

Objective of research

The objective is to design alloy compositions for the enhancement of strength and corrosion properties
The design of compositions is based solely on alloy thermodynamics

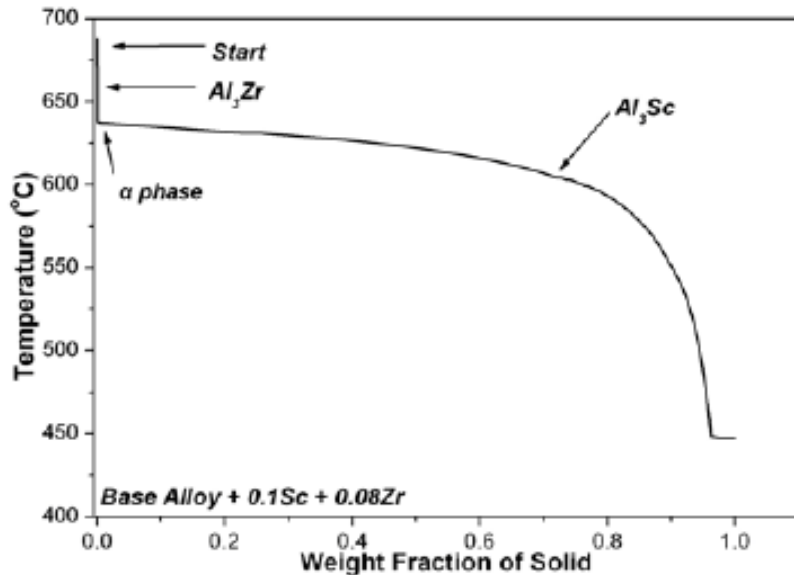
Methodology

- The Al-Mg system (5xxx alloy series) is taken as an example with additions of Zr and Sc.
- The effect of intermetallic compounds Al_3Sc and Al_3Zr on the grain refinement and recrystallization resistance is assessed with computational thermodynamics
- The driving force for precipitation of Al_3Sc and Al_3Zr is computed as a function of alloy composition and temperature. Driving force maps are constructed
- A grain refining index M_{GR} is defined based on the amount of primary intermetallics used for heterogeneous nucleation of the matrix phase
- A recrystallization resistance index M_{RX} is defined based on the Zener drag imposed by the intermetallics

Alloy design microstructural indices

Grain Refining Index M_{GR}

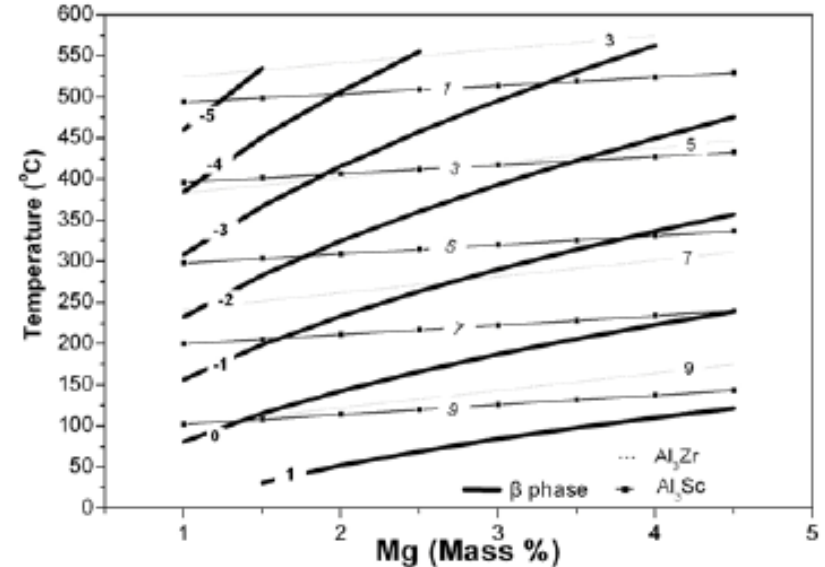
$$M_{GR} = (f_{bsa})_{Al_3Zr} + (f_{bsa})_{Al_3Sc}$$



Scheil simulations for M_{GR} index

Rycrystallization Resistance Index M_{RX}

$$M_{RX} = (f_{bal} \Delta G_m)_{Al_3Zr} + (f_{bal} \Delta G_m)_{Al_3Sc}$$



Precipitation driving force maps for M_{RX} index

Alloy variant	f_{ac}		f_{bsa}		f_{eq}		f_{bal}		ΔG_m		$f_{bal}\Delta G_m$		M_{GR}	M_{RX}	M
	Al ₃ Zr	Al ₃ Sc	Al ₃ Zr	Al ₃ Sc	Al ₃ Zr	Al ₃ Sc	Al ₃ Zr	Al ₃ Sc	Al ₃ Zr	Al ₃ Sc	Al ₃ Zr	Al ₃ Sc			
0.1Sc-0.08Zr	0.048	0.031	0.048	0	0.06	0.153	0.012	0.122	865	2120	10.58	258.64	0.048	269.02	12.91
0.4Sc-0.08Zr	0.051	0.591	0.051	0.16	0.06	0.877	0.009	0.286	854	1433	7.68	409.83	0.211	417.51	88.09
0.1Sc-0.15Zr	0.132	0.029	0.132	0	0.142	0.154	0.010	0.125	865	2120	8.65	265	0.132	273.65	36.12
0.4Sc-0.15Zr	0.136	0.600	0.136	0.16	0.143	0.877	0.007	0.277	854	1433	5.97	396.94	0.296	402.91	119.27

f_{ac} : mole fraction of phase in as-cast microstructure

f_{bsa} : mole fraction of phase formed during solidification before α -phase

f_{eq} : mole fraction of phase at equilibrium at 500°C

$f_{bal} = f_{eq} - f_{ac}$ balance mole fraction of phase left for precipitation at 500°C

ΔG_m : precipitation driving force at 500°C

$M_{GR} = (f_{bsa})_{Al3Zr} + (f_{bsa})_{Al3Sc}$ grain refining index

$M_{RX} = (f_{bal}\Delta G_m)_{Al3Zr} + (f_{bal}\Delta G_m)_{Al3Sc}$ recrystallization resistance index

$M = M_{GR} M_{RX}$ alloy performance index

More Info:

G.N. Haidemenopoulos, A. Katsamas and H. Kamoutsi,
Thermodynamics-Based Computational Design of Al-Mg-
Zr-Sc Alloys, Metallurgical and Materials Transactions A,
Vol.41(4), p.888-899, 2010