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Diffusion in Ni-HEAs

The transition from pure Ni to the Cantor-HEA

Josua Kottke, Adnan Fareed, Sergiy V. Divinskiy, Gerhard Wilde
Institute of Materials Physics, WWU Münster

Daniel Utt, Alexander Stukowski, Karsten Albe
Materials Modelling Division, TU Darmstadt

Tom Keil, Enrico Bruder, Karsten Durst
Institute of Materials Science, TU Darmstadt

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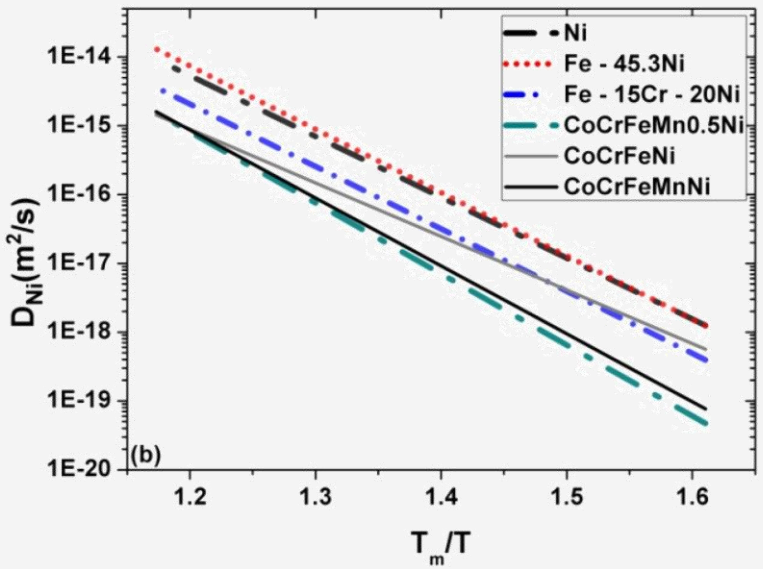
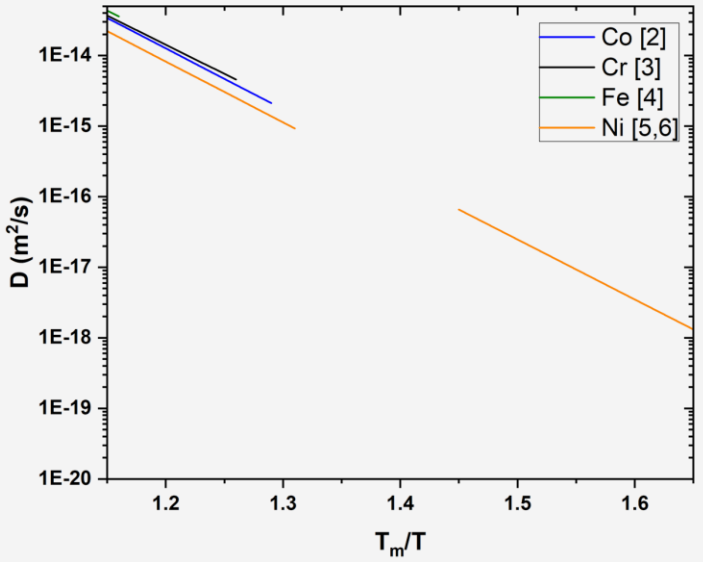
Pure elements forming equiatomic compositions



