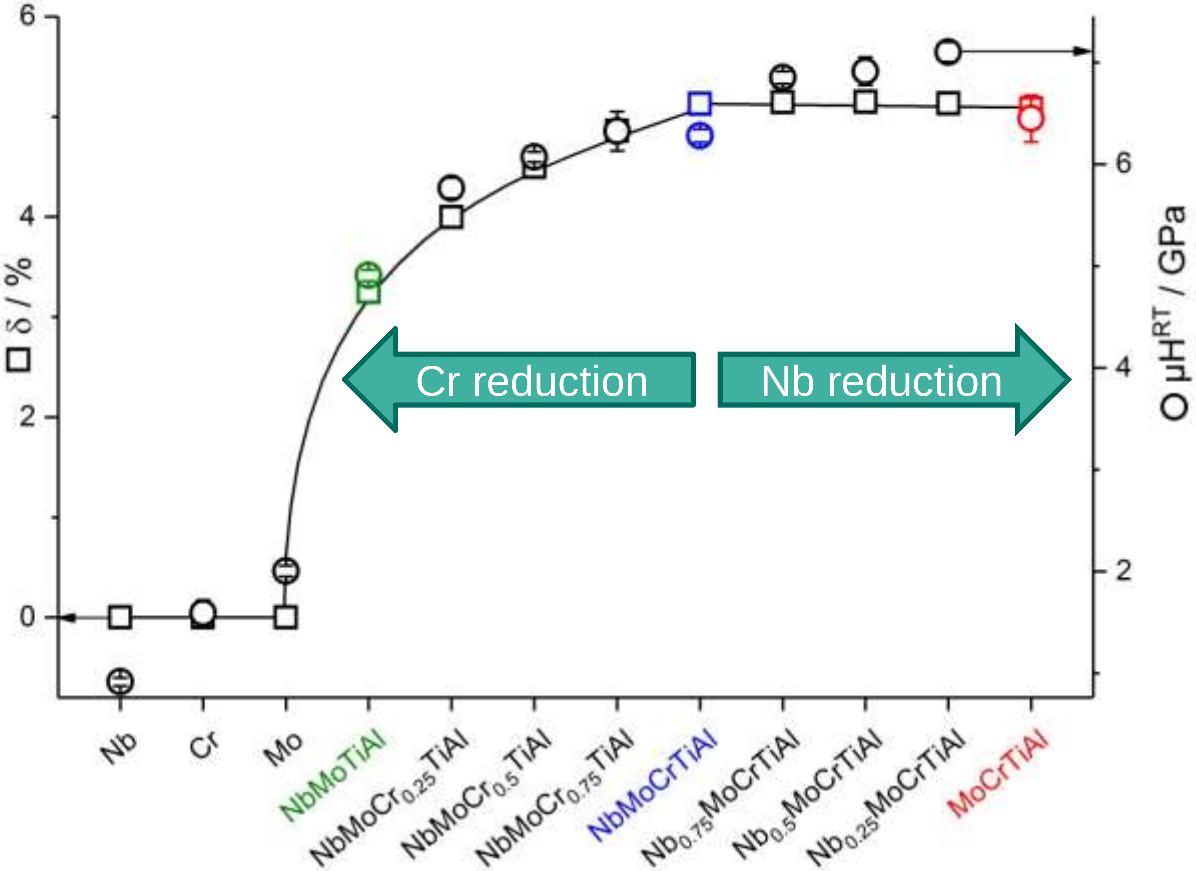
$Nb_{0.75}MoCrTiAl$

$Nb_{0.5}MoCrTiAl$

$Nb_{0.25}MoCrTiAl$

MoCrTiAl

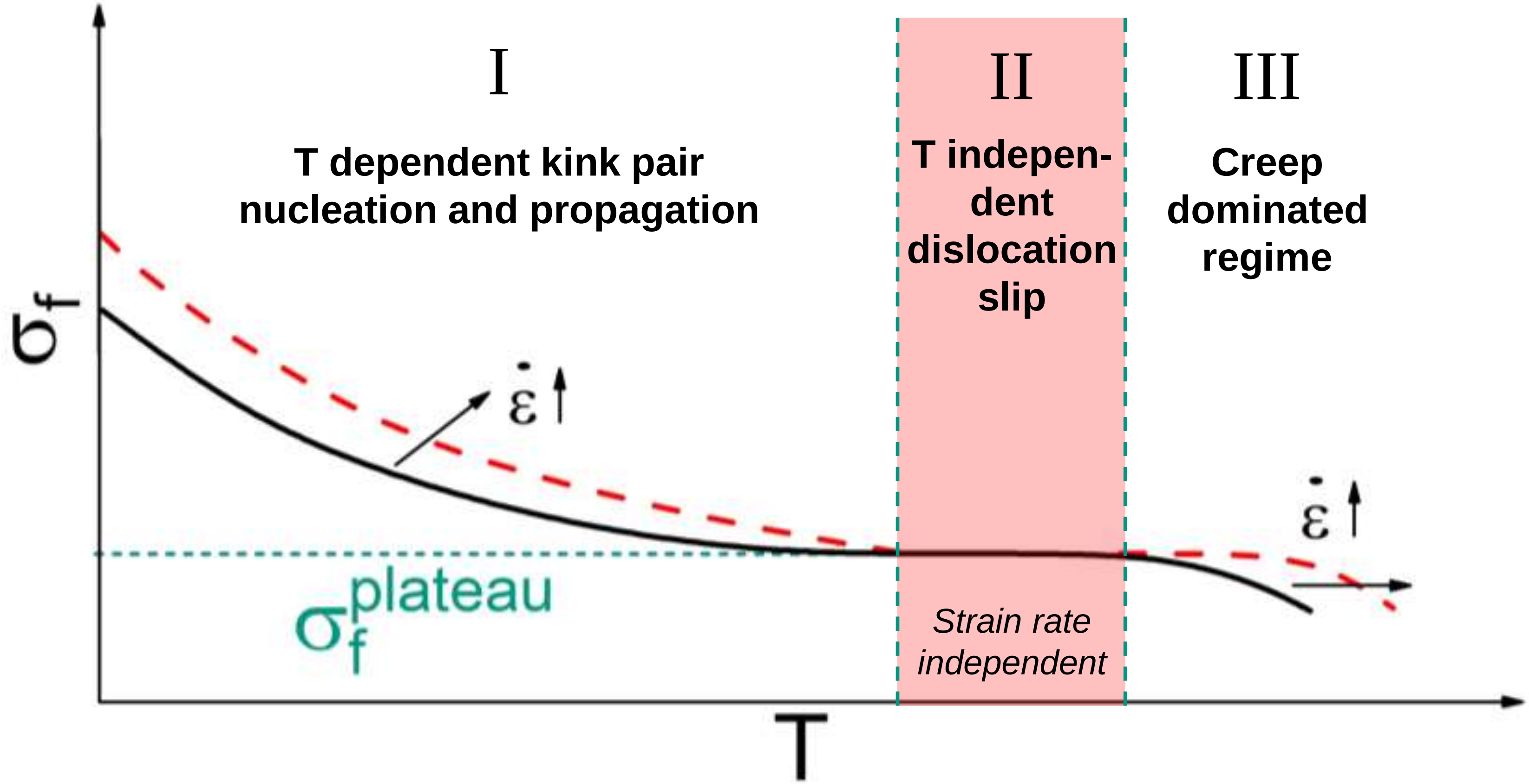
$\delta \leftrightarrow \mu H^{RT}$



- Asymmetric trend of δ
- Microhardness at RT μH^{RT}
- μH^{RT} in good accordance with δ

➡ Contribution of T dependency of mechanical properties in bcc alloys not considered, so far

T dependency of mechanical properties

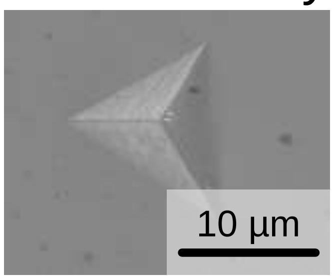


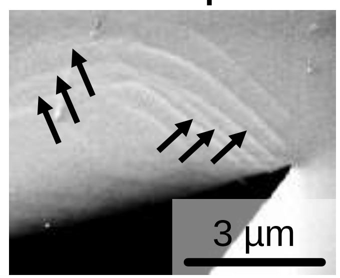
- Section II: Lattice – dislocation interactions are revealed
- Responsible mechanism regarding solid solution strengthening

