



Interstitial Doping in High-entropy Alloys



Yan Ma, Chang Liu, and Dierk Raabe

Simulation support: Fritz Körmann

Acknowledgement: Zhiming Li, Wenjun Lu, Zhifeng Lei, Paraskevas Kontis

SPP2006, 2nd phase kick-off meeting, 13.04.2021

Interstitial doping in high-entropy alloys



1. Interstitials in FCC high-entropy alloys

- Tuning deformation mechanisms through alloy design
- Design of thermally stable bulk nanostructured iHEA

2. Interstitials in BCC high-entropy alloys

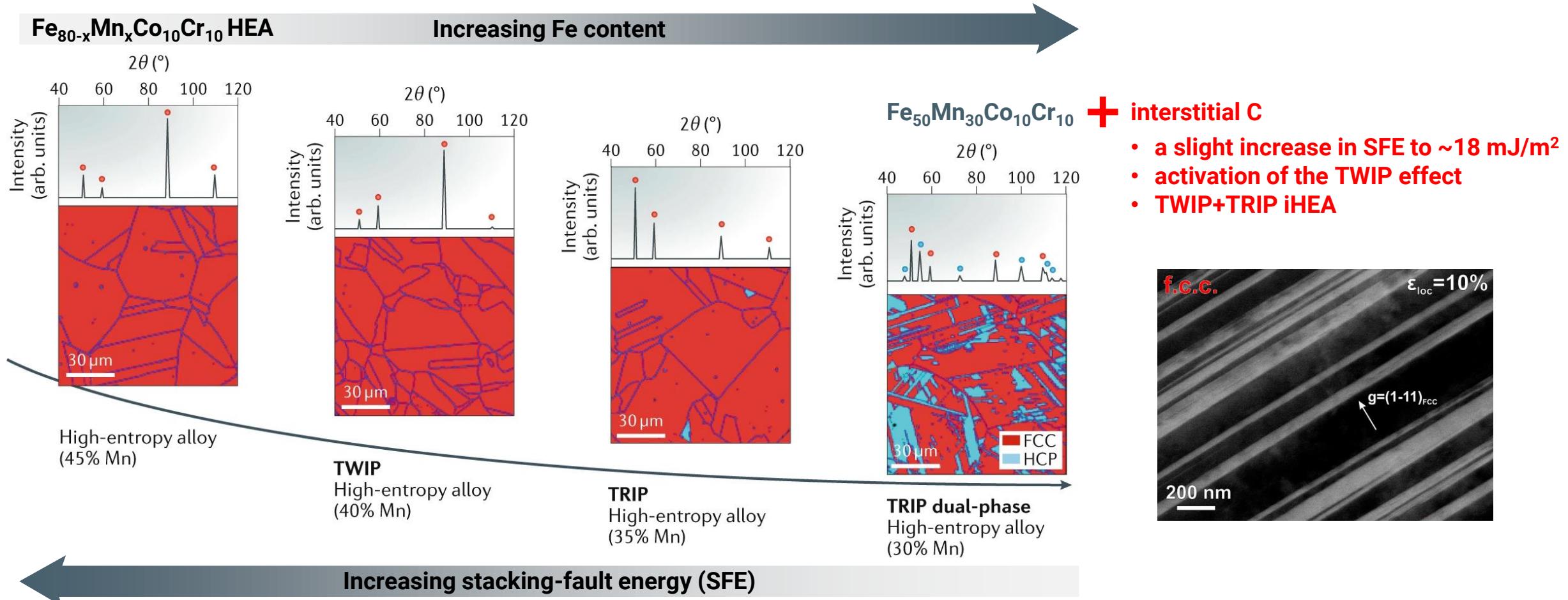
- Tuning deformation mechanisms via ordered oxygen complexes