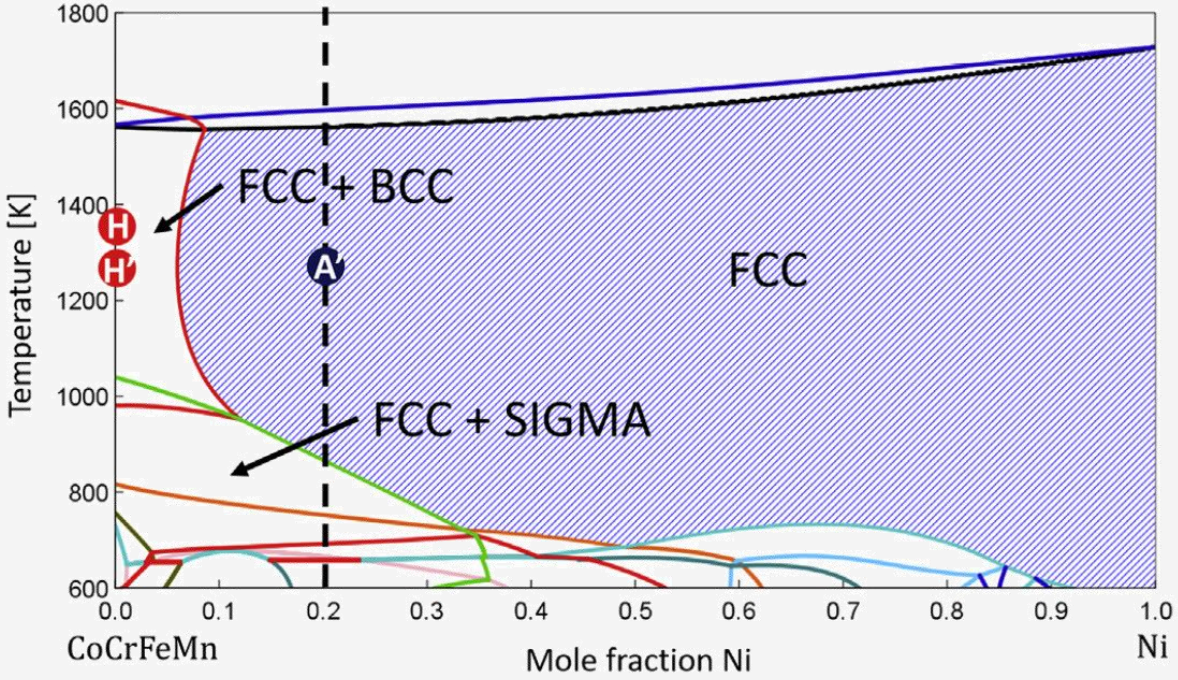
Equiatomic Cantor alloy:
Mechanical properties and diffusion is intensively investigated
„Sluggish“ diffusion?

