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Radiotracer studies of diffusion in multi-principal element alloys

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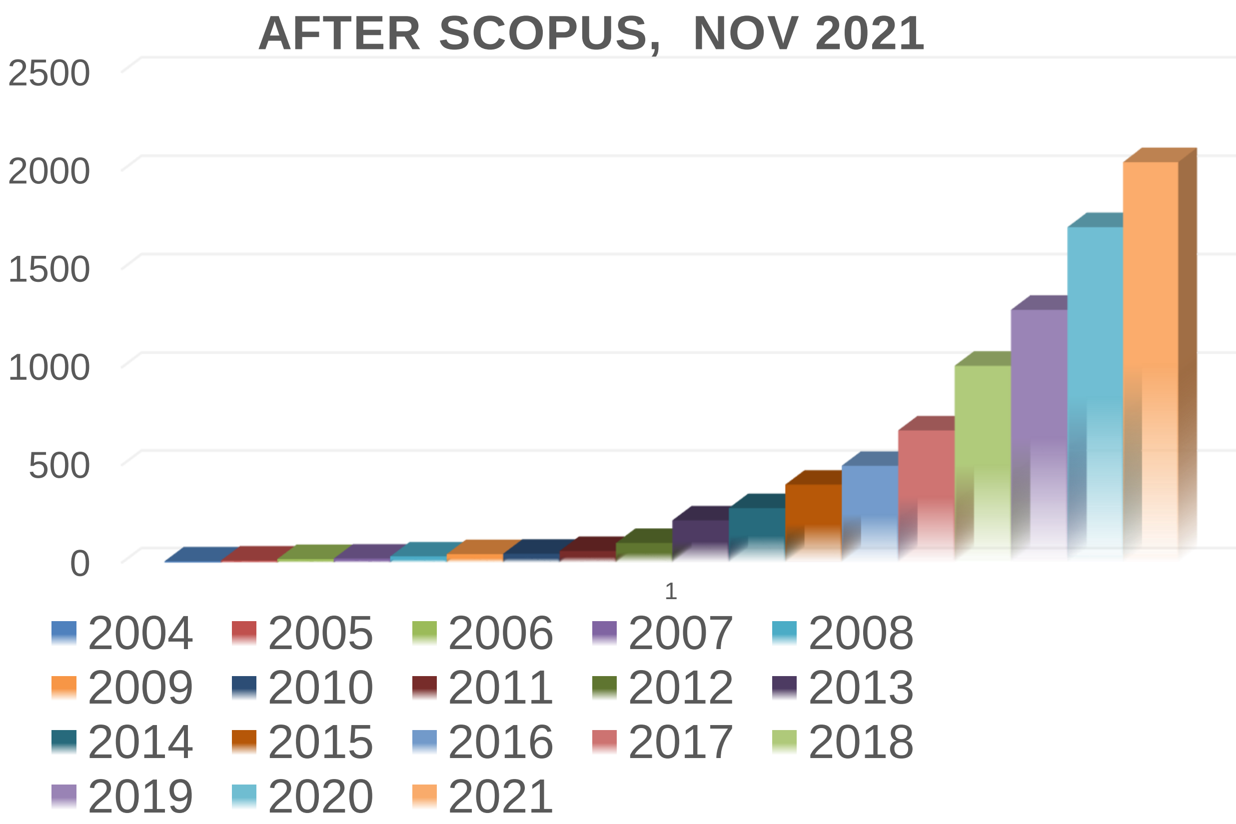
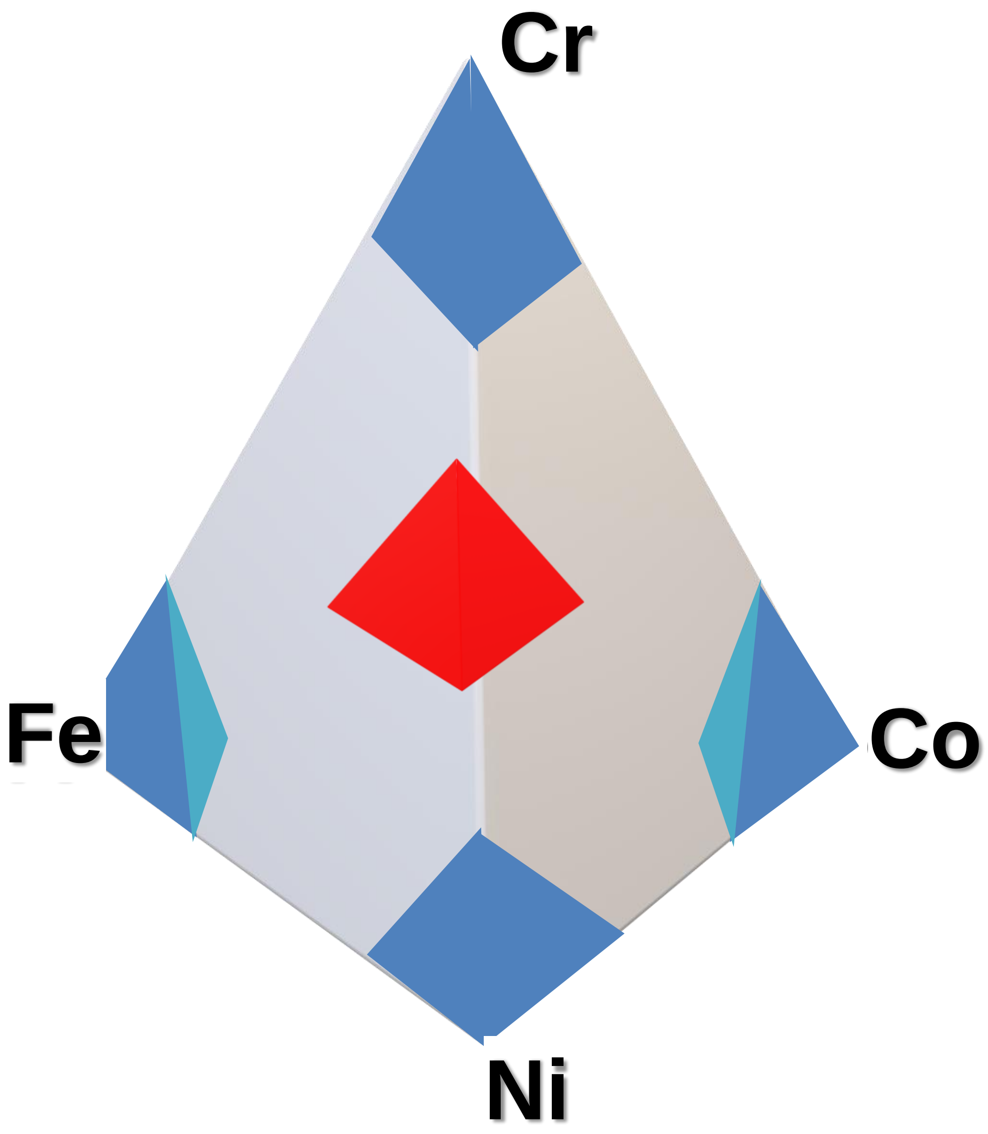
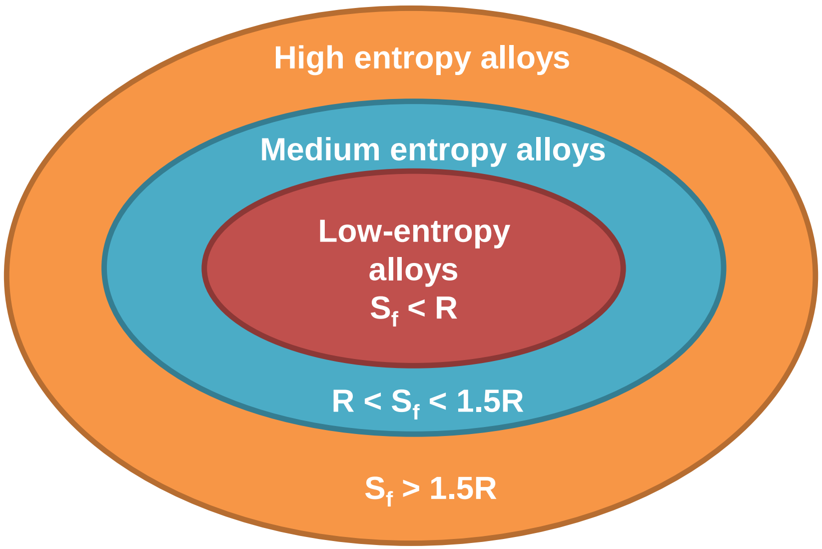
Number of publications devoted to HEAs