3. Summary

From HEA to iHEA



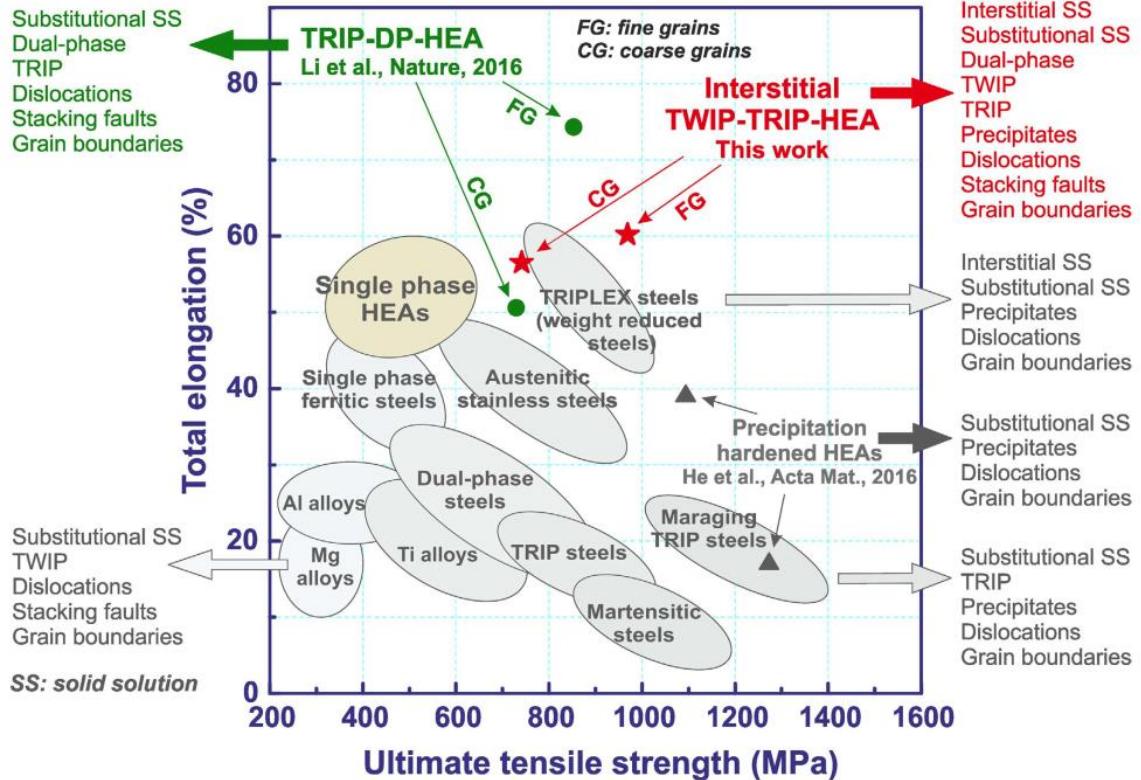
Tuning deformation mechanisms through alloy design (SFE-guided alloying concept)





