Stability and interstitial doping in high-entropy alloys from ab initio – Project: “MULTI-TRIP CCAs”

Ab initio calculations: Yuji Ikeda*, Fritz Körmann

Experimental counterpart: Yan Ma, Chang Liu, and Dierk Raabe

April 2021 – SPP kick-off meeting

(*) now at University of Stuttgart

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Overview

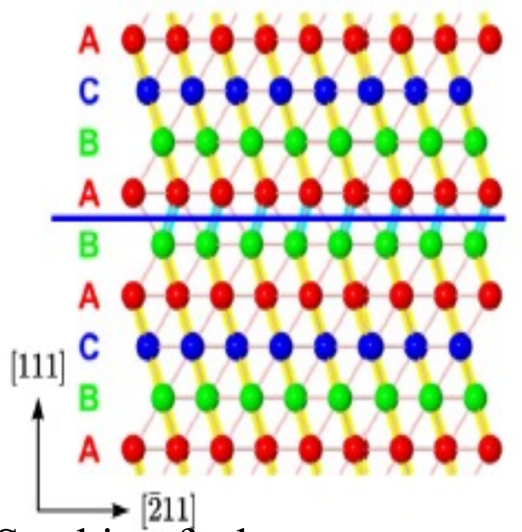
1. **Main focus in first SPP round**

2. **Some applications FCC alloys**

3. **Some applications BCC alloys**

1st SPP: Transformation-induced-plasticity-HEAs <-> SFEs

- **Main part: *Ab initio* simulations → Stacking fault energies**



Stacking faults

Varying composition

Impact of interstitials (C, N, …)

Impact of finite-temperature contributions

FCC Alloys (mainly Cantor-family)

Previous investigations

- **Stacking fault energies → screening for TRIP-HEAs [1]**
- **Impact interstitials on SFE** (C, N) **SFE [2]**
- Lattice distortions [3] and short-range order (VCoNi)

Next steps

- **MULTI-TRIP CCAs** : dual phase HEAs with fcc->hcp + hcp->fcc transformation
  (computing generalized stacking fault energy surface, …)
- Continue SFEs and interstitial calculations
- (short-range order and coupling to SFEs)

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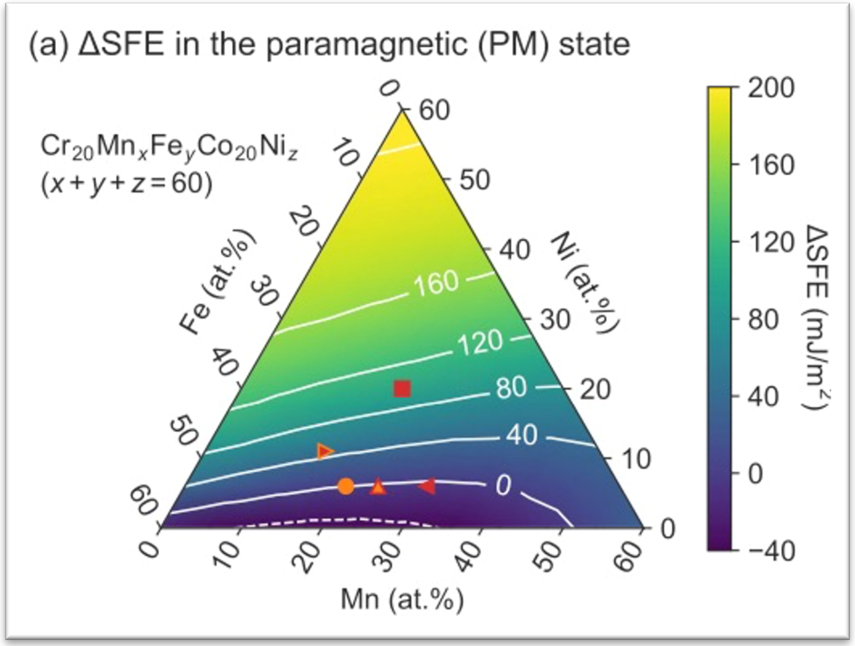

[1] Wu, Li, Rao, Ikeda, Körmann, Dutta, Neugebauer, Raabe, Phys. Rev. Mat. 4, 033601 (2020)