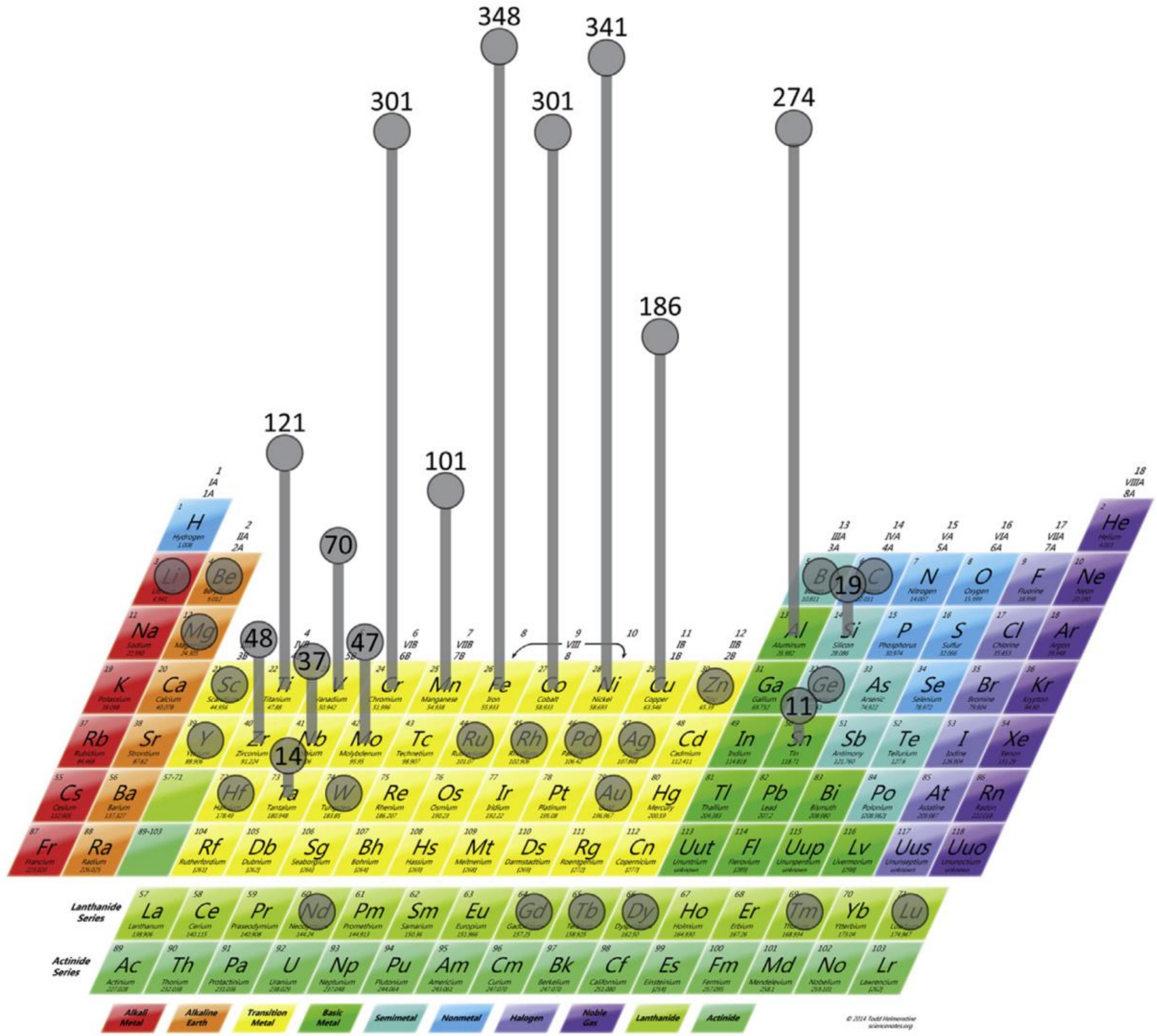


127 publications: diffusion (title) + HEA (topic)
697 publications: diffusion + HEA (topic)

Why multi-principal element (high-entropy) alloys?







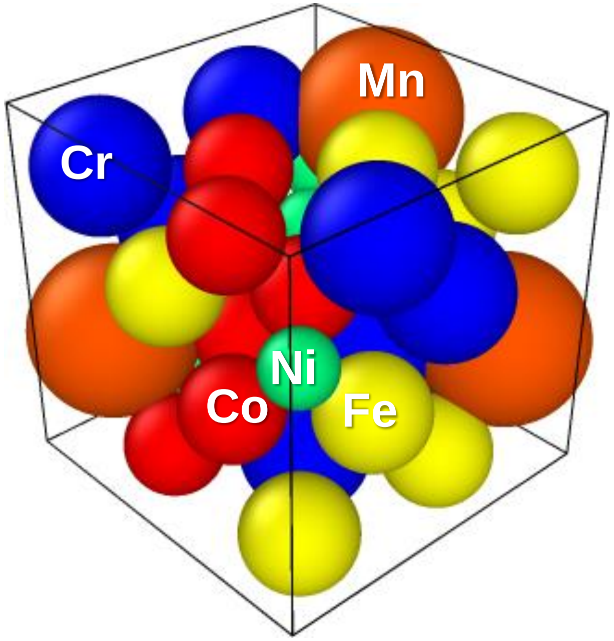
D.B. Miracle, O.N. Senkov / Acta Materialia 122 (2017) 448–511

High-Entropy Alloys

Main principles of HEAs:

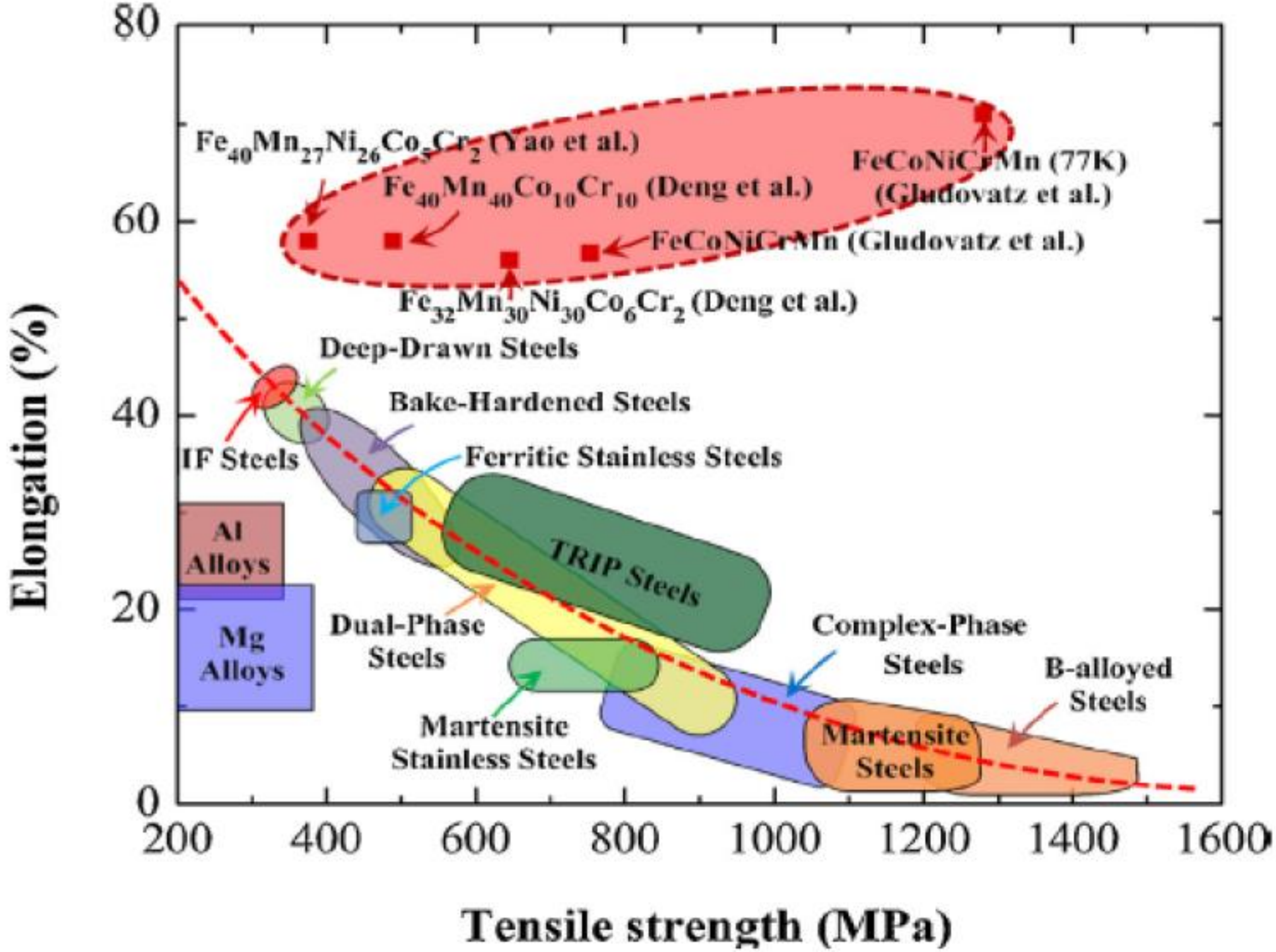
- **high configurational entropy** (five and more components in equiatomic proportion)
- **sluggish diffusion**
- **severe lattice distortion**
- **cocktail effect**