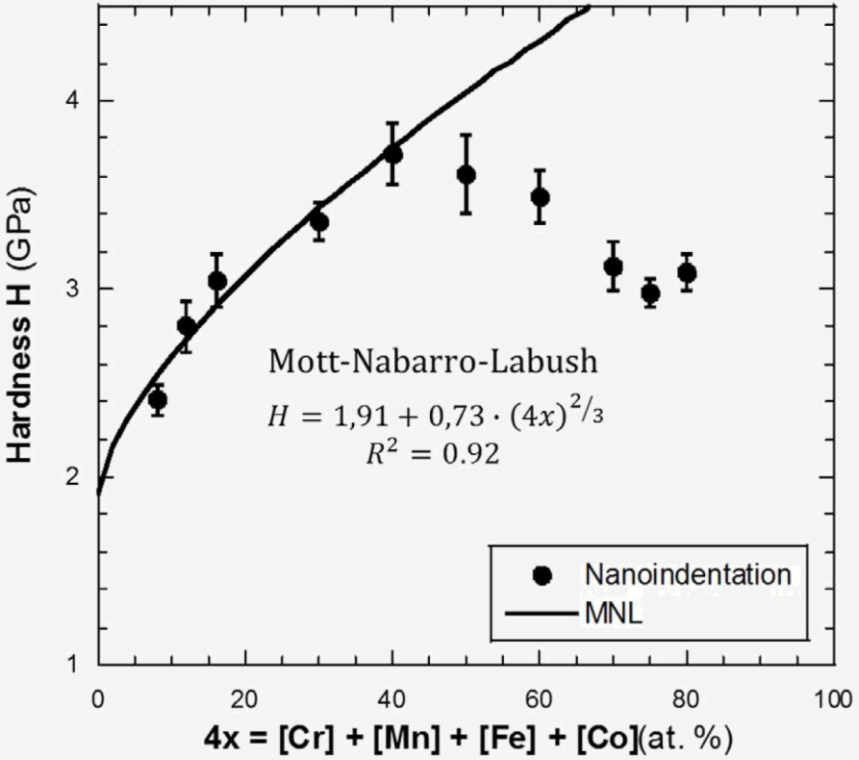


Pure Elements (Ni):
Solute diffusion – Le Claire model [7]
Mn was not measured

[1] M. Vaidya et al., *Journal of Alloys and Compounds* **688**, (2016): 994-1001.
[2] A. Vladimirov et al., *Fiz. Met. Metalloved.* **46**, (1978): 1232–1239.
[3] K. Monma, et al., *J. Jpn. Inst. Metals* **28**, (1964): 188–192.
[4] H. Bakker et al., *Phys. Status Solidi B* **45**, (1971): 633–638.
[5] M. Bronfin, G. Bulatov, I. Drugova, Fiz. Met. Metalloved. 40 (1975) 363–366.
[6] K. Maier et al., *Physica Status Solidi B* **78.2**, (1976): 689-698.
[7] A.D.Le Claire, *Journal of Nuclear Materials* **69–70**, (1978), 70-96.