Ab initio SFE maps → new TRIP-HEAs

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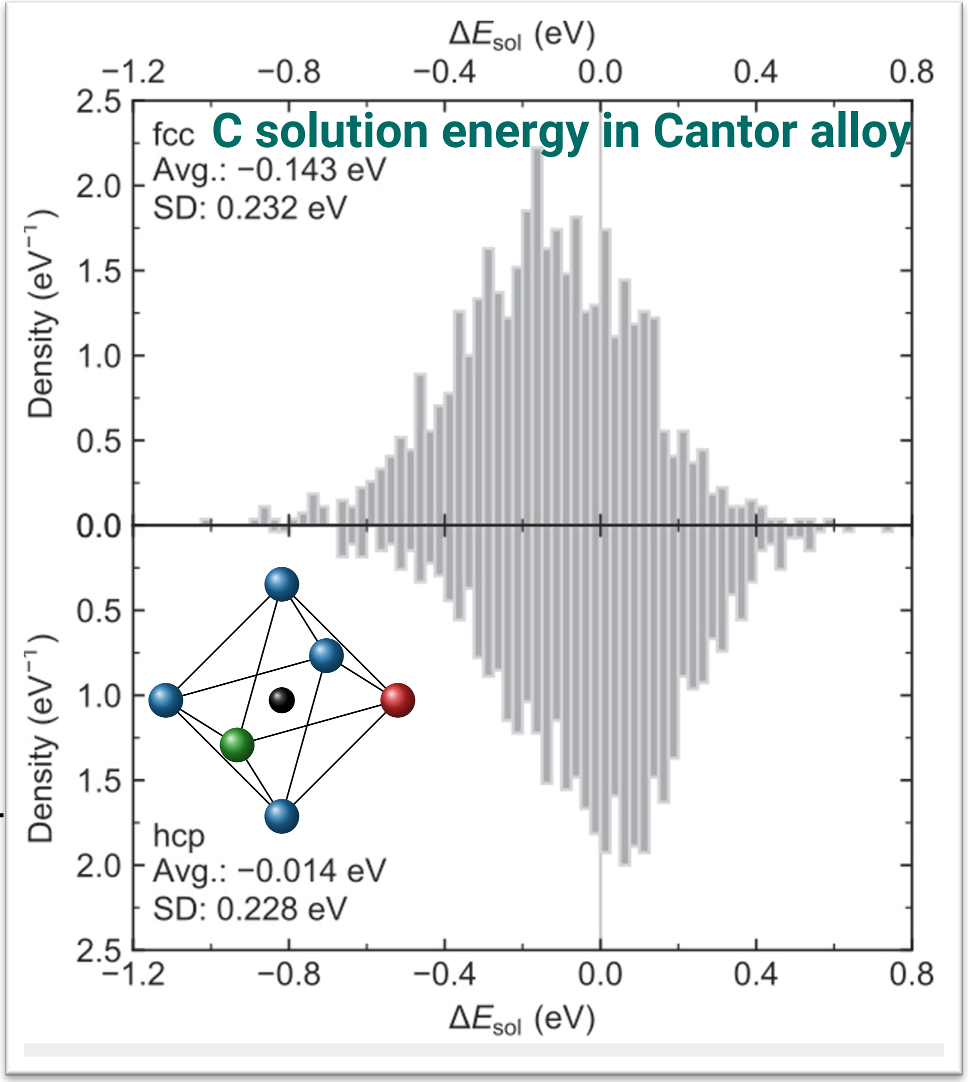

[2] Ikeda, Tanaka, Neugebauer, Körmann, Phys. Rev. Mat. 3, 113603 (2019)
C increase SFE for Cantor, but decreases for Al0.5CoFeMnNi [Kies, Hallstedt, Körmann, Haase, et al., Scripta Mat. 178, 366 (2020)].