Yeh (2004)



CoCrFeMnNi Cantor alloy

Mechanical properties of HEAs



After Miracle & Senkov, Acta Mater (2017)

Content of the talk

Tracer diffusion in homogeneous alloys:

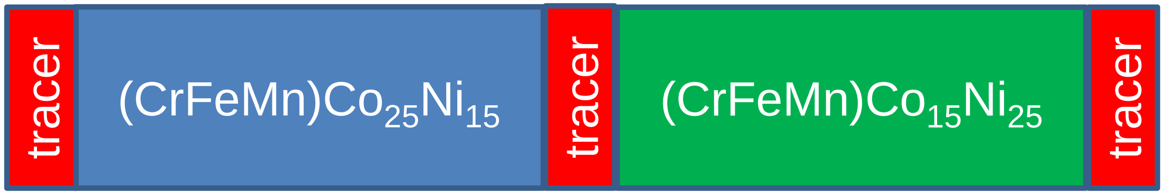
- FCC CoCrFeNi & CoCrFeMnNi — Vaidya et al JALCOM (2016); Vaidya et al, Acta Mater (2018); Gaertner et al, Scr Mater (2020)

  (poly-, single- and bi- crystals)

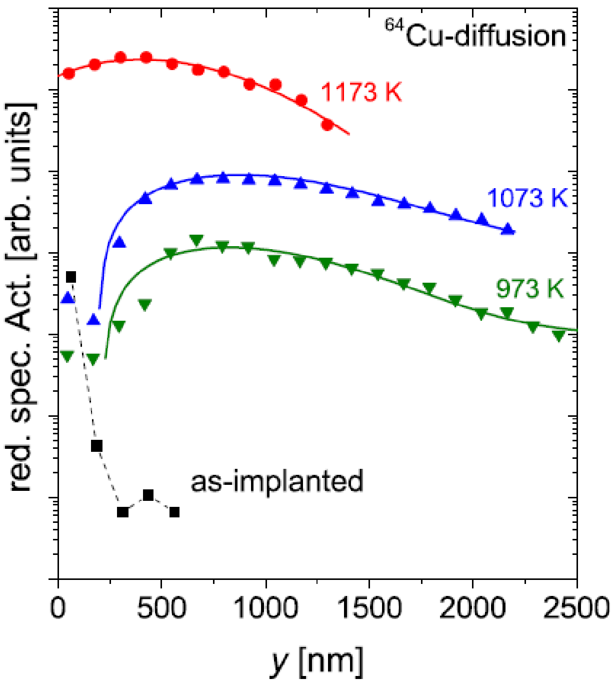
- σ-phase CoCrFeMnNi — Zhang et al, Acta Mater (2020)
- FCC $(CoCrFeMn)_{100-x}Ni_x$ — Kottke et al, Acta Mater (2020)
- FCC & BCC& B2 $Al_xCoCrFeNi$
- HCP AlScHfTiZr — Vaidya et al, Acta Mater (2020); Sen et al (2021) in preparation
- BCC HfTiZrTaNb — J.Zhang et al (2021) submitted

Tracer diffusion under concentration gradient

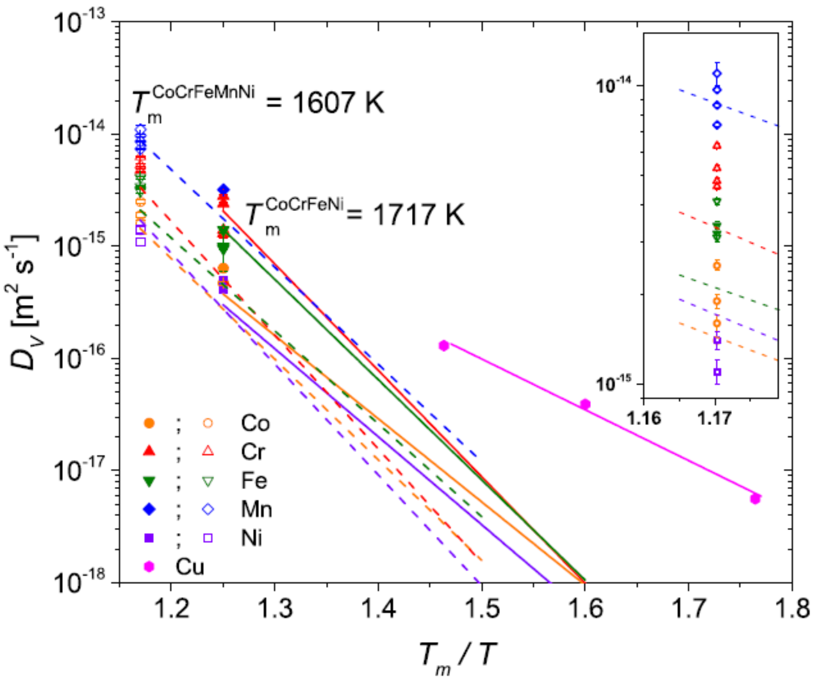
Augmented tracer-interdiffusion couple — Gaertner et al Acta Mater (2019)



FCC CoCrFeMnNi system

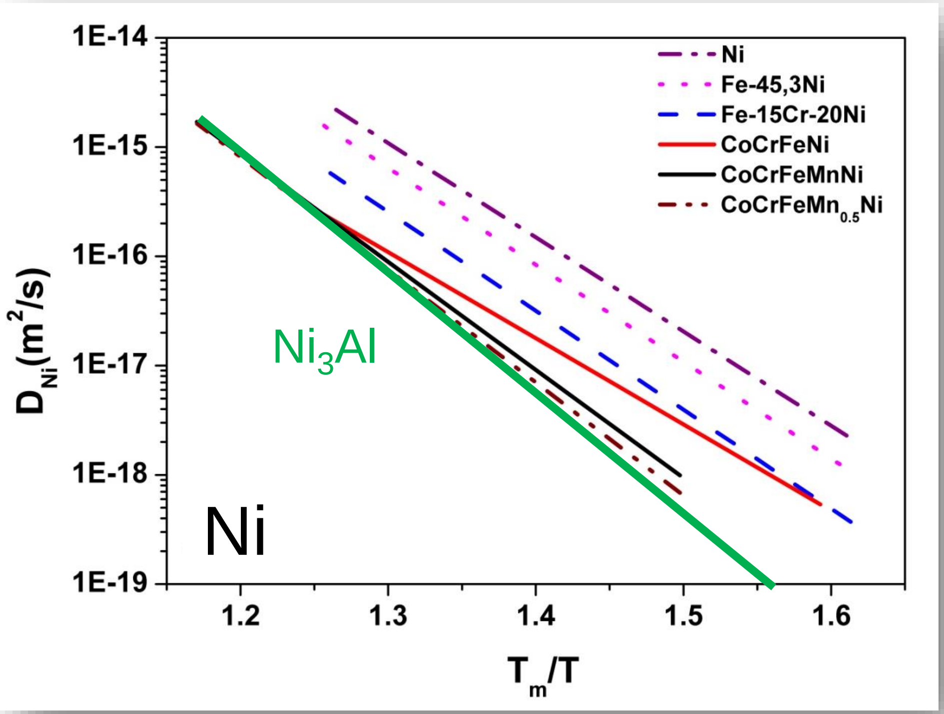


Penetration profiles measured for Cu diffusion in single crystalline CoCrFeNi using on-line Diffusion Chamber at ISOLDE