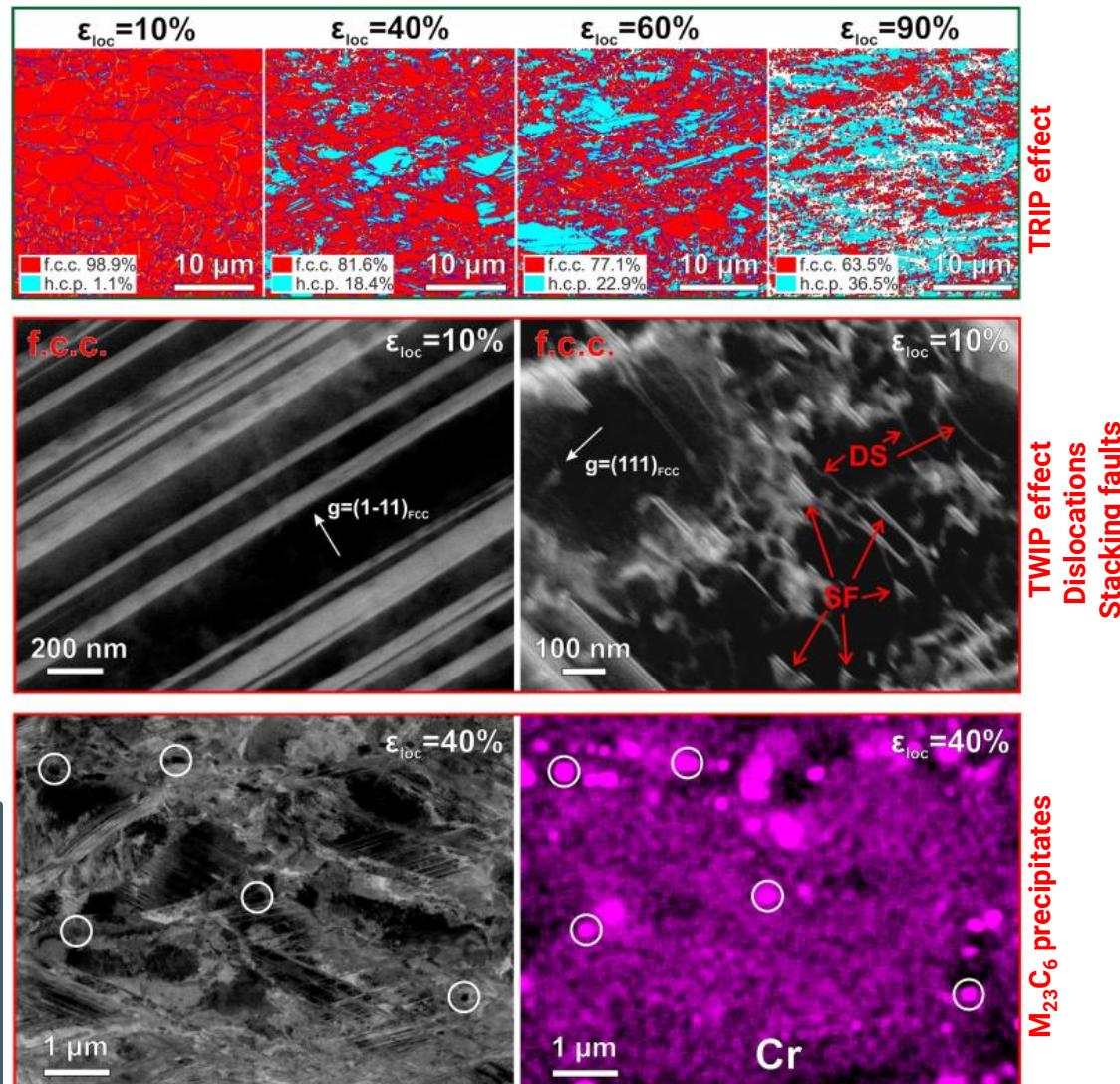
Interstitials in FCC HEA

Tuning deformation mechanisms through alloy design



- **Carbon addition** effectively tunes the stability of the metastable FCC matrix.
