UNIVERSITY OF CAMBRIDGE

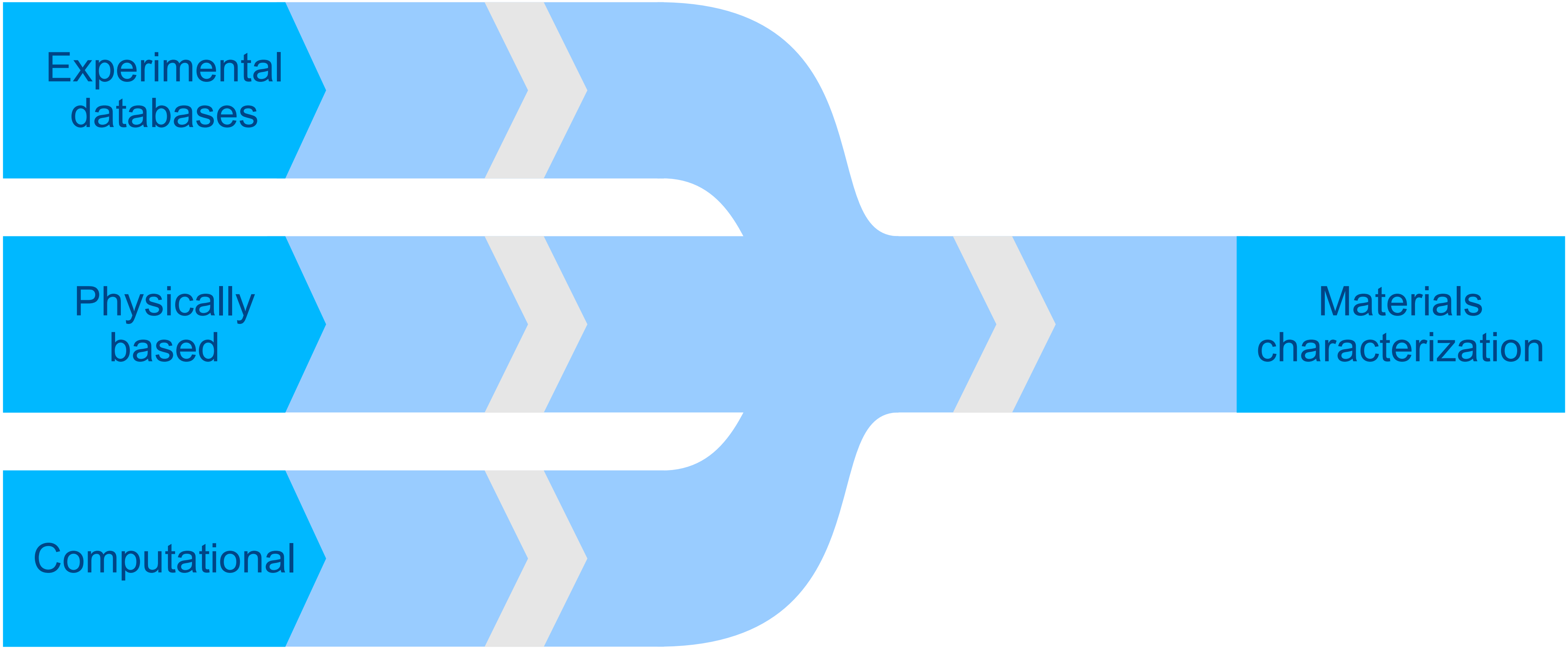
Concurrent materials design

Gareth Conduit

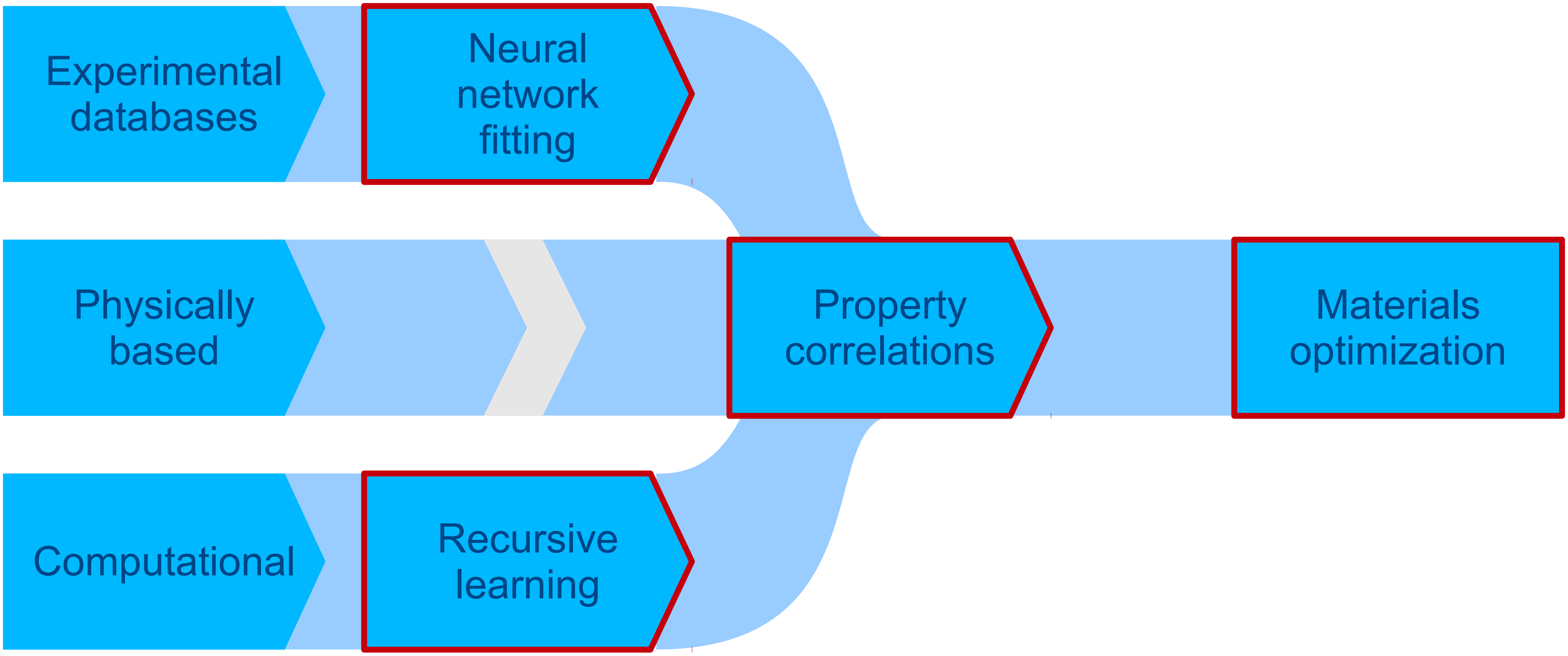
Patent GB1302743.8 (2013)
Patent GB1307533.8 (2013)
Patent GB1307535.3 (2013)
Patent US 2013/0052077 A1 (2013)
Acta Materialia, **61**, 3378 (2013)
Intermetallics, advanced online publication (2013)