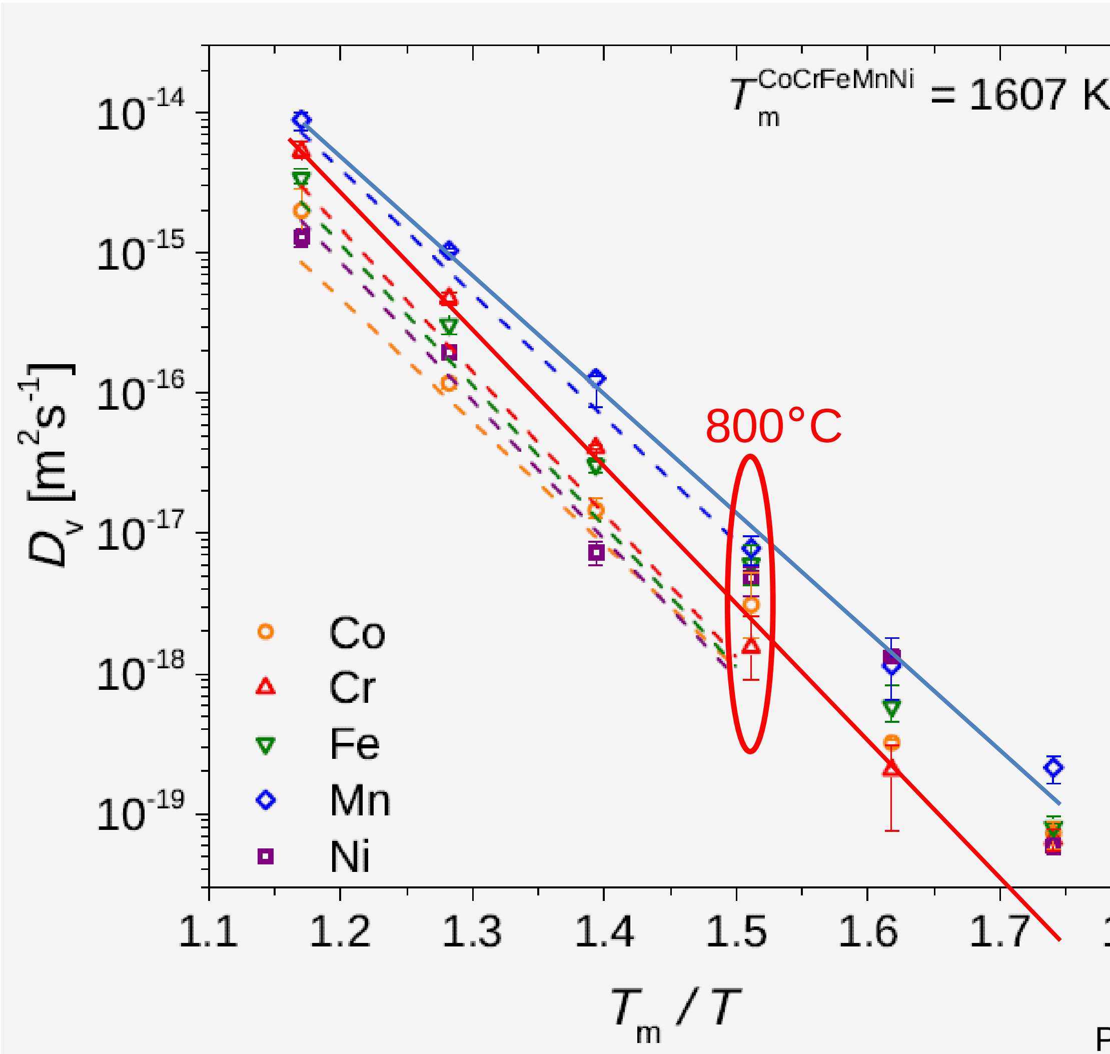
Co, Cr, Fe, Mn, Ni and Cu tracer diffusion in HEA single crystals
(filled symbols correspond to CoCrFeNi and open symbols correspond to CoCrFeMnNi)

Diffusion in HEAs and other FCC systems (homologous T scale)

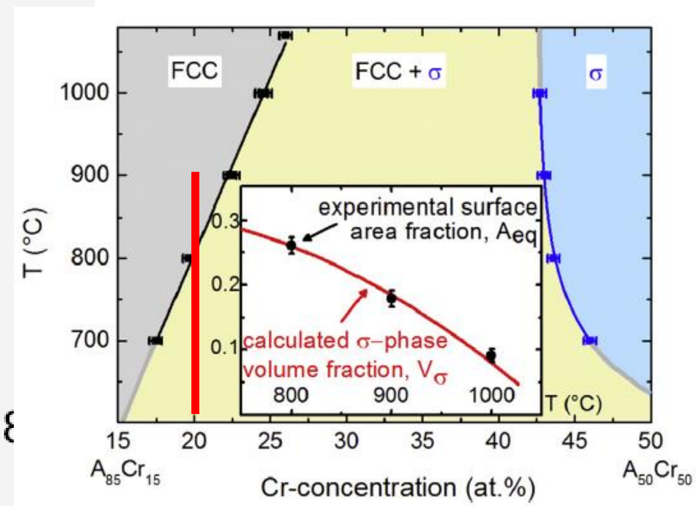


Ni: *M.B. Bronfin, G.S. Bulatov and I.A. Drugova, Fiz. Met. Metalloved. 40 (1975) 363-366.*
B. Million, J. Růžičková, J. Velíšek, and J. Vřešťál, Mater. Sci. Eng. 50 (1981) 43-52.
S.J. Rothman, L.J. Nowicki and G.E. Murch, J Phys F Met Phys. 10 (1980) 383.
K.Y. Tsai, M.H. Tsai, J.W. Yeh Acta Materialia (2013) 61, 4887–4897
Vaidya et al JALCOM (2016)

Everything clear?



- Deviations from linear plots at about 800°C
- Something special?

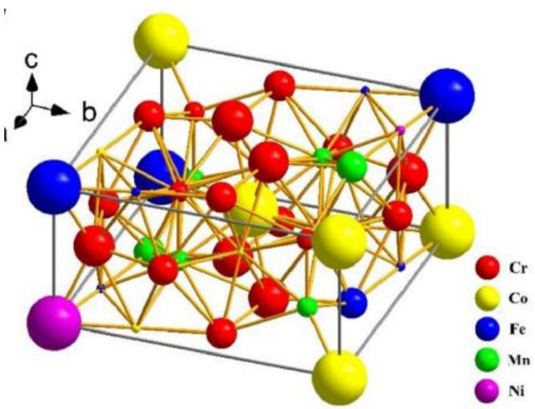


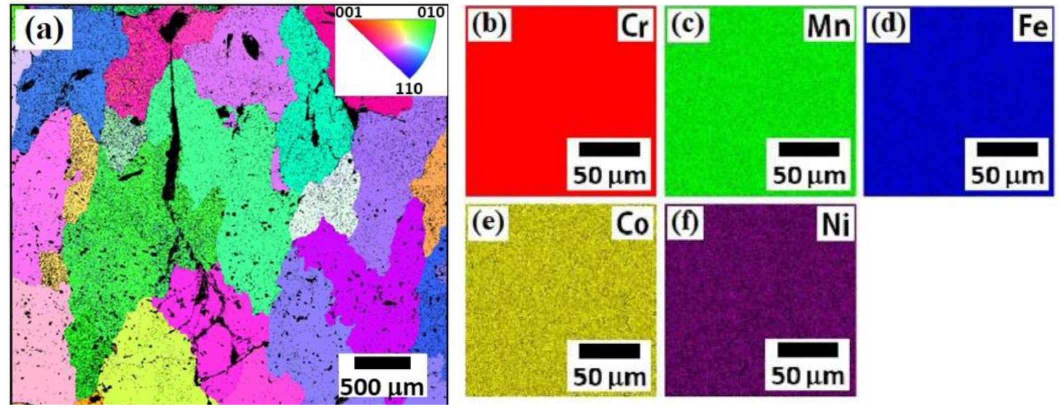
Phase stability and kinetics of σ-phase precipitation in CrMnFeCoNi high-entropy alloys, G. Laplanche et al, Acta Mater (2019)

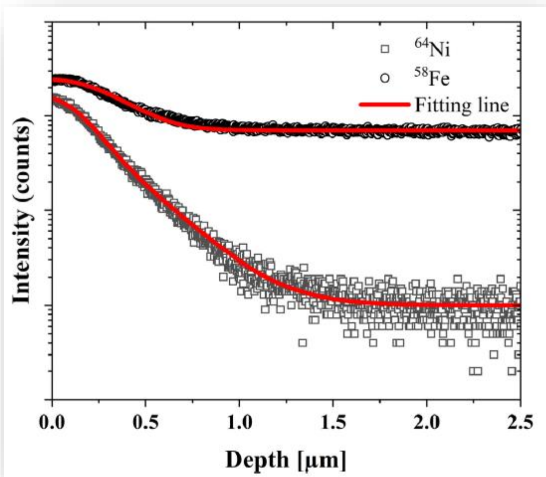
Gaertner et al, Scr Mater (2020)

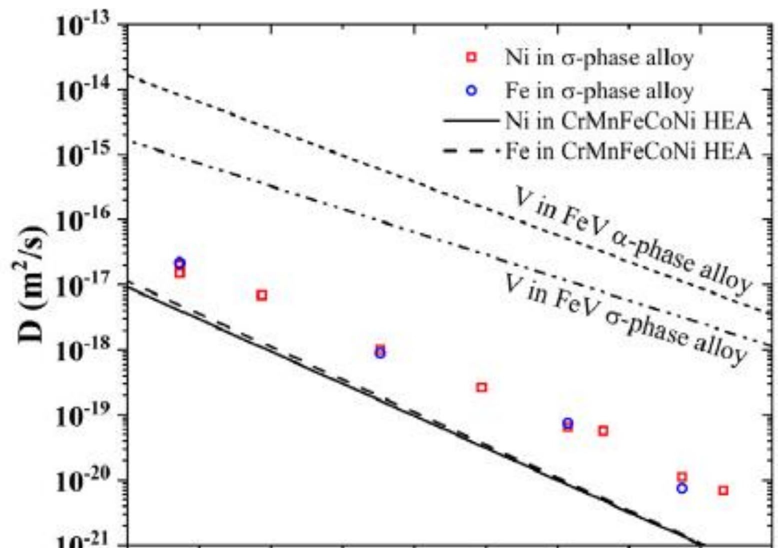
A = Co + Fe + Mn + Ni

Diffusion in sigma phase of the CoCrFeMnNi system (Cr-rich)