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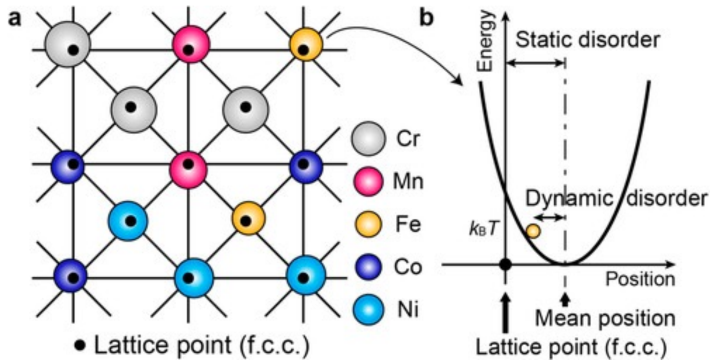
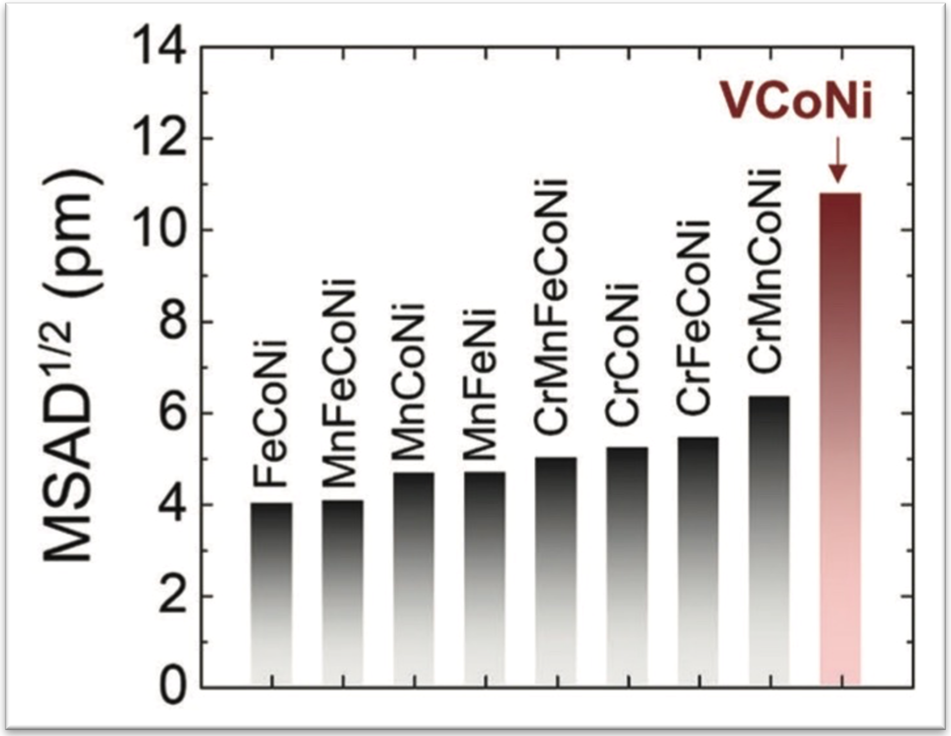
Lattice distortions from DFT



Okamoto et al. (2016)



[3]Sohn, Körmann, Raabe, *et al.*, Adv. Mat. 31, 1807142 (2019)

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COMMUNICATION

ADVANCED MATERIALS

Alloys

www.advmat.de

Bidirectional Transformation Enables Hierarchical Nanolaminate Dual-Phase High-Entropy Alloys