➡ Determining T-range of athermal plateau properties $\sigma_f^{plateau}$

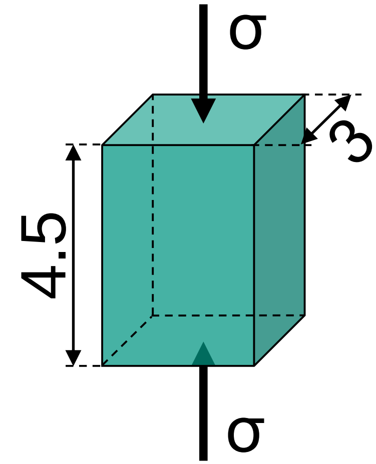
T dependency of mechanical properties

- Alloys: NbMoCrTiAl, MoCrTiAl, NbMoTiAl
- 400 °C – 1200 °C
  - Compression tests → T dependent flow stress σ_f
- RT - 400 °C
  - Lack of ductility on macroscopic scale



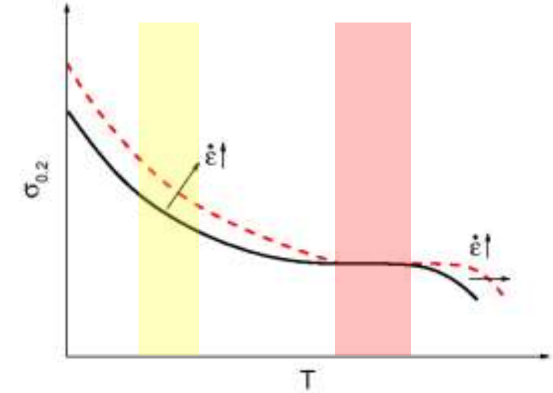


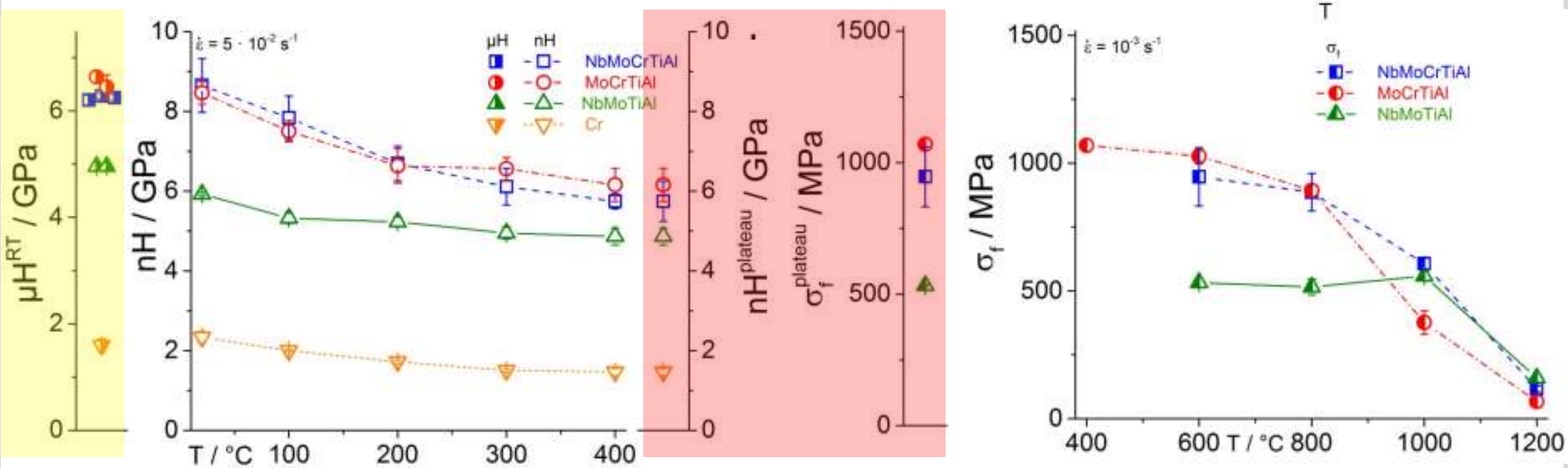
  - Nanoindentation → T dependent nanohardness nH