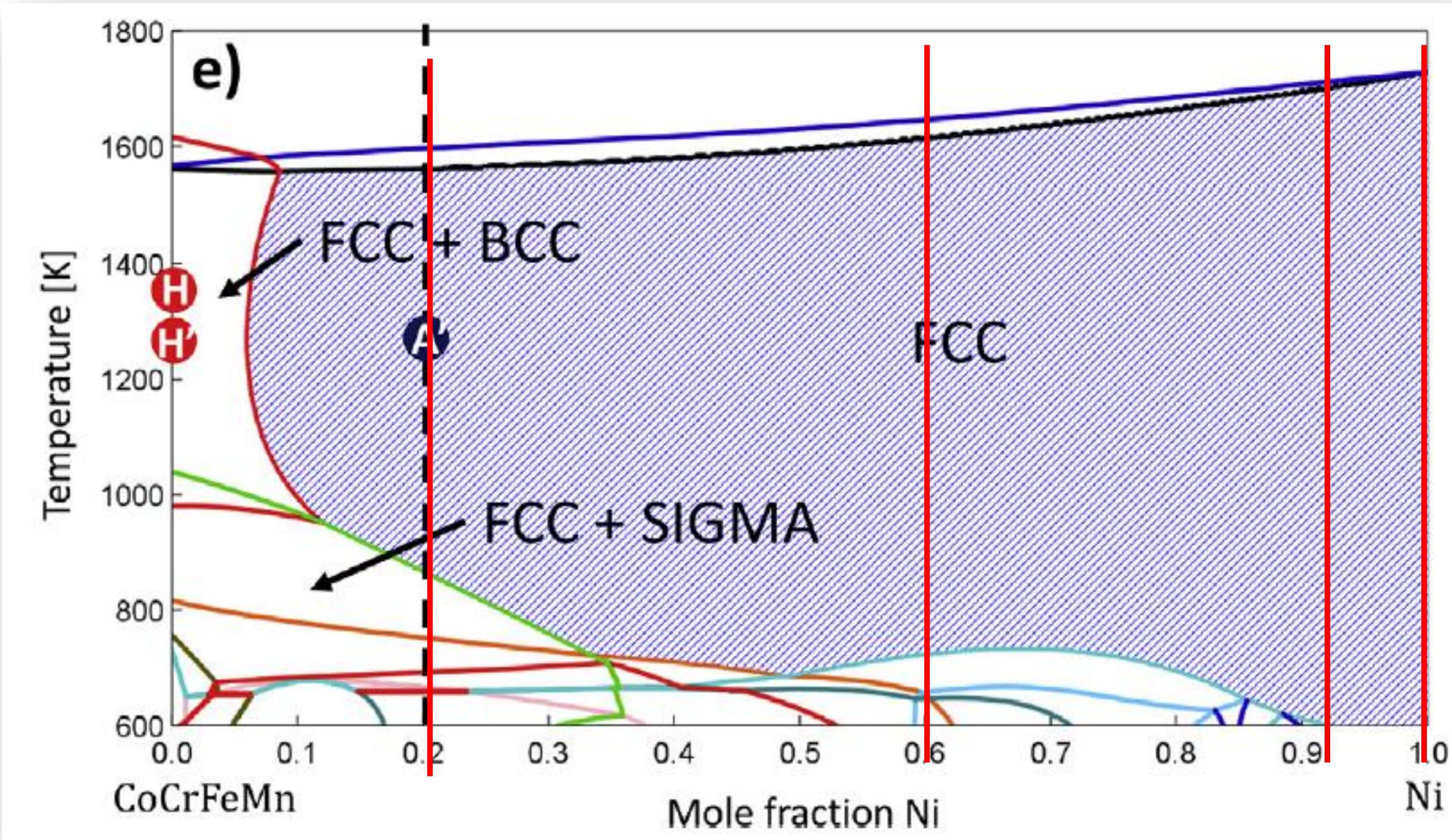




On a homologous temperature scale, diffusion of Fe and Ni in (Cr-rich) sigma-CoCrFeMnNi phase is faster as in equiatomic FCC CoCrFeMnNi

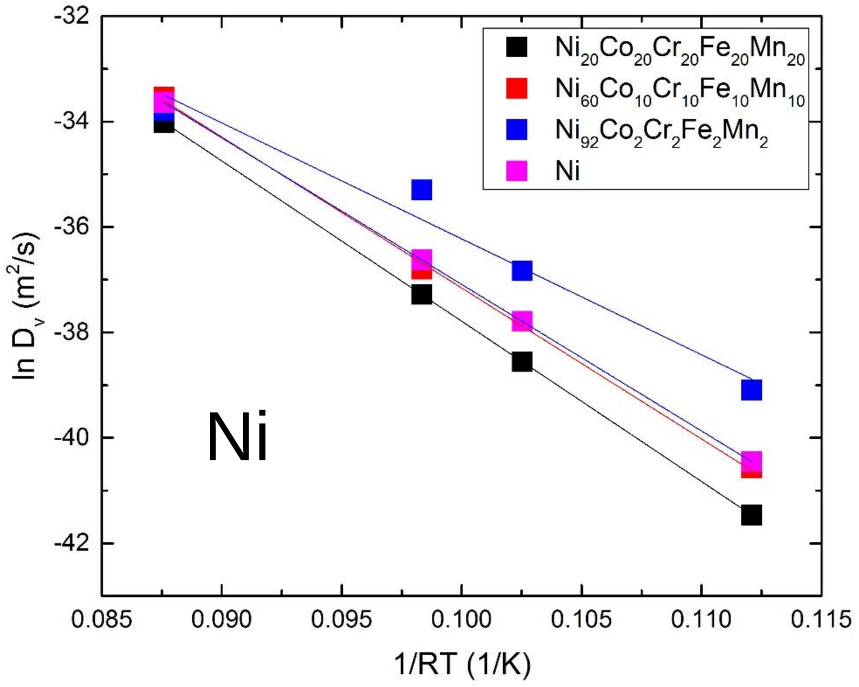
J. Zhang et al, Acta Mater (2021)

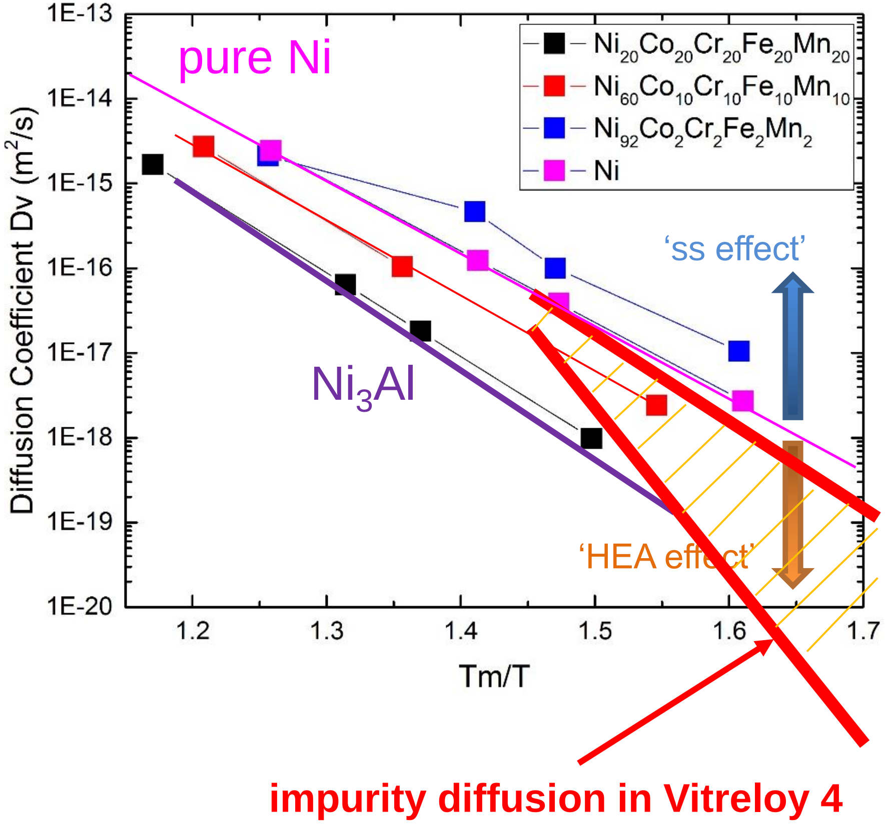
Appearance of a HEA effect



The fcc solid solution stability in the Co-Cr-Fe-Mn-Ni multi-component system
G. Bracq, M. Laurent-Brocq, L. Perriere, R. Pires, J.-M. Joubert, I. Guillot, Acta Materialia 128 (2017) 327-336