Theory of Condensed Matter Group, Department of Physics

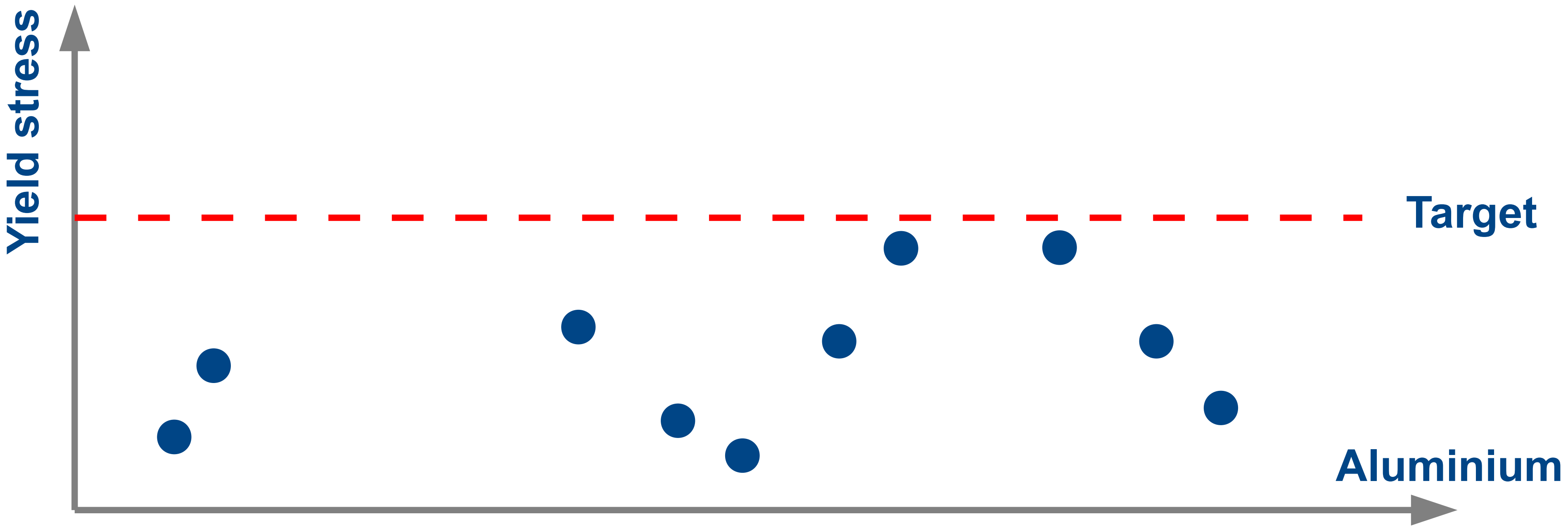
Four new tools



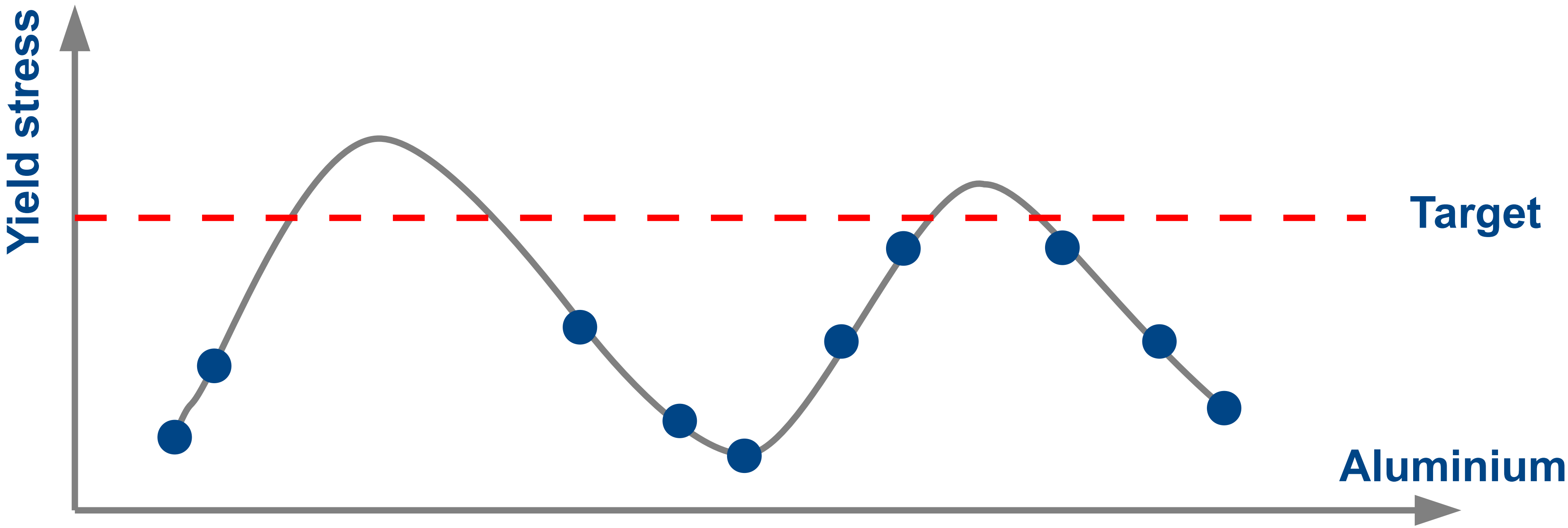
Four new tools