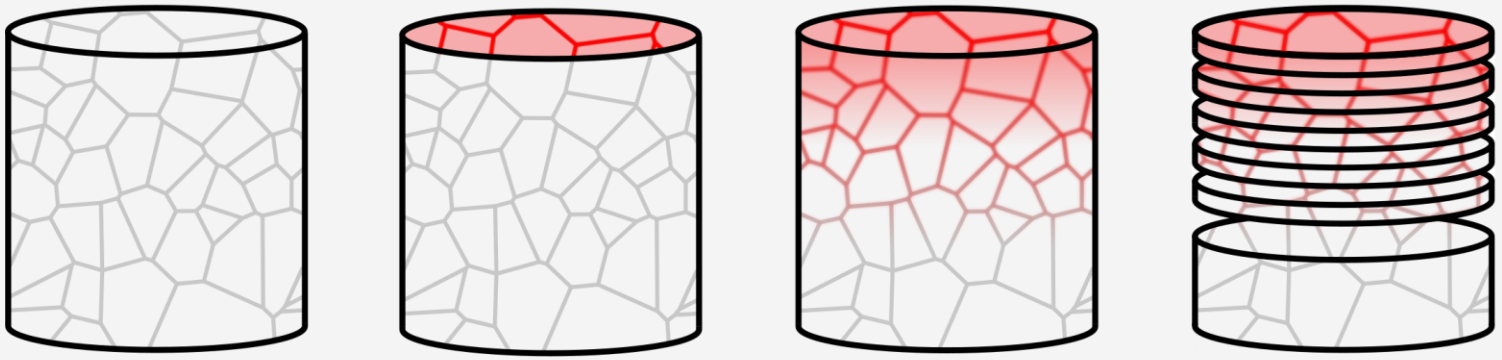
The transition from elements to HEAs

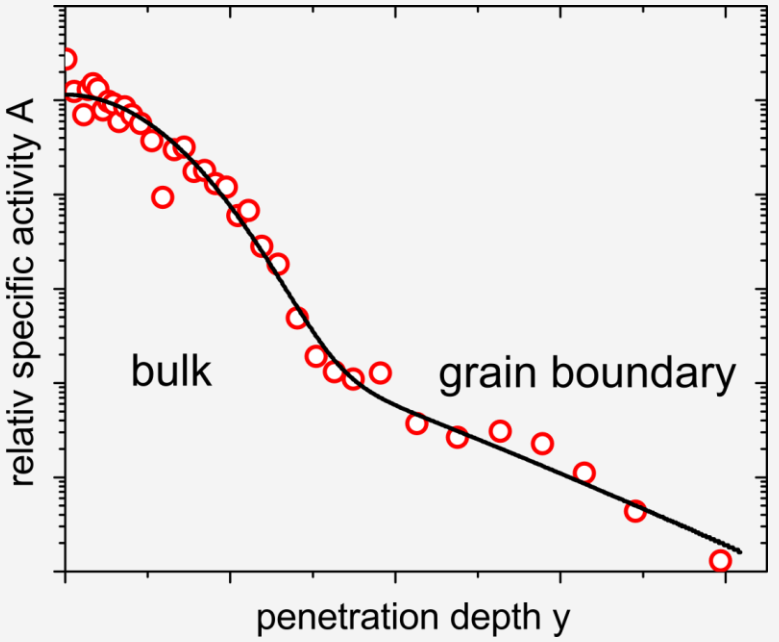




[8] G. Bracq et al., *Acta Materialia* **128**, (2017): 327-336.
[9] M. Laurent-Brocq et al., *Materials and Design* **103,** (2016): 84–89.

Radiotracer technique

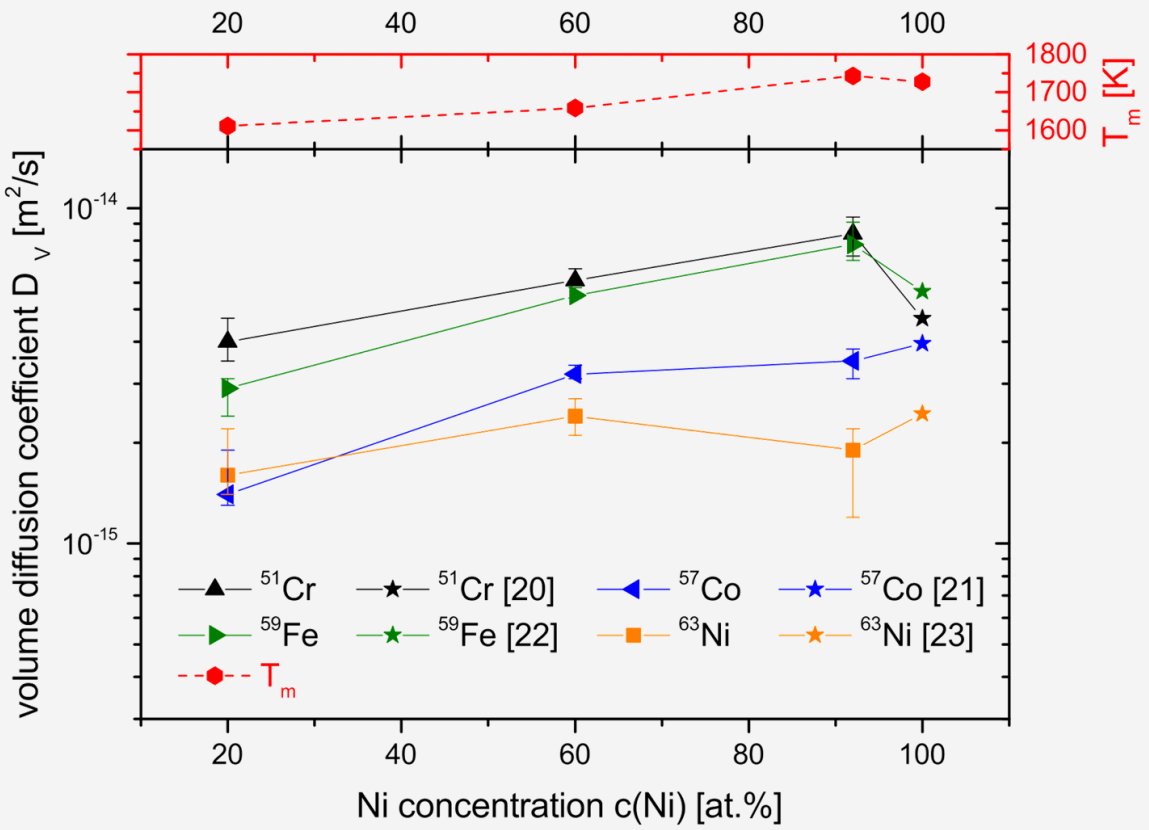




Concentration dependent diffusion coefficients

- usually: enhancement of solute diffusion in diluted FCC alloys due to the increased vacancy concentration