→ Determination of $nH^{plateau}$ / $\sigma_f^{plateau}$

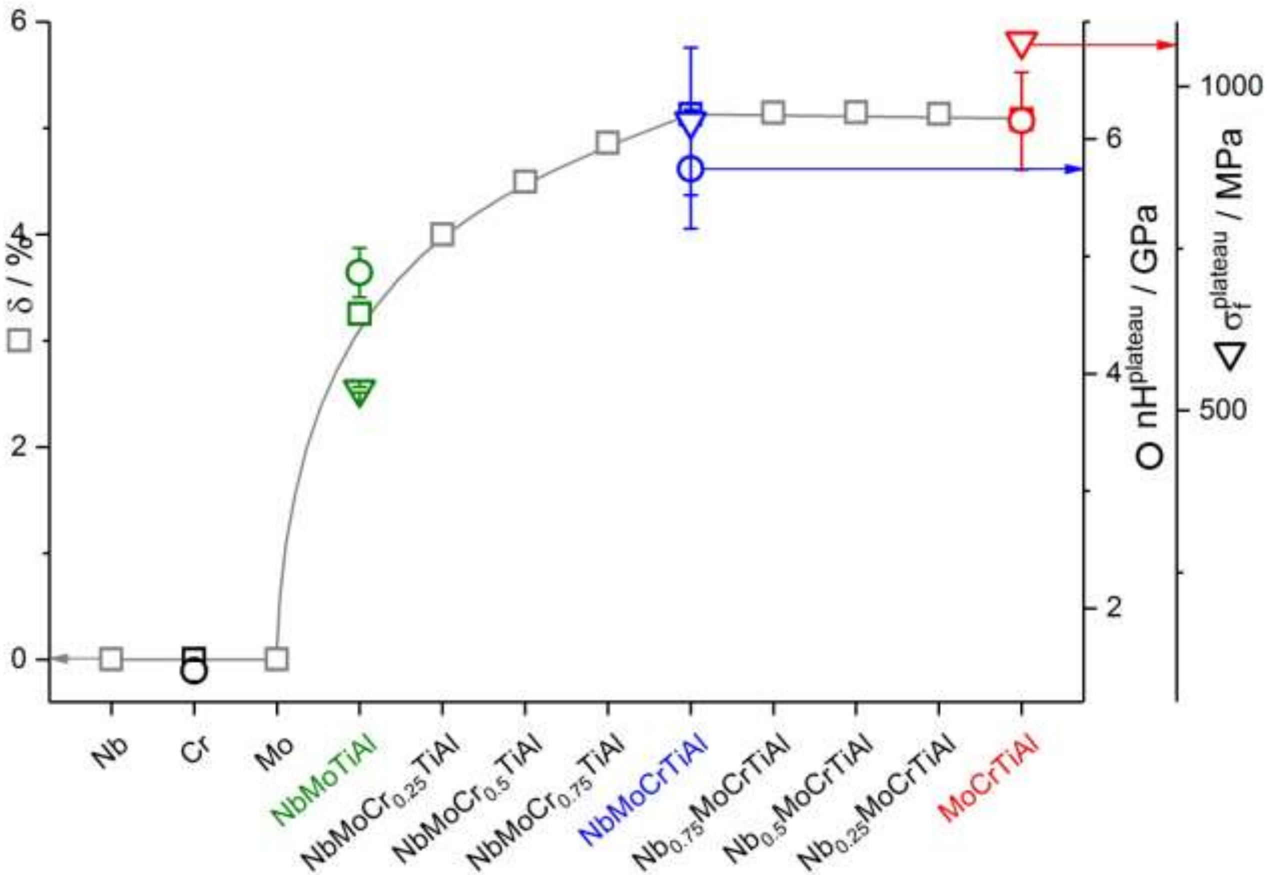
T dependency of mechanical properties





- RT – 400 °C: Varying increase of mechanical properties of respective alloys
- 400 °C – 600 °C: $nH^{plateau}$ / $\sigma_f^{plateau}$

$\delta \leftrightarrow nH^{plateau}$ $\sigma^{plateau}$



Scattering: varying contributions of…

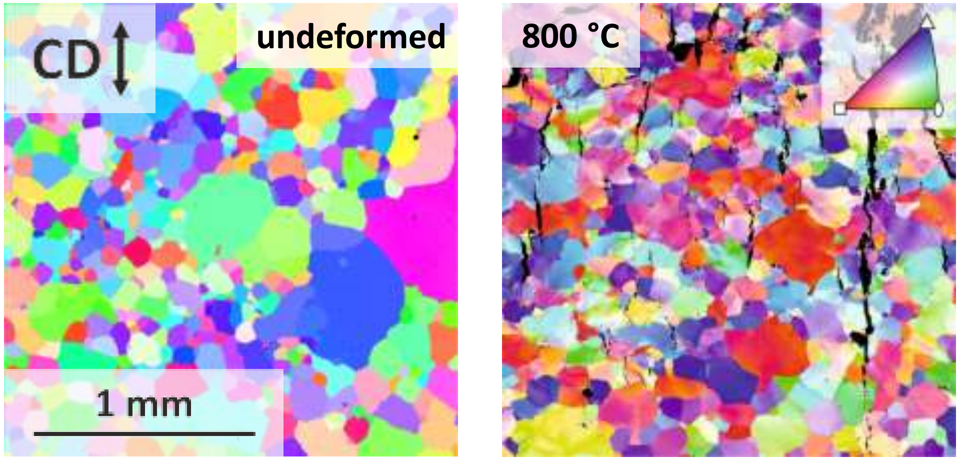
- Short range ordering
- Work hardening
- Shear modulus