- SFE is $\sim 18 \text{ mJ/m}^2$, triggering both **TRIP and TWIP effects**.
- **All strengthening mechanisms** are realized in one HEA.

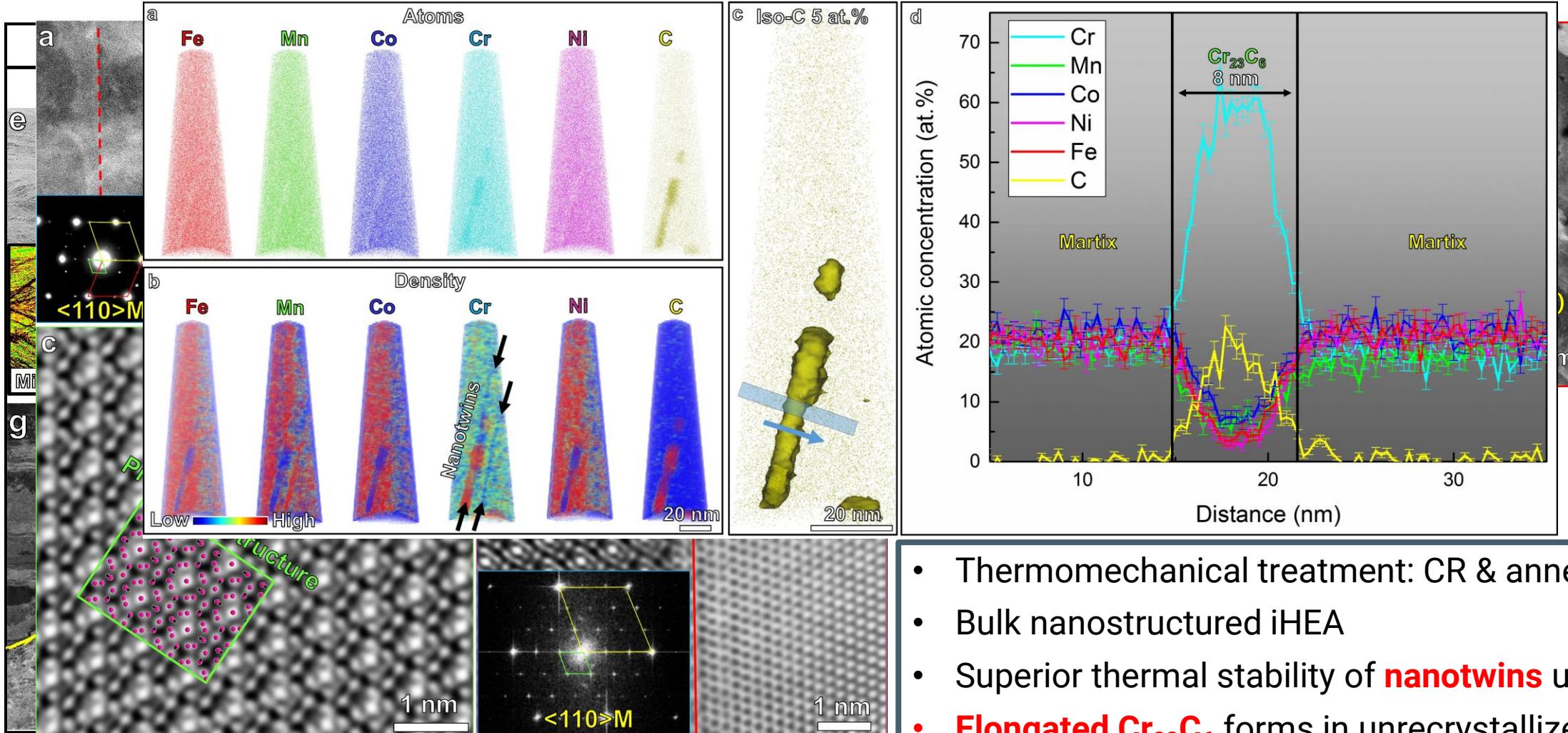
$\text{Fe}_{49.5}\text{Mn}_{30}\text{Co}_{10}\text{Cr}_{10}\text{C}_{0.5}$, CR&RX, GS=4 μm