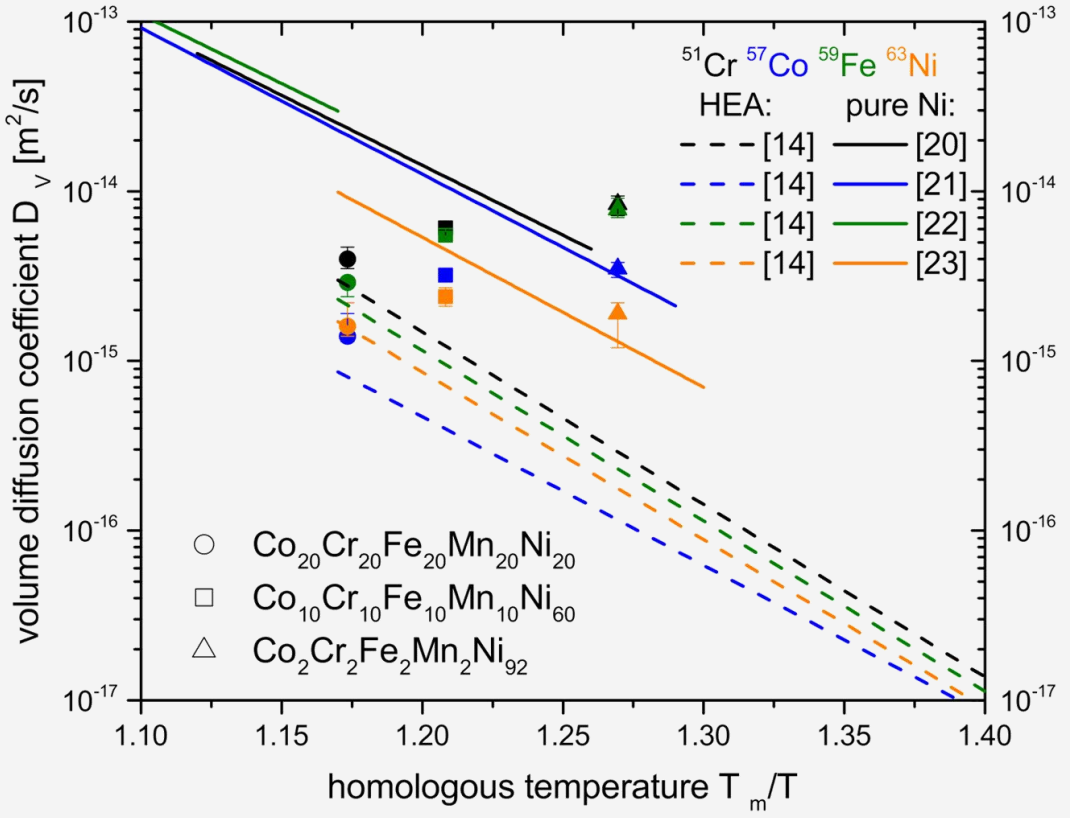
- HEAs: opposite trends are partially seen
- Slower elements (Co, Ni) decrease monotonously
- Faster diffusing elements (Cr, Fe) increase and are significantly decreased at more equiatomic compositions



[10] J. Kottke et al., *Scripta Materialia* **159** (2019): 94-98.

Diffusion behavior at homologous temperature T_m

- ‘true’ differences between diffusion rates are revealed due to a decrease of the melting temperatures
- D_v of solutes (Cr, Co, and Fe) are slower in the high-entropy alloy than in the dilute solid solution

