Designing and understanding novel high-entropy alloys towards superior properties

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Designing novel high-entropy alloys

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100 years public-private partnership
1. Background of high-entropy alloys (HEAs)

2. TRIP-assisted dual-phase HEAs

3. Interstitially alloyed TWIP-TRIP-HEAs

4. Summary and outlook
1. Background of high-entropy alloys (HEAs)

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Single-phase solid solution

High-entropy alloy (HEA)

$$\Delta S_{\text{conf}}^{\text{mix}} = R \ln(n)$$

$$\text{Fe}_{20}\text{Mn}_{20}\text{Ni}_{20}\text{Co}_{20}\text{Cr}_{20}$$

FCC
High entropy alloys (HEAs)

• Definition:
  – multi-component alloy systems;
  – high configurational entropy $S_c (> R)$.

• Alloy design criteria: solid solution formation
  – primary components $\geq 5$;
  – equiatomic or near equiatomic (5-35 at.%);
  \[ \Delta G_{\text{mix}} \downarrow = \Delta H_{\text{mix}} - T\Delta S_{\text{mix}} \uparrow \]
  – some proposed rules: $\delta, \Delta H_{\text{mix}}, \Delta S_{\text{mix}}, \Delta \chi, \text{VEC...}$

• Candidates for many applications
  – high compressive strength;
  – excellent wear and oxidation resistance;
  – thermal resistance to softening up to ...
HEAs-Background

Single-phase FCC Fe$_{20}$Mn$_{20}$Ni$_{20}$Co$_{20}$Cr$_{20}$


Unchanged toughness
Single-phase solid solution

High-entropy alloy (HEA)

\[ \Delta S_{\text{conf}}^{\text{mix}} = R \ln(n) \]

\[
\text{Fe}_{20}\text{Mn}_{20}\text{Ni}_{20}\text{Co}_{20}\text{Cr}_{20}
\]

FCC

BCC

HCP

* Lanthanide series

** Actinide series
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Motivations

Single-phase HEA

Solid solution strengthening + Dislocation

Multi-phase HEA

Phase-interface strengthening + Twinning

Displacive transformation

Stress

Single-phase

Multi-phase

Strain
Phase formation in HEAs

Single phase solid solution

Ni → Cu
Cr → Mo

Configurational entropy ↑ Solid solution

Motivations

Non-equiaatomic HEAs

\[ \text{Fe}_{20}\text{Mn}_{20}\text{Ni}_{20}\text{Co}_{20}\text{Cr}_{20} \rightarrow \text{Fe}_{80-x}\text{Mn}_x\text{Co}_{10}\text{Cr}_{10} \]
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Fe$_{20}$Mn$_{20}$Ni$_{20}$Co$_{20}$Cr$_{20}$ $\rightarrow$ Fe$_{80-x}$Mn$_x$Co$_{10}$Cr$_{10}$

$\Delta G^{\gamma \rightarrow \varepsilon} = 1928$ J/mol for single phase Fe$_{20}$Mn$_{20}$Ni$_{20}$Co$_{20}$Cr$_{20}$

SFE: $\Gamma = 2\rho\Delta G^{\gamma \rightarrow \varepsilon} + 2\sigma^{\gamma/\varepsilon} + 2\rho\Delta G_{ex}$
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Fe$_{20}$Mn$_{20}$Ni$_{20}$Co$_{20}$Cr$_{20}$ → Fe$_{80-x}$Mn$_x$Co$_{10}$Cr$_{10}$


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Fe\textsubscript{50}Mn\textsubscript{30}Co\textsubscript{10}Cr\textsubscript{10} (TRIP-DP-HEA)

**Elemental distribution**


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**Compositionally-equivalent high-entropy phases**
Mechanical behavior


Deformation mechanisms


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Deformation mechanisms

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Quinary TRIP-HEAs $\text{Fe}_{40-x}\text{Mn}_{20}\text{Ni}_x\text{Co}_{20}\text{Cr}_{20}$ (X=6 at%)
Rather than focusing on phase stabilization and single-phase formation, HEA design could have rewarding guidelines from phase metastability and ductile multi-phase configurations.
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Possible solution:
Adding interstitial atoms → introducing interstitial solid solution (SS) strengthening
Interstitial atoms: C, N, B…; Content: 0.2 at.% / 0.5 at.% / 0.8 at.%
TRIP-DP-HEA + 0.5at% C $\rightarrow$ Fe$_{49.5}$Mn$_{30}$Co$_{10}$Cr$_{10}$C$_{0.5}$