Interstitials in FCC HEA

Design of thermally stable bulk nanostructured iHEA

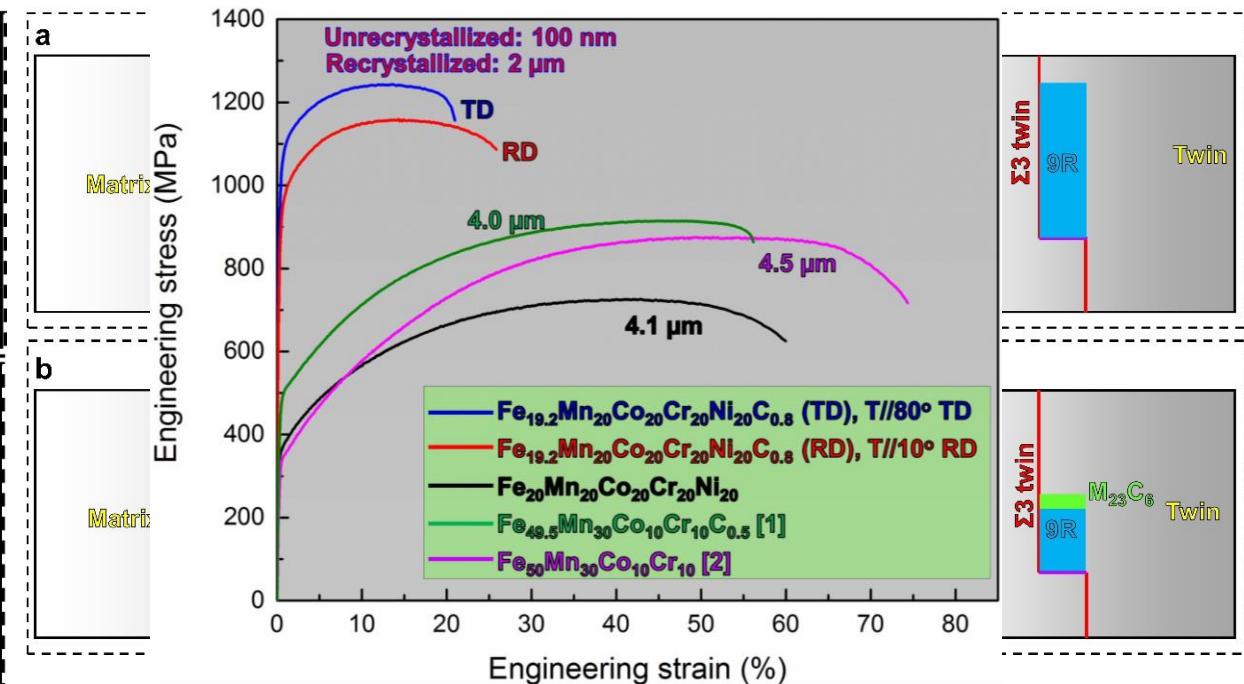
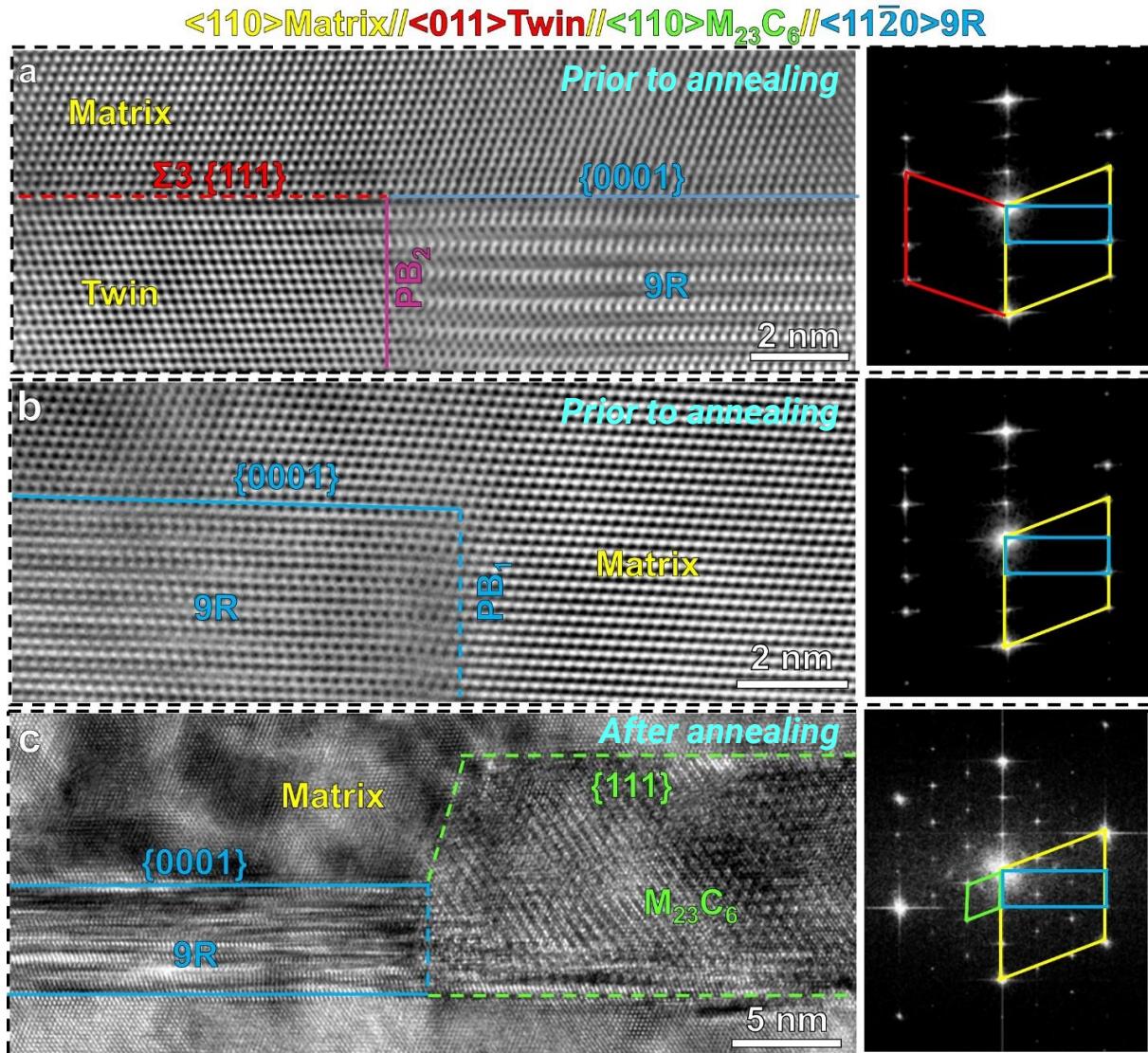


- Thermomechanical treatment: CR & annealing
- Bulk nanostructured iHEA
- Superior thermal stability of **nanotwins** up to 900°C
- **Elongated Cr_{23}C_6** forms in unrecrystallized region.
- Nano-carbides retards mobility of twin boundary.