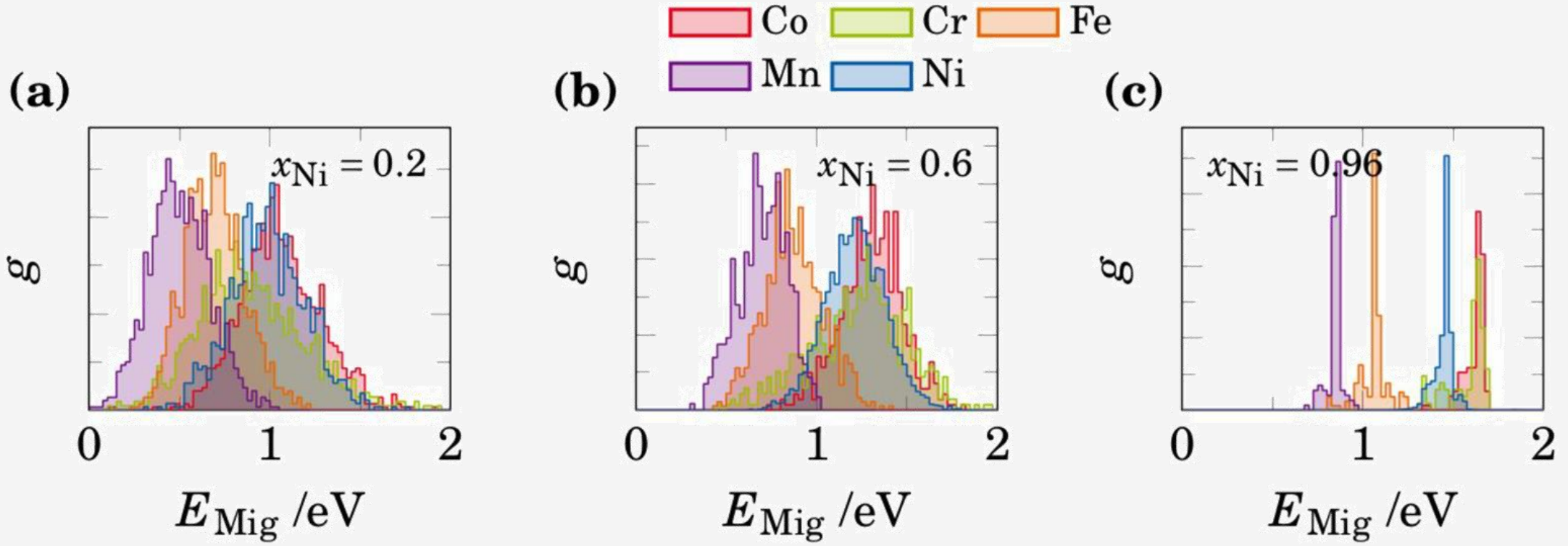


[10] J. Kottke et al., *Scripta Materialia* **159** (2019): 94-98.

Experiment Simulation

Modelling the findings

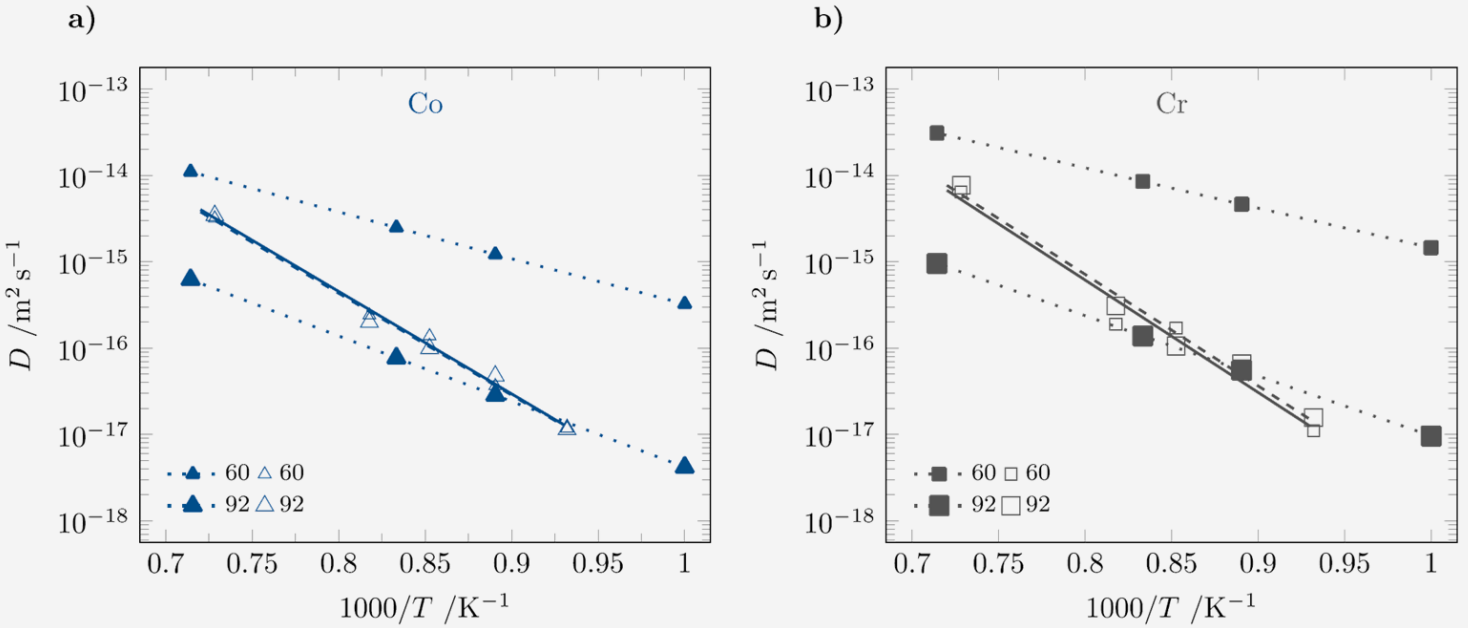
$$D = D_0 e^{-Q/RT} = c_{\mathrm{vac}} f g a^2 \nu_0 e^{-G_M/k_B T}$$



