On the Appearance of a High-Entropy Effect: Tracer Diffusion and Microstructure Analysis of $(\text{CoCrFeMn})_{100-x}\text{Ni}_x$ ($20 \leq x \leq 100$)

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Tracer Diffusion and Microstructure Analysis of (CoCrFeMn)$_{100-x}$Ni$_x$ $(20 \leq x \leq 100)$

Coopération

Priority program collaborations:
- Divinski/Grabowski (diffusion & ab initio modelling)
- Freudenberger (noble-metal HEA)
- Stukowski, MM (atomistic modelling)
- Wilde, WWU (defect structures & diffusion)
- Durst, PhM (deformation mechanisms)
- M. Laurent-Brocq (synthesis)
- Raabe/Zhiming (segregation analysis)
- Feuerbacher (synthesis)
- Glatzel (mechanical & diffusion data)

Schematic of Collaboration between different institutes.
Appearance of the HEA effect

- lattice parameter follows Vegard’s law from 20 at.% ≤ x ≤ 60 at.%;
  Vegard’s law:

\[
a_{\text{Vegard}}(x) = a_{\text{Ni}} \cdot \frac{x}{100} + \frac{100 - x}{4 \cdot 100} \cdot (a_{\text{Cr}} + a_{\text{Co}} + a_{\text{Fe}} + a_{\text{Mn}})
\]

(1)

- hardness follows Mott-Nabarro- Labush law from 20 at.% ≤ x ≤ 60 at.%

\[
x = 100 - 4s, \quad s = \frac{100 - x}{4} \quad \text{s concentration of solutes.}
\]

\[1\text{Laurent-Brocq et al., “From diluted solid solutions to high entropy alloys: On the evolution of properties with composition of multi-components alloys”, 2017}

Josua Kottke
Radiotracer method

concentration/activity profile for volume diffusion

\[ c = \frac{M}{\sqrt{2\pi Dt}} \exp \left( -\frac{y^2}{4Dt} \right) \]  

(2)
Radiotracer profiles
Tracer Diffusion and Microstructure Analysis of (CoCrFeMn)$_{100-x}$Ni$_x$ ($20 \leq x \leq 100$)

$^{63}$Ni diffusion

![Graph showing $^{63}$Ni diffusion coefficients as a function of Ni concentration for $T = 1373$ K. The graph includes data points and a trend line. The x-axis represents the Ni concentration in at.%, and the y-axis represents the diffusion coefficient ($D_v$) in m$^2$/s. The graph also includes a comparison to Bronfin 1975 data.](image-url)
57 Co diffusion

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$D_v$ [m$^2$/s]

$T_m$ [K]

$c$(Ni) [at. %]
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$^{59}$Fe diffusion

![Graph showing $^{59}$Fe diffusion data at $T = 1373$ K](image)
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$^{51}$Cr diffusion

![Graph showing $D_v$ (m^2/s) vs. c(Ni) [at.%] at T = 1373 K]
From pure nickel to Cantor alloy

Bronfin, Bulatov, and Drugova, “Self-diffusion of Ni in the intermetallic compound Ni 3 Al and pure Ni”, 1975


Monma, Suto, and Oikawa, “Diffusion of Ni63 and Cr51 in nickelchromium alloys”, 1964

Vaidya et al., “Bulk tracer diffusion in CoCrFeNi and CoCrFeMnNi high entropy alloys”, 2018

Gaertner et. al., in prep (project Divinski)
Conclusion

i $^{63}\text{Ni}$ and $^{57}\text{Co}$ diffusion is slowest, $^{59}\text{Fe}$ and $^{51}\text{Cr}$ are faster and $^{54}\text{Mn}$ is fastest diffusor

ii no special features in diffusion at $x = 60$ at.%, solute enhancement effects at $x \rightarrow 100$ at.% (reminder: kinks in hardness and lattice parameter at $x = 60$ at.%)
Outlook

- clarify $^{54}$Mn diffusion
- *remarkable increase at low solute concentrations*: further diffusion experiments with $\text{Co}_1\text{Cr}_1\text{Fe}_1\text{Mn}_1\text{Ni}_{96}$ and $\text{Co}_3\text{Cr}_3\text{Fe}_3\text{Mn}_3\text{Ni}_{88}$
- *Arrhenius behaviour*: radiotracer measurements at different temperatures
- *time dependency*: effects of grain boundary diffusion in HEA
Acknowledgment

Thank you for your kind attention.
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