Interstitials in FCC HEA

Interfacial nanophase design enables thermally stable nanotwins

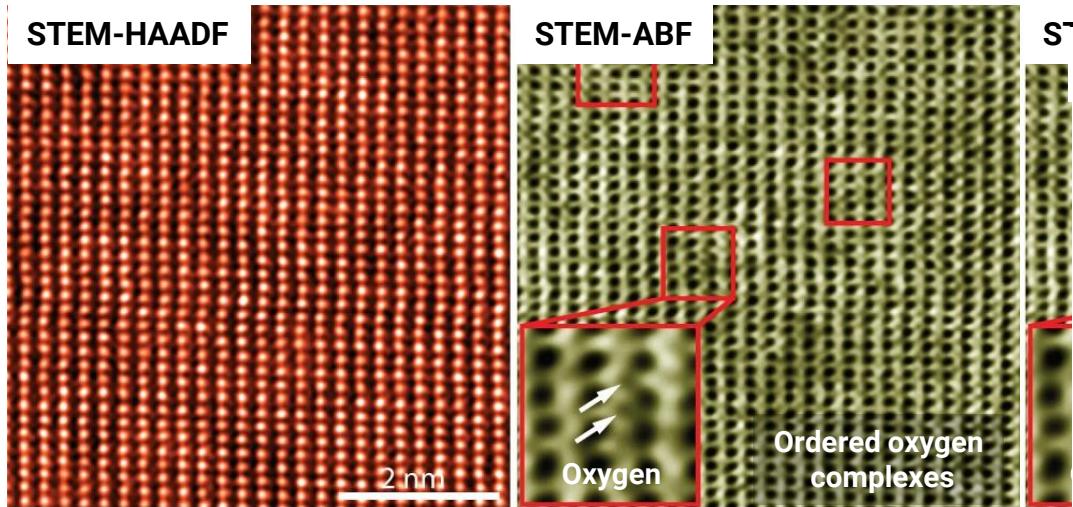


- Co-segregation of Cr and C to **9R structures**
- Formation of elongated nano-carbides at **ICT Σ3 boundary** and grow along {0001} habit plane of 9R
- **Nano-carbides retards de-twinning process**, resulting in superior high-strength.