[11] J. Kottke, D. Utt et al., *Acta Materialia* **194**, (2020): 236-248.

Comparison with simulations

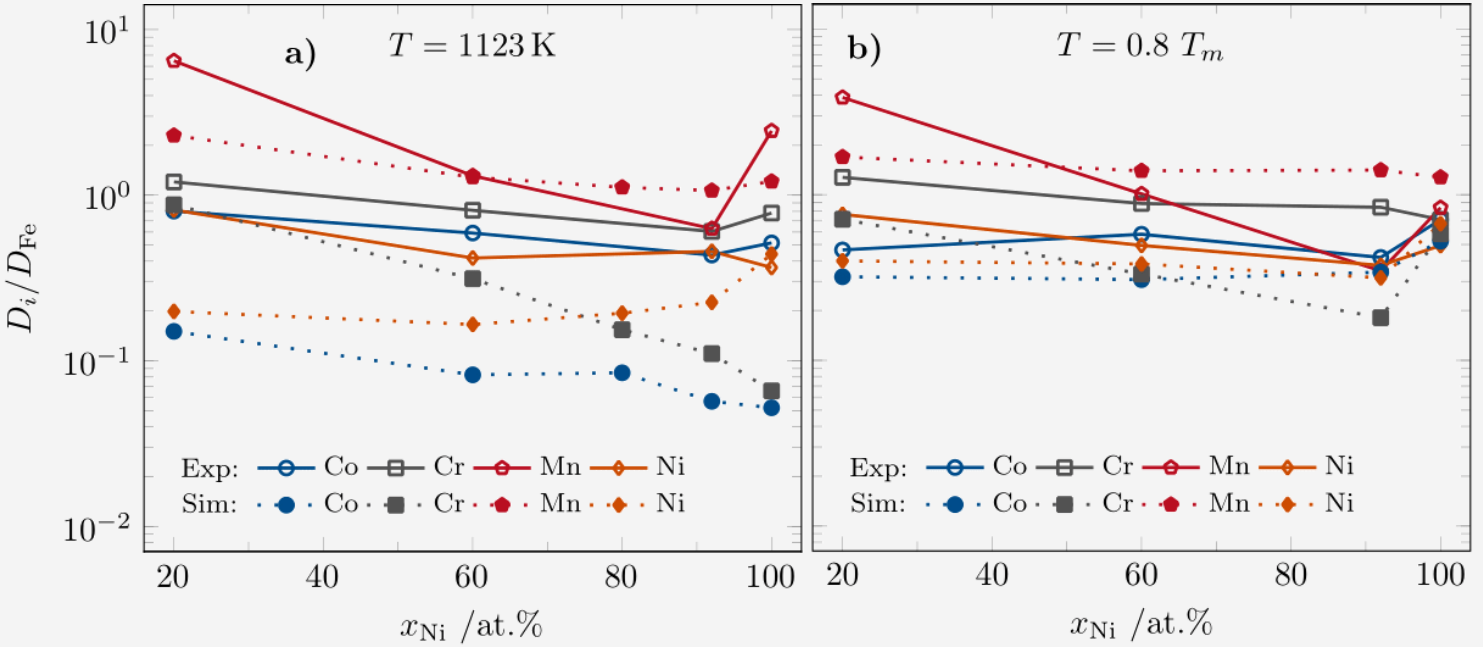
- General increasing trend of the normalized diffusion coefficients for all solutes