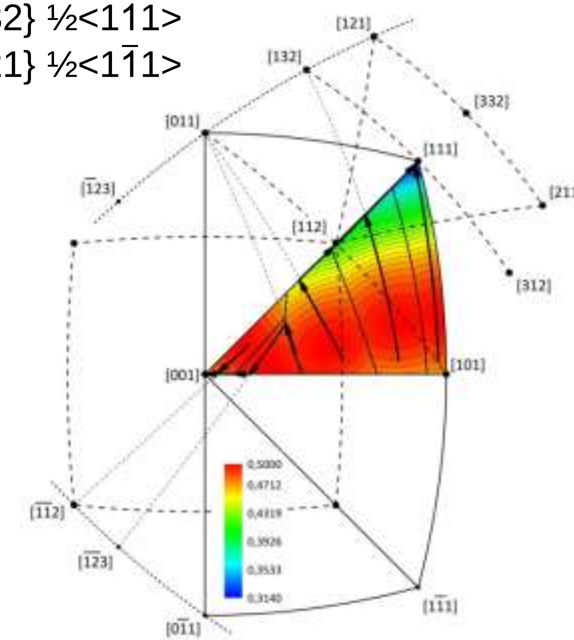
…to respective alloys

➡ δ tends to correlate with athermal properties $nH^{plateau}$ / $\sigma_f^{plateau}$

Deformation mechanism by EBSD

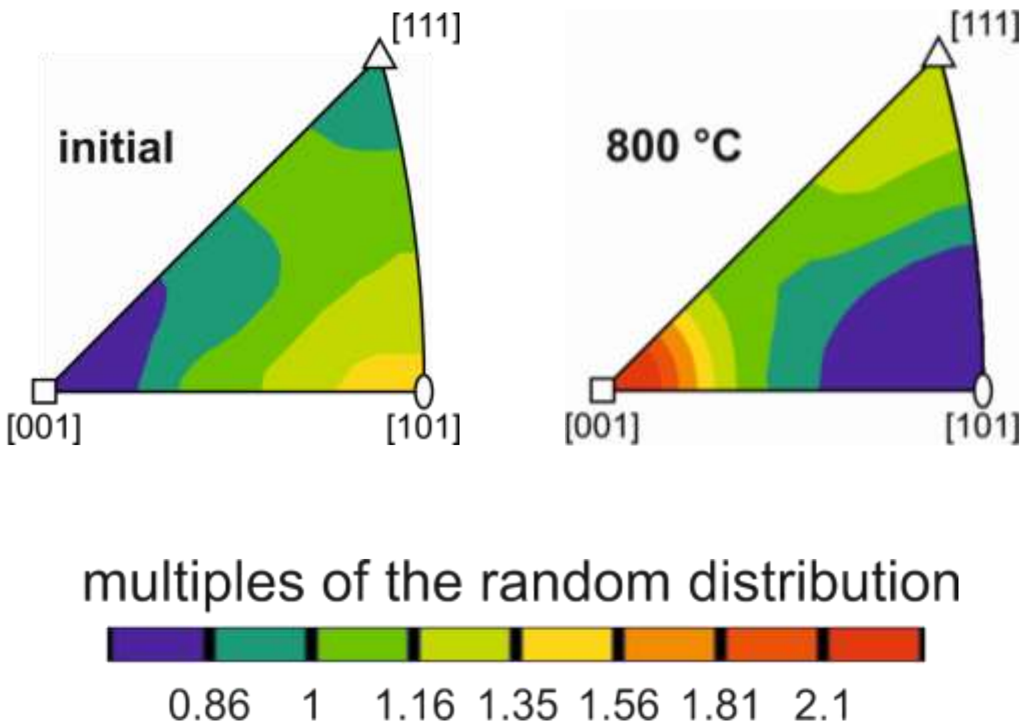
BCC
„pencil glide“
{011} ½<$1\bar{1}1$>
{132} ½<$1\bar{1}1$>
{121} ½<$1\bar{1}1$>