*Wenjun Lu, Christian H. Liebscher, Gerhard Dehm, Dierk Raabe, and Zhiming Li**

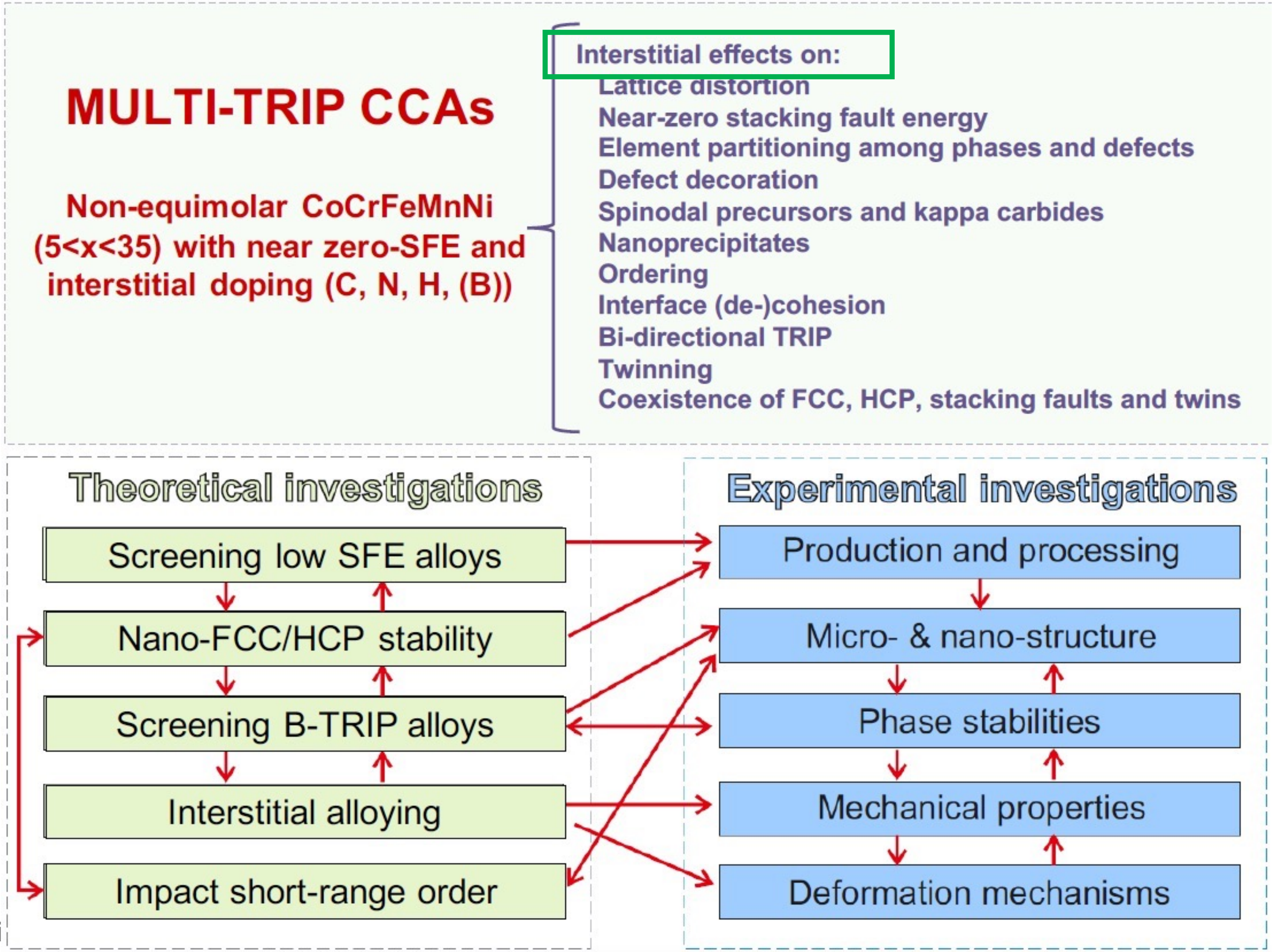
FCC Fe50Mn30Co10Cr10

"This is achieved by triggering both, dynamic forward transformation from a faced-centered-cubic matrix into a hexagonal-close-packed nanolaminate structure and the dynamic reverse transformation from ε into γ. This new mechanism is referred to as the "**bidirectional transformation induced plasticity**" (B-TRIP) effect, which is enabled through a near-zero yet positive stacking fault energy of γ."

→Can we exploit and screen for B-TRIP HEAs?

Lu, Liebscher, Dehm, Raabe, Li, Adv. Mat. 30, 1804727 (2018)

MULTI-TRIP CCAs – Project Overview



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BCC Alloys

Previous investigations

- Phase stability + short-range order,
  e.g., BCC NbMoTaW [4], AlNbTiV [5],
- omega-BCC-HCP stability in Ti-HEAs

Next steps

- Continue short-range order / stability, e.g.,
  B2 phase in Al-containing HEAs

BCC Alloys

DFT → on-lattice machine learning potentials → Monte Carlo simulations

Bcc AlNbTiV → B2 ordering (and sublattice disorder)