[11] J. Kottke, D. Utt et al., *Acta Materialia* **194**, (2020): 236-248.

Comparison with simulations

- General increasing trend of the normalized diffusion coefficients for all solutes
- Qualitatively agreement between the experiment and the simulations(especially well for Mn and Ni)
- Cr shows a significantly stronger increase is predicted by our model



[11] J. Kottke, D. Utt et al., *Acta Materialia* **194**, (2020): 236-248.

Summary

- diffusion measurements reveal a significant difference already at 92 at.% Ni-alloys (mechanical properties at 60 at.%)
  - Diffusion rates are increased in slightly diluted alloys and then decreased decreased for larger amounts of solutes

- Developed a model, which can predict the trends for HEA and its behavior while mixing

Thank you for your kind attention.

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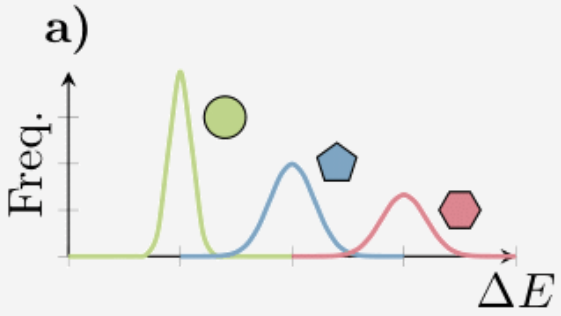
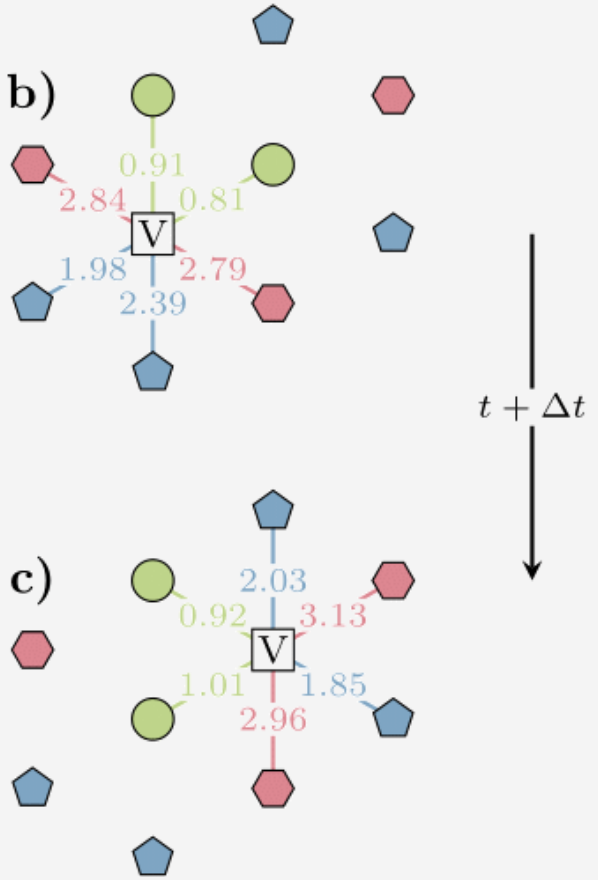
DFG Deutsche Forschungsgemeinschaft

Kinetic Monte-Carlo simulations – variable barrier model





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