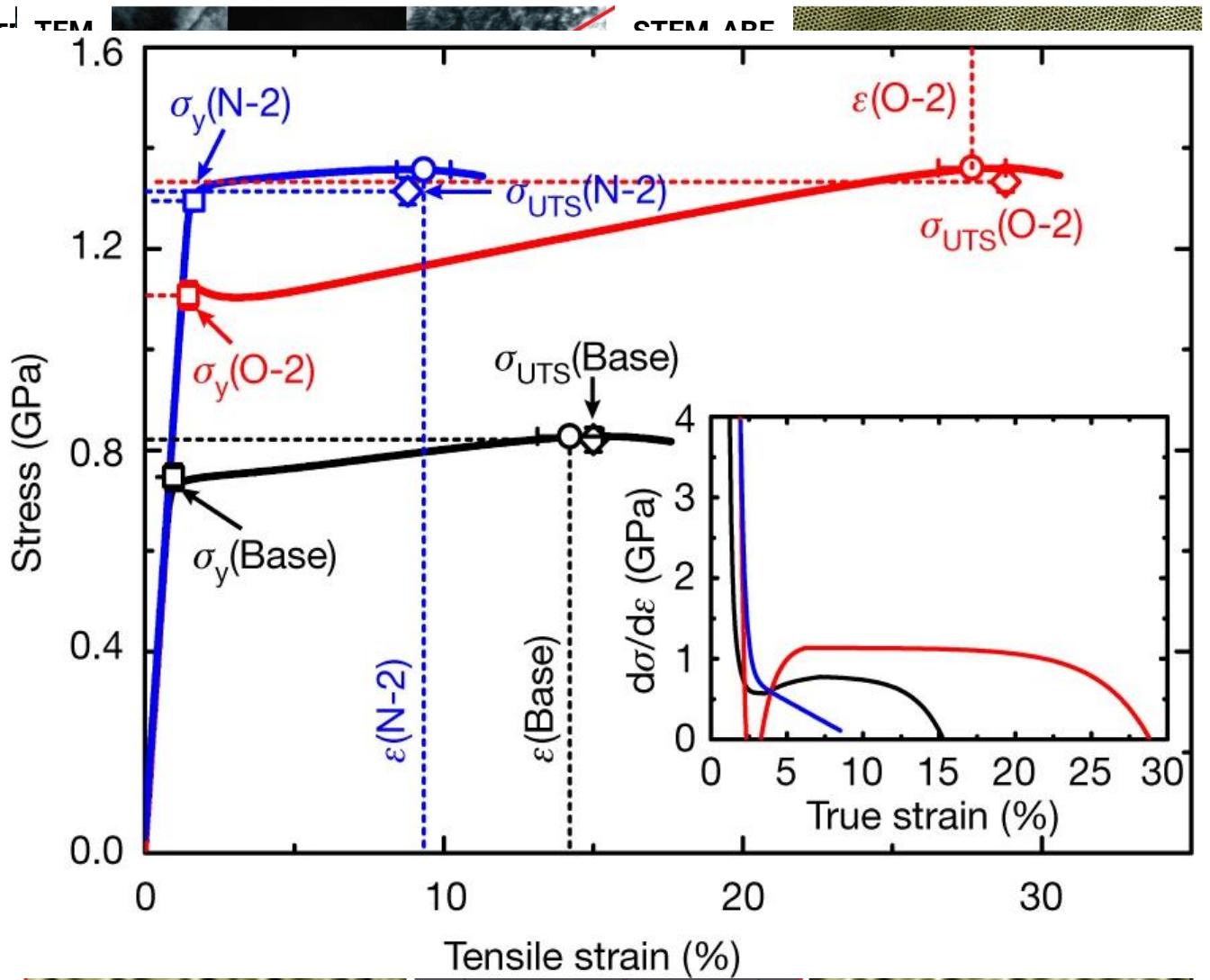
Interstitials in BCC HEA



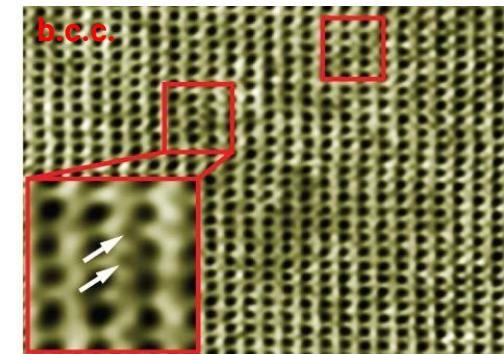
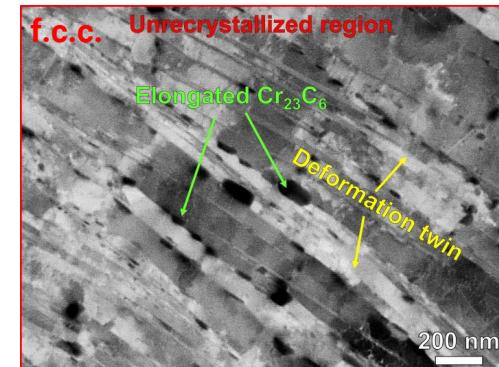
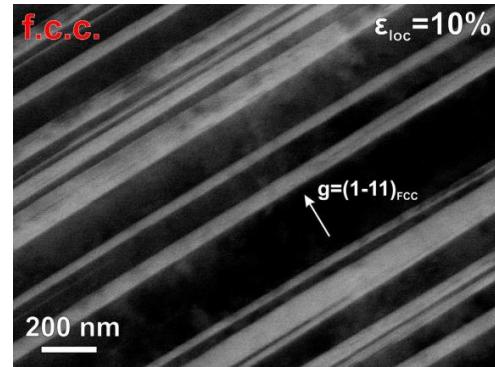
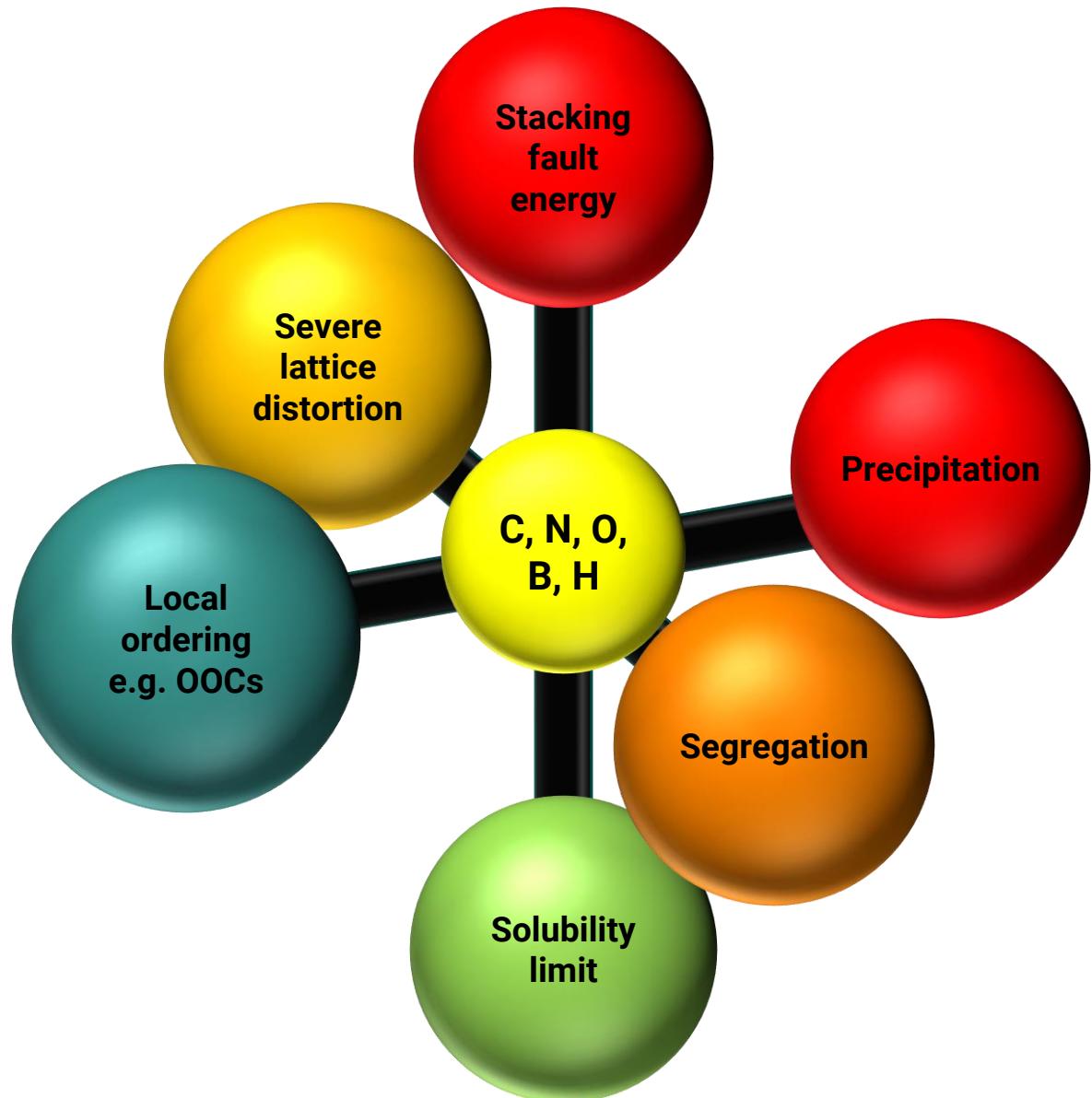
Tuning deformation mechanism via ordered oxygen complexes (OOCs) in $(\text{TiZrHfNb})_{98}\text{O}_2$ HEA



- O prefers interstitial sites in **light-atom-rich (i.e. Ti and Zr) lattices** and form OOCs with size of 1-3 nm and space of 2-4 nm.
- OOCs effectively pin dislocations, promoting **cross slip and massive dislocation multiplication**.
- Homogeneous deformation and high strain hardening result in high strength and superior ductility.



Fascinating impacts of interstitials on HEAs



b.c.c.
TiZrNbHfTa + B
Grain refinement
GB segregation
Hydrogen embrittlement

b.c.c.
TiZrNb + O
Solubility limit
SRO/OOCs
Deformation modes



MAX-PLANCK-INSTITUT
FÜR EISENFORSCHUNG GmbH

Thank you for your kind attention!



Funded by



Deutsche
Forschungsgemeinschaft
German Research Foundation

Contact: Dr.-Ing. Yan Ma

y.ma@mpie.de