Casting

Hot-rolling

(50% / 900 °C)

Homogenization

(2 h / 1200 °C with Ar + Water quenching)

Chemical analysis results (at. %):

<table>
<thead>
<tr>
<th>Alloy</th>
<th>C</th>
<th>Cr</th>
<th>Co</th>
<th>Ni</th>
<th>Mn</th>
<th>Fe</th>
</tr>
</thead>
<tbody>
<tr>
<td>FeMnCoCrC</td>
<td>0.56</td>
<td>10.35</td>
<td>10.22</td>
<td>0</td>
<td>29.87</td>
<td>49.01</td>
</tr>
</tbody>
</table>
Interstital TWIP-TRIP-HEAs

As-homogenized (1200°C, 2h, water-quenched)

CG C-HEA

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Grain-refined (Cold-rolled 70%; annealed at 900°C/3 min, water-quenched)

FG C-HEA

Carbide: M$_{23}$C$_6$

Element | At.%
--- | ---
Mn | 17.82%
Cr | 47.16%
Co | 1.92%
Fe | 13.64%
Metal | 80.54%
C | 19.46%

50~100 nm, ~1.5 vol.%

C in the Matrix: 0.35 at%

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Interstitial TWIP-TRIP-HEAs

iHEA


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Interstitial TWIP-TRIP-HEAs \textit{iHEA}

\begin{tabular}{cccc}
\hline
$\varepsilon_{\text{loc.}} = 10\%$ & $\varepsilon_{\text{loc.}} = 40\%$ & $\varepsilon_{\text{loc.}} = 60\%$ & $\varepsilon_{\text{loc.}} = 90\%$ \\
\hline
\end{tabular}


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**Interstitial TWIP-TRIP-HEAs iHEA**

![Graph showing the relationship between ultimate tensile strength and total elongation across different alloys and phases.](image)

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Summary

- Ultimate tensile strength, MPa
- Total elongation, %

#1: Fe$_{40}$Mn$_{27}$Ni$_{26}$Co$_5$Cr$_2$
  Single FCC, 35 μm
#2: Co$_{20}$Cr$_{20}$Fe$_{20}$Mn$_{20}$Ni$_{20}$
  Single FCC, 140 μm
#3: Fe$_{35}$Mn$_{45}$Co$_{10}$Cr$_{10}$
  Single FCC, 90 μm
#4: Fe$_{49.5}$Mn$_{30}$Co$_{10}$Cr$_{10}$C$_{0.5}$
  Single FCC, 100 μm

Tuning mechanisms ↔ NE-HEAs design

Substitutional SS Dislocations Grain boundaries
Substitutional SS Dislocations Grain boundaries TWIP
Substitutional SS Dual-phase Dislocations Grain boundaries TRIP TWIP Stacking faults
Substitutional SS Interstitial SS Dual-phase Dislocations Grain boundaries TRIP TWIP Stacking faults Nano-precipitates

SS: solid solution
New HEAs design

- New quinary TRIP-DP-HEAs
- Interstitial quinary TRIP-HEAs (Dr. Xiaoxiang Wu)
- Light-weight high-strength HEAs (Dr. Jing Su, Dr. Zhangwei Wang)
- High-temperature refractory HEAs (Mr. Yueling Guo)
- Functional (magnetic/thermal) HEAs (Mr. Ziyuan Rao)

Further studies on current HEAs

- Hydrogen fracture behavior of HEAs (Dr. Hong Luo)
- Grain boundary segregations in HEAs (Dr. Linlin Li)
- High cyclic fatigue of HEAs (Dr. Xu Zhang)
- ……
Thanks for your attention!

Zhiming Li, Dierk Raabe, Cem Tasan, Konda G. Pradeep, Yun Deng, Hauke Springer, Baptiste Gault, Fritz Körmann, Blazej Grabowski, Jörg Neugebauer, Hong Luo, Linlin Li, Jing Su, Xiaoxiang Wu, Zhangwei Wang, Xu Zhang, Wenjun Lu, Silva Basu