Ni diffusion in $Ni_x(CoCrFeMn)_{1-x}$ alloys

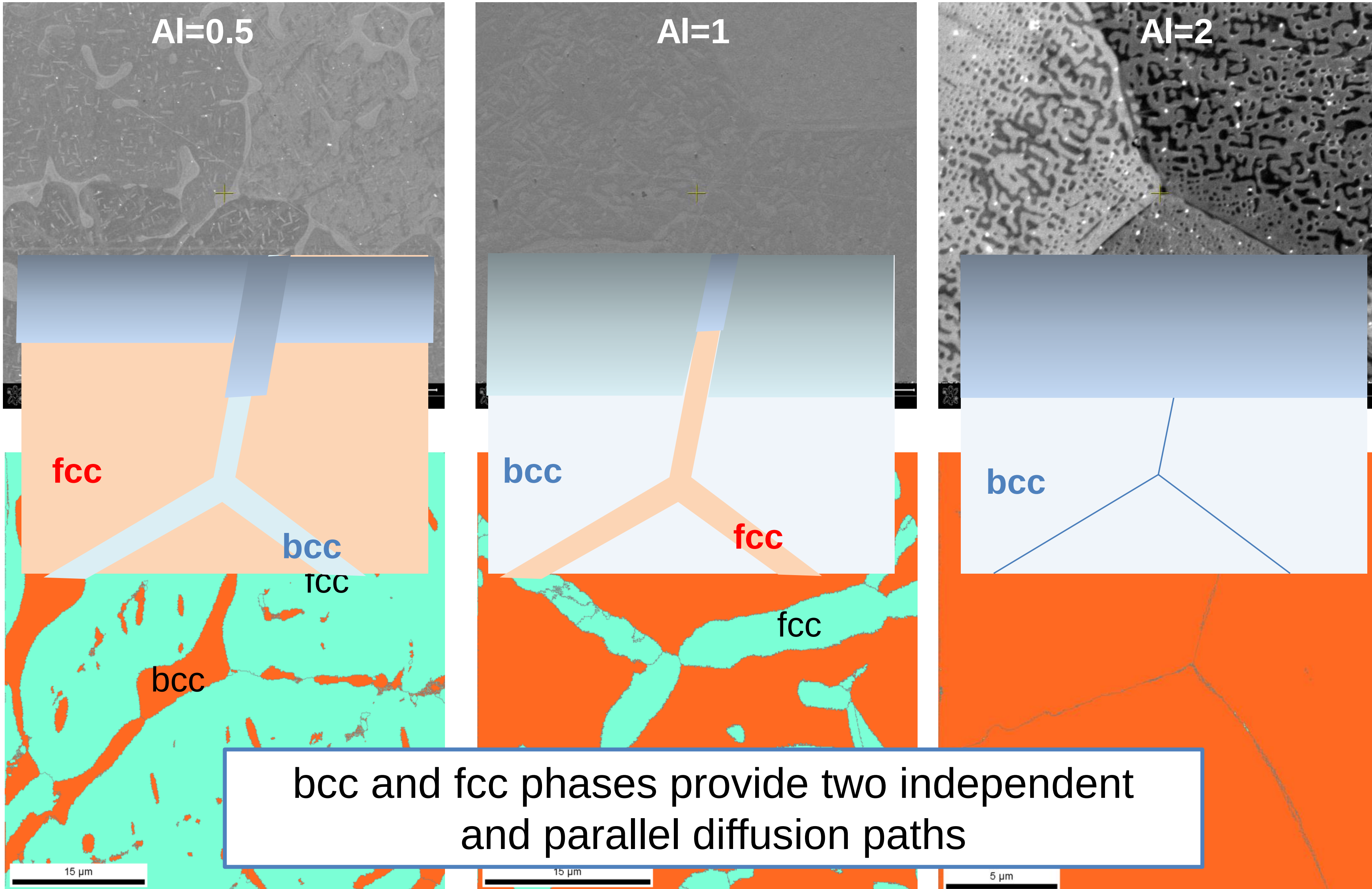




Kottke et al Acta Mater (2020)

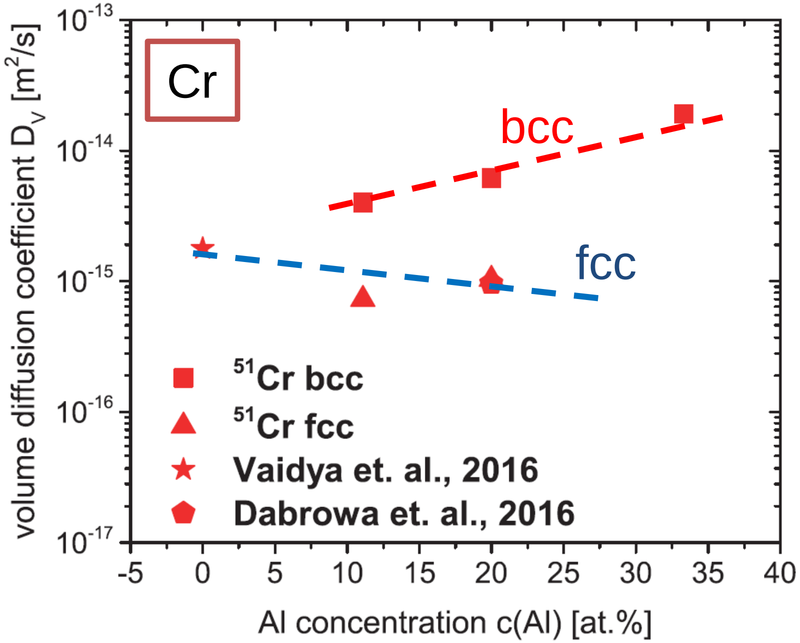
FCC / BCC / B2 phases in $Al_xCoCrFeNi$

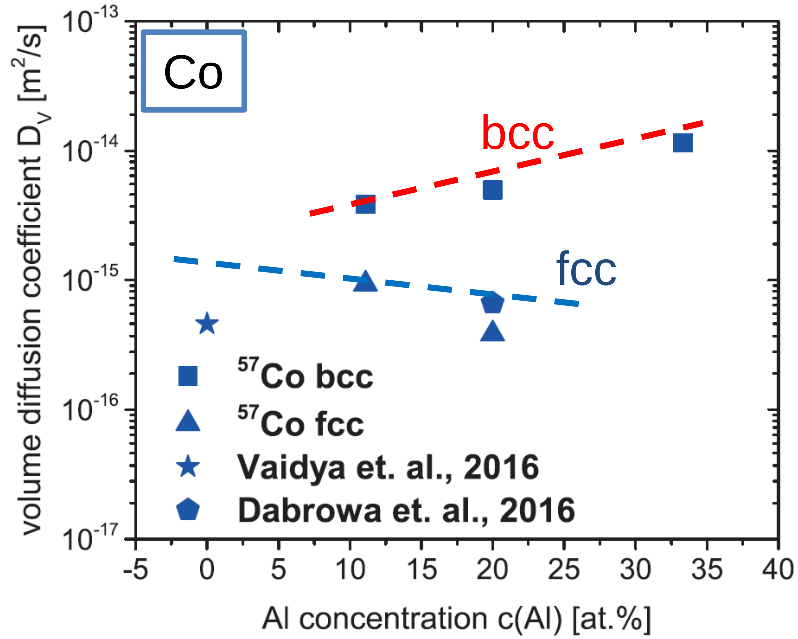
Ni diffusion in $Al_xCo_1Cr_1Fe_1Ni_1$ (x = 0.5, 1, 2)

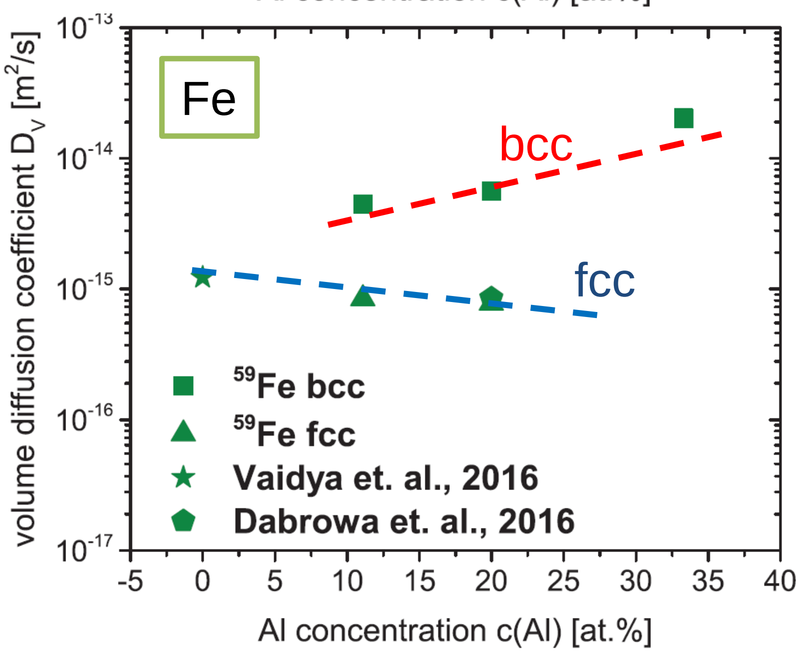


bcc and fcc phases provide two independent and parallel diffusion paths

Element diffusion at $T = 0.8\ T_m$







"entropy effect" on diffusion (i.e. addition of a further principal alloying component)