- EBSD maps show orientation of the grains
- Undeformed: Random distribution of grain orientations
- Deformed: Amount of orientation with [001] and [111] crystallographic axes parallel to the compression direction increased

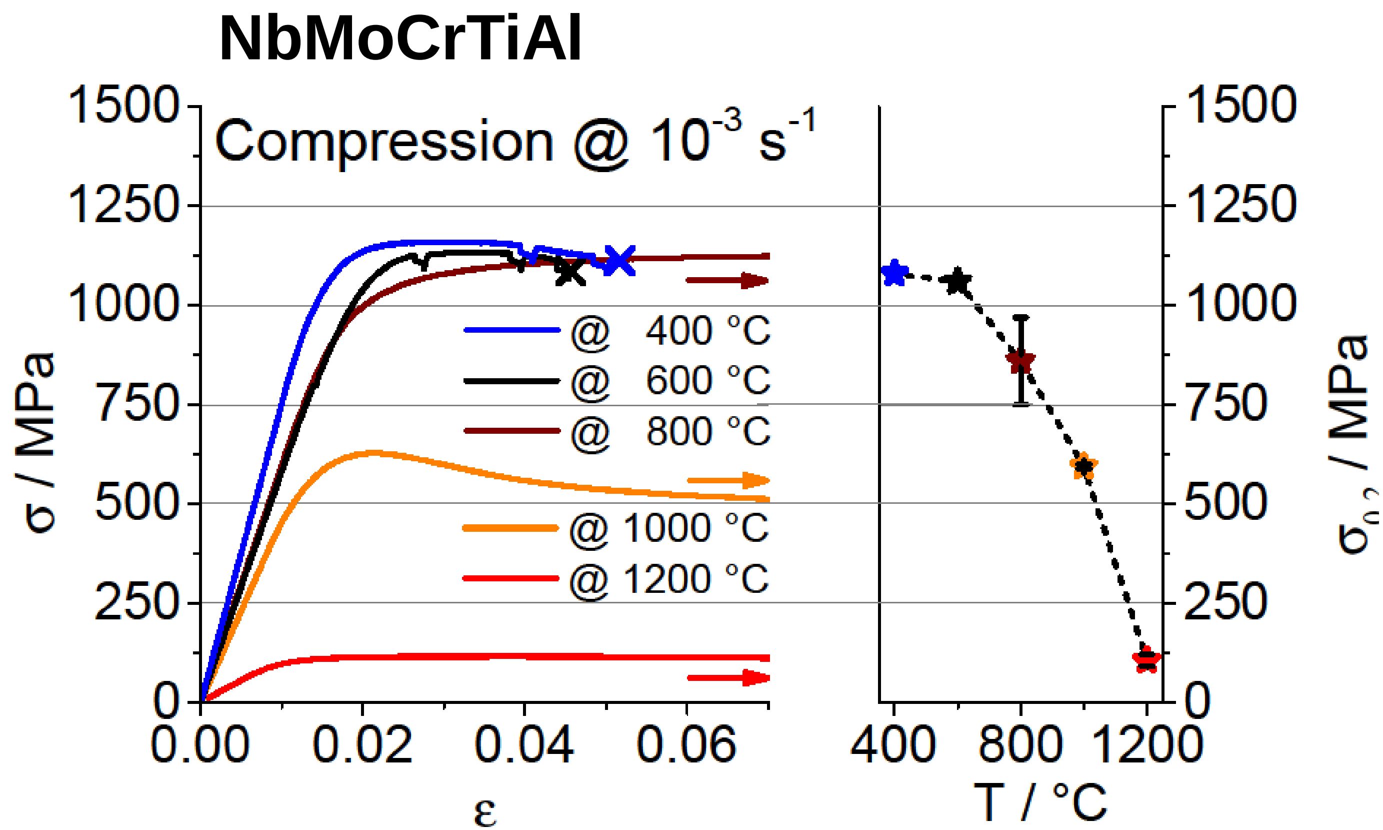
Deformation behavior



- EBSD: Inverse pole figures
  - Increase of orientation density at [001] and [111] crystallographic axes parallel to compression direction
  - Deformation by dislocation slip with <111> slip direction is observed

➡ EBSD: Dislocation mediated plasticity within solid solution

Deformation behavior



- No plastic deformation on macroscopic scale below 400 °C
- Temperature-dependent strength

➡ Macroscopic plasticity between 400 °C and 1200 °C