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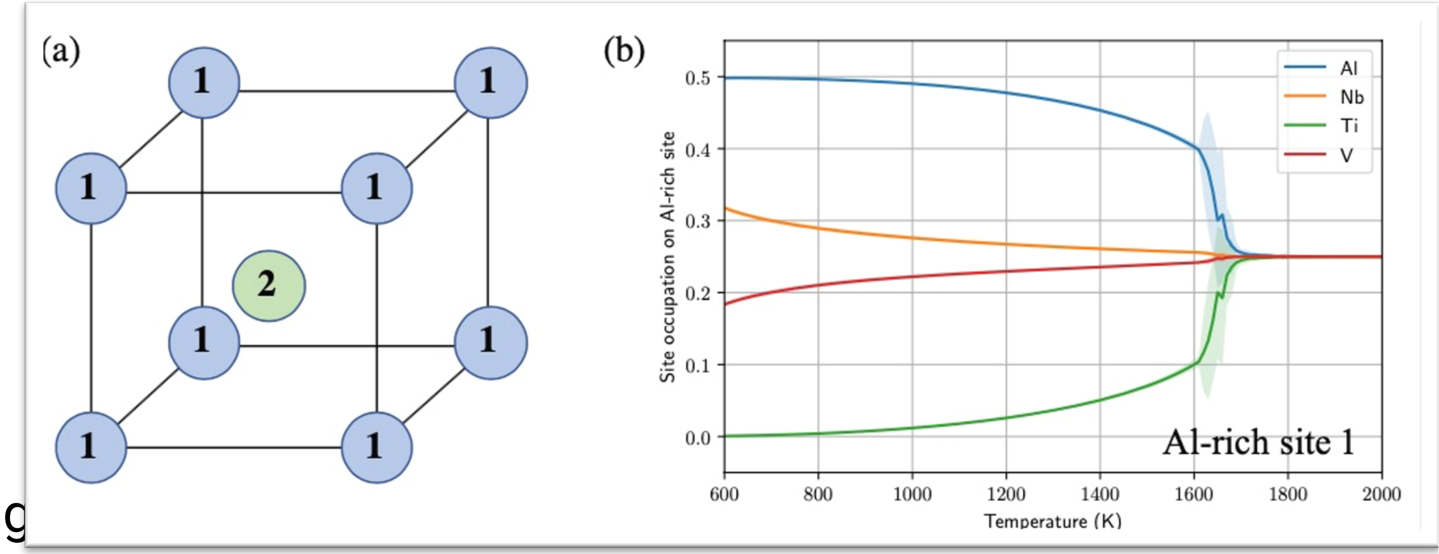
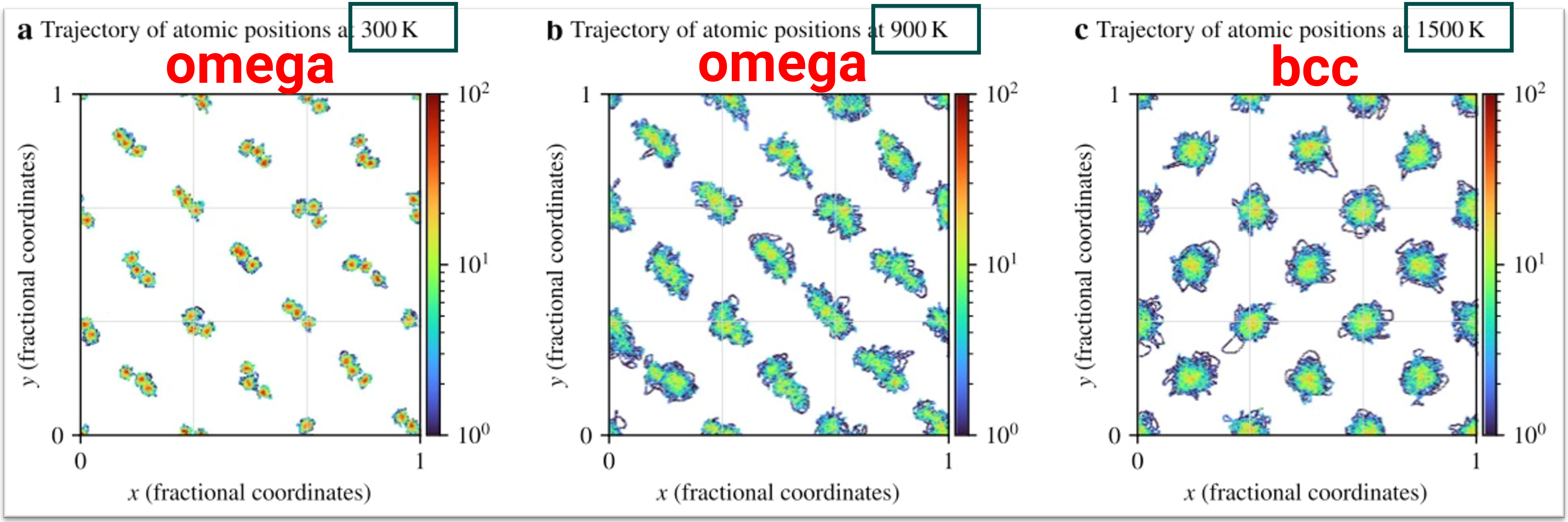


