Designing Nanostructured Metallic Bulk Alloys via First Principles Simulations and Atomic Scale Characterization: The Basis of Modern Manufacturing

Dawn of the iron age in the Mediterranean

Hittite empire: iron age

1274 BC:
- Iron weapons
- Large chariots

Egypt empire: bronze age

20,000 soldiers, 4 divisions
- Largest Egypt army ever

37,000 soldiers, Hittite and other kingdoms

Legend:
- Muwatalli
- Quadesh
- Ramses II.
Treaty of Kadesh (Quadesh), mankind’s first documented peace treaty. It signified the end of a conflict between Egypt and the Hittites and dates from 1269 BC.
- First principles guided design of structural alloys
  Mg-Li
  Mg-Y
  TWIP steel
  Phase transformation at lattice defects

- RAP (Rapid Alloy Prototyping)
  Combinatorial design of bulk alloys
  Density-reduced TRIPLEX steels

- Conclusions
Ab-initio design of Mg-Li alloys: a ‘treasure‘ map


Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany

Weak under normal load
Weak under shear load

Y: Young’s modulus
ρ: mass density
B: compressive modulus
G: shear modulus
Ab-initio design of Mg-Li alloys: a ‘treasure’ map

Weak under normal load

Weak under shear load


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Mg vs. Mg-Y: > 5 times higher ductility at same stress level
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Deformation - dislocation activity

TEM images of <c+a> dislocations in Mg 3 wt-% Y (3.5 % CR)

- Red arrows: cross-slip events
- Blue arrows: dislocation dissociation on pyramidal planes
\{0001\}<1\overline{1}-20>
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Twins
Double cross slip
\[ \tau_{tw} = \frac{\gamma_{sf} e}{3b_s} + \frac{3G b_s}{L_0} \]

Diagram showing the relationship between stress and strain withlegend:
- USF: Upper Slip System
- ISF: Inter-Slip Facet

Texture map with scale bar 20 \( \mu m \)

Graph showing True Stress (GPa) vs. True strain with data from different temperatures:
- 296K Experiment
- 573K Experiment
- 673K Experiment
- 296K Simulation
- 573K Simulation
- 673K Simulation
Effect of aging on ductility

Engineering Stress (MPa) vs. Engineering Strain (%)

- as-quenched
- aged 450°C/48h

Strain: 0% → 15%

Precipitation hardening
Increase of austenite fraction during aging

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Increase of austenite fraction during aging

Effect of aging on ductility

D. Raabe et al. Scripta Materialia 60 (2009) 1141

Table:

<table>
<thead>
<tr>
<th>C</th>
<th>Ni</th>
<th>Mo</th>
<th>Ti</th>
<th>Al</th>
<th>Mn</th>
<th>Fe</th>
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<td>0.01</td>
<td>2.0</td>
<td>1.0</td>
<td>1.0</td>
<td>0.15</td>
<td>12</td>
<td>bal.</td>
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</tbody>
</table>
Mn atoms
Ni atoms
Mn iso-concentration: 18 at.%

Scale: nm

70 million ions Laser mode (0.4nJ, 54K)

APT results: Atomic map (12%Mn, aged 450°C/48h)

Mn segregation at grain boundary, (450°C/65h)

9Mn-2Ni-0.15Al-1Ti-1Mo (wt.%)
Iso-concentration surfaces at 10 at.%Ni and 18 at.%Mn

9Mn-2Ni-0.15Al-1Ti-1Mo (wt.%)
Growth of retained austenite 450°C/48h. 12MnPH

Mn profile

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Thin intergranular FCC layer among two martensite crystals, APT

20 nm

martensite – martensite boundary

\( C_{Mn}^\gamma \approx 28\% \)

\( C_{Mn}^0 = 9\% \)

Mn

Distance [nm]

Mn content [at.\%]

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Mn segregation at dislocations, (450°C/48h)

12Mn-2Ni-0.15Al-1Ti-1Mo (wt.%) iso-conc surfaces at 14at.%Mn and 8at.%Ni.
650 MPa to 2 GPa

400°C aging:
Ms-relaxation + precipitation + austenite reversion

Fe-13.6Cr-0.44C (wt.%)
Prior Austenite Grain Boundary

[111]α

[110]γ

1 μm
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How can we close this loop and efficiently probe the composition – processing – microstructure – property - phase space?

RAP: Rapid alloy prototyping
combinatorial design
complex alloys
thermomechanical processing
tensile testing
35 hours instead of 6 months
Rapid alloy prototyping: combinatorial design of complex alloys

1. Multi-ingot vacuum or inert gas inductive melting and casting

2. Homogenization and hot rolling

3. Heat treatment and / or thermomechanical processing

2. Discharge sample preparation

3. Tensile testing (3 test per state)
Rapid alloy prototyping: multiple ingot casting

5 Cu-moulds, 60 kW vacuum induction furnace (vacuum, Ar, air)

10 x 50 x 150 mm³
Rapid alloy prototyping: applied to TRIPLEX Fe-Mn-Al-C steels

(a) YS / MPa vs. Alloy (wt.% Fe–30Mn–1.2C–)
(b) UTS / MPa vs. Alloy (wt.% Fe–30Mn–1.2C–)
(c) TE / % vs. Alloy (wt.% Fe–30Mn–1.2C–)
(d) Hardness / HBW vs. Alloy (wt.% Fe–30Mn–1.2C–)

Aging treatments: 
- as-homogenised
- 450°C, 1h
- 500°C, 1h
- 500°C, 24h
- 550°C, 1h
- 550°C, 24h
- 600°C, 1h
- 600°C, 24h
Rapid alloy prototyping: applied to TRIPLEX Fe-Mn-Al-C steels.
Rapid alloy prototyping: applied to TRIPLEX Fe-Mn-Al-C steels

Fe-24Mn–0.5C–8.6Al (wt%)

Courtesy of Dr. Koyama (NIMS, MPI)
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