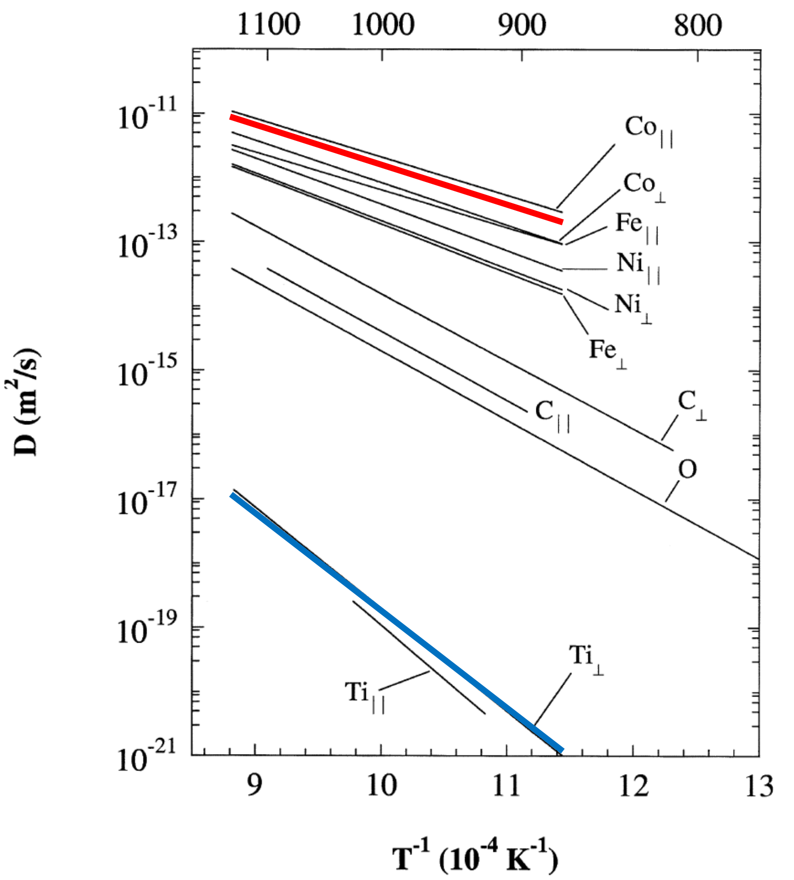
- Tracer diffusion is **enhanced** in bcc lattice if considered at the same homologous temperature
- Tracer diffusion is **retarded** in fcc lattice if considered at the same homologous temperature

Kottke et al. (2021) in preparation

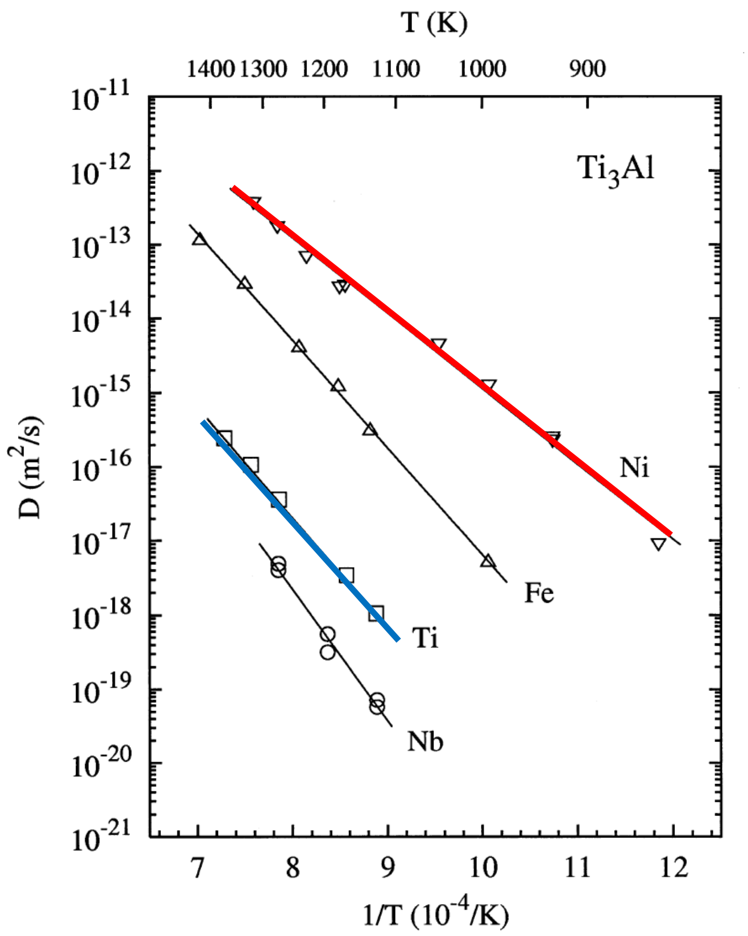
hcp AlScHfTiZr

Ultra-fast diffusion in hcp Ti aluminides

diffusion in α-Ti

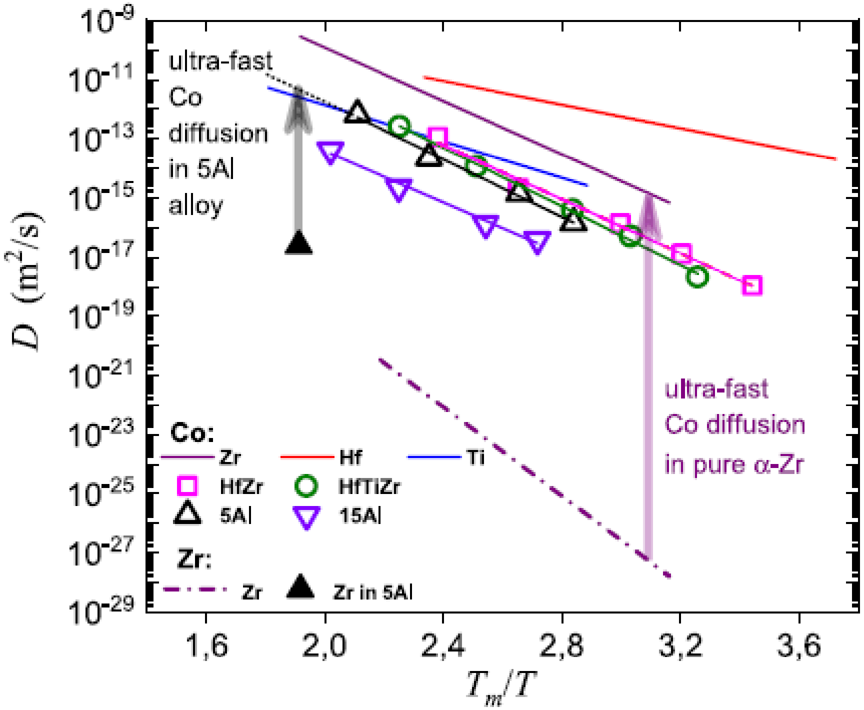


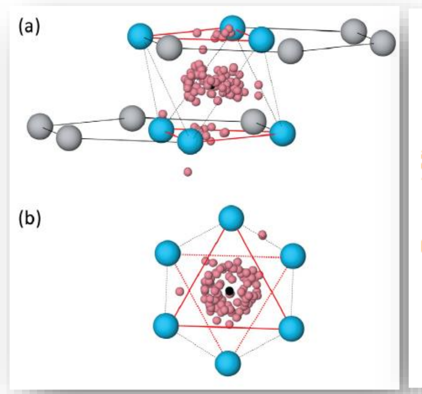
diffusion in α_2-Ti_3Al

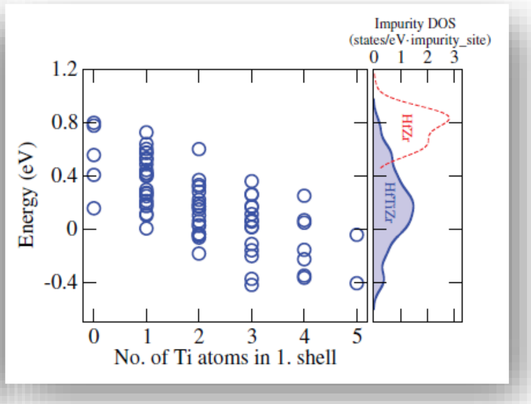


Herzig & Divinski (2005)

Ultra-fast diffusion in hcp-HEAs







Ultra-fast diffusion of Co in HCP HEAs does exist!
⇒ A sensitive and unique probe of local order!