[5] Körmann et al., (under review)

BCC Alloys

Example: TiZrHf



[5] Ikeda, Gubaev, Neugebauer, Grabowski, Körmann, npj Comp Mat **34** , 1 (2021)

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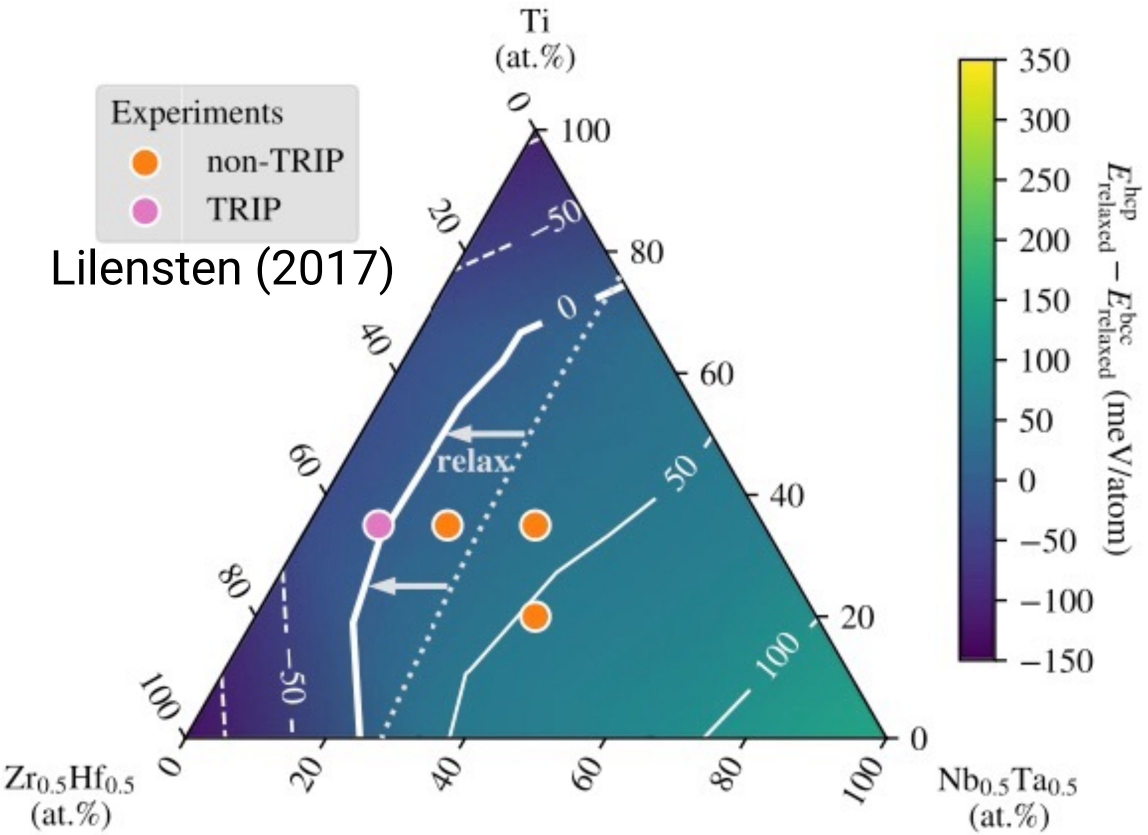
TiZrHfNbTa: BCC – HCP stability (T=0K)



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Thank you for your attention!

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