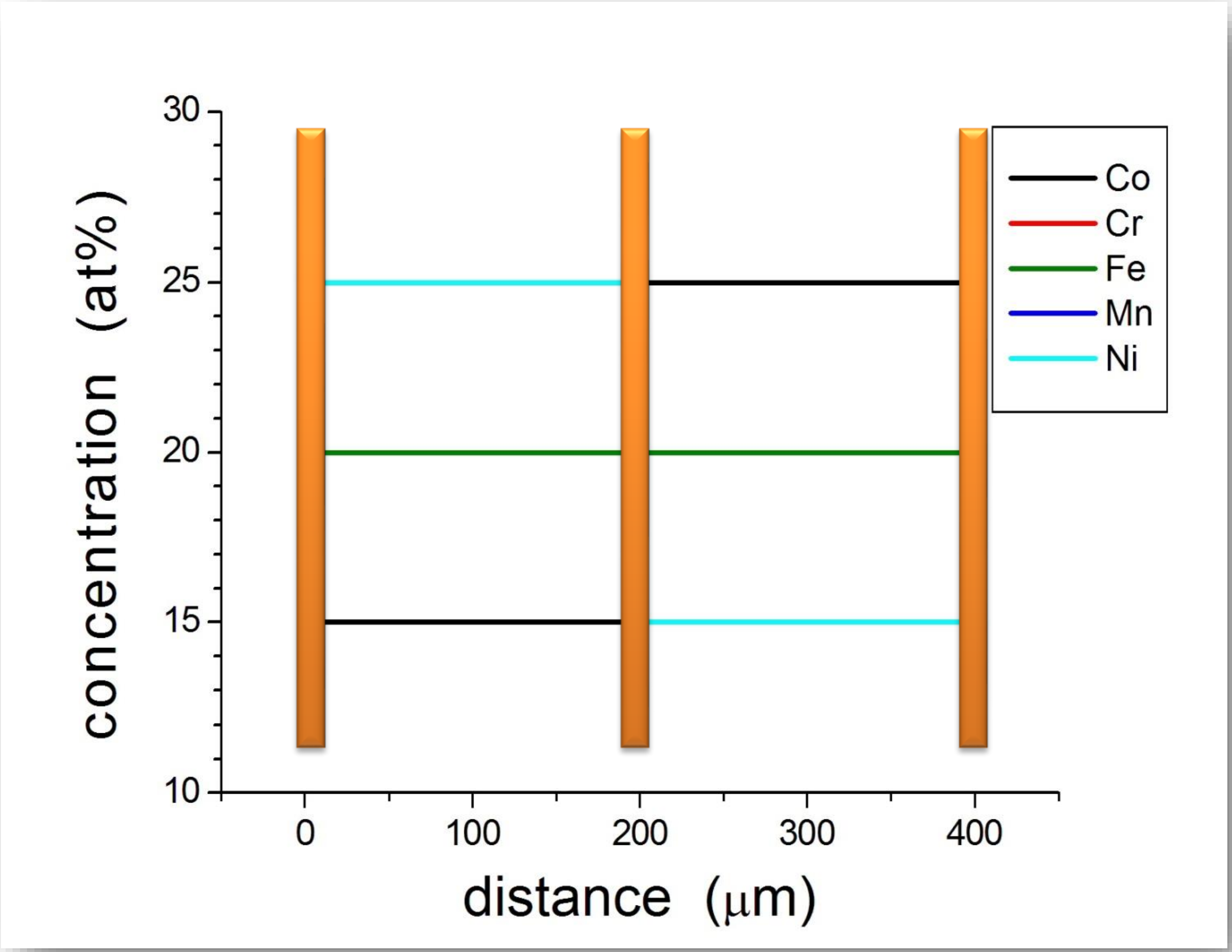
Vaidya, Sen, Zhang, et al, Acta Mater (2020)

Tracer vs chemical (inter-)diffusion

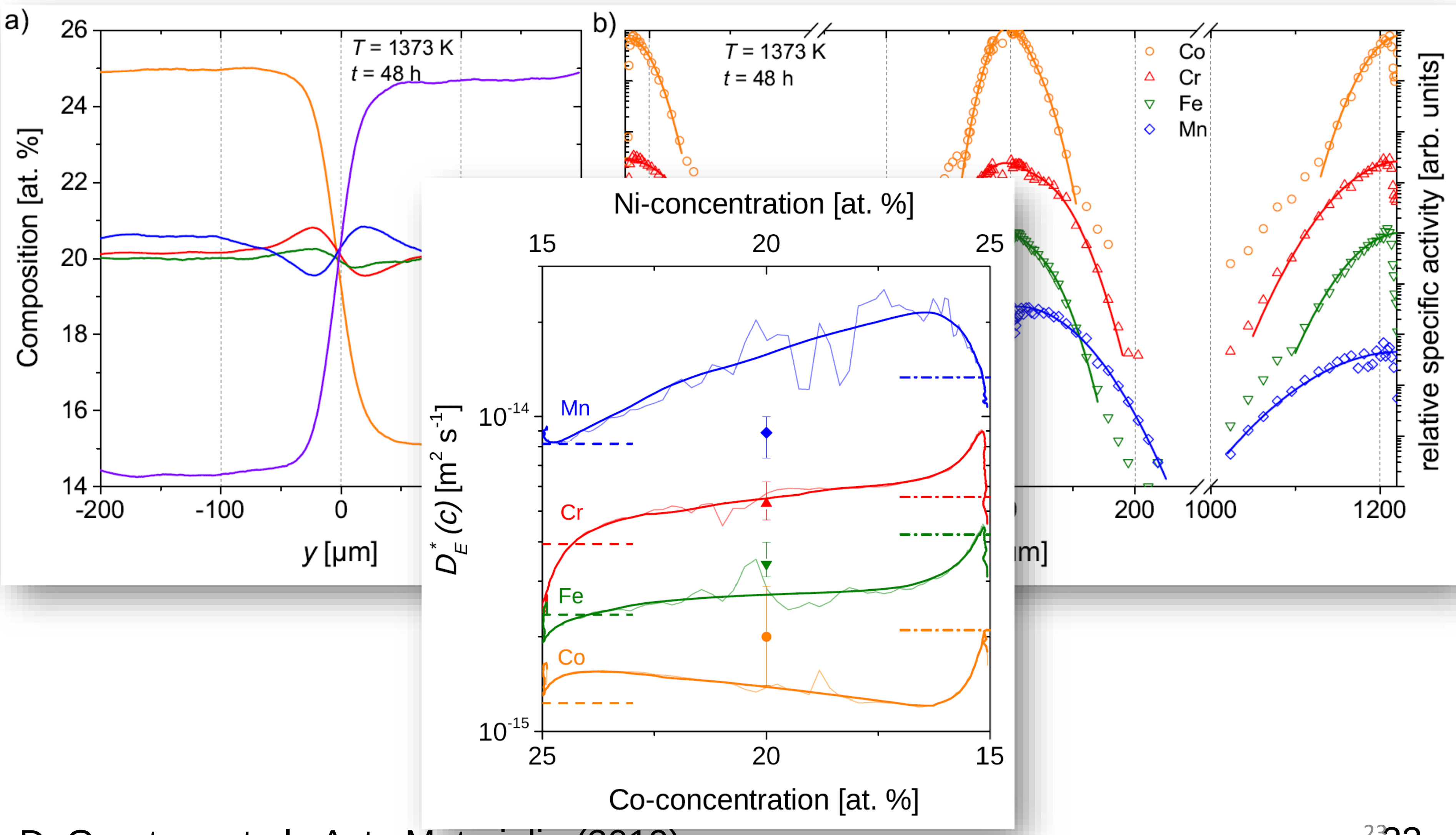
$\Rightarrow$

a pathway to high-throughput determination of the concentration-dependent tracer diffusion coefficients

Composition dependent atomic mobilities: combination of tracer and chemical diffusion measurements



Interdiffusion and tracer diffusion



D. Gaertner et al. Acta Materialia (2019)

Conclusions

- Tracer diffusion in HEAs is “normal”, not “sluggish”
- diffusion “retardation” in fcc and “acceleration” in bcc & hcp

  (at T/T_m = const)
- systematic variation of Ni amount in $Ni_x(CoCrFeMn)_{100-x}$ affects the diffusion rates ->

  no abrupt transition from “solid solution”-like to “HEA-like” behavior
- ultra-fast diffusers in hcp HEAs
- concentration-dependent tracer diffusivities
- Tracer diffusion: precision differentiation between bulk and GB diffusion

Unresolved/open problems

- Diffusion in different crystalline lattices
- Solute diffusion
- Relation of diffusion and nucleation/short range ordering/decomposition
- GB diffusion
- Mobility / thermodynamic databases
- …

Thank you!

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