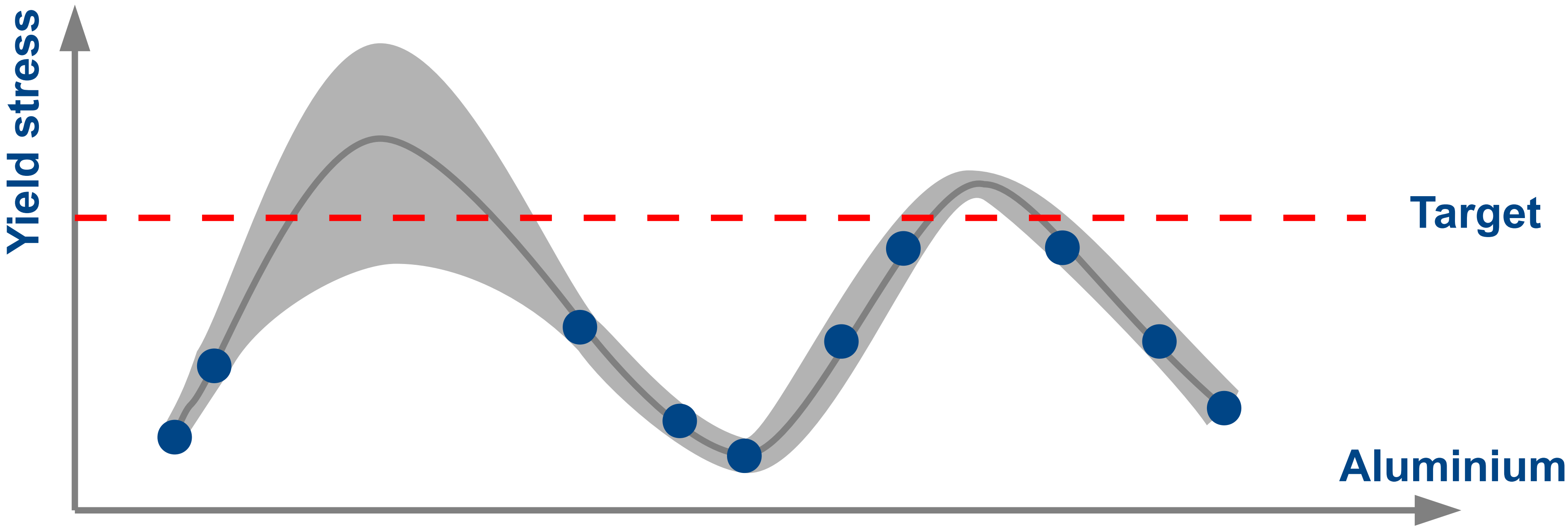
Neural network fitting & optimization



Neural network fitting & optimization



Neural network fitting & optimization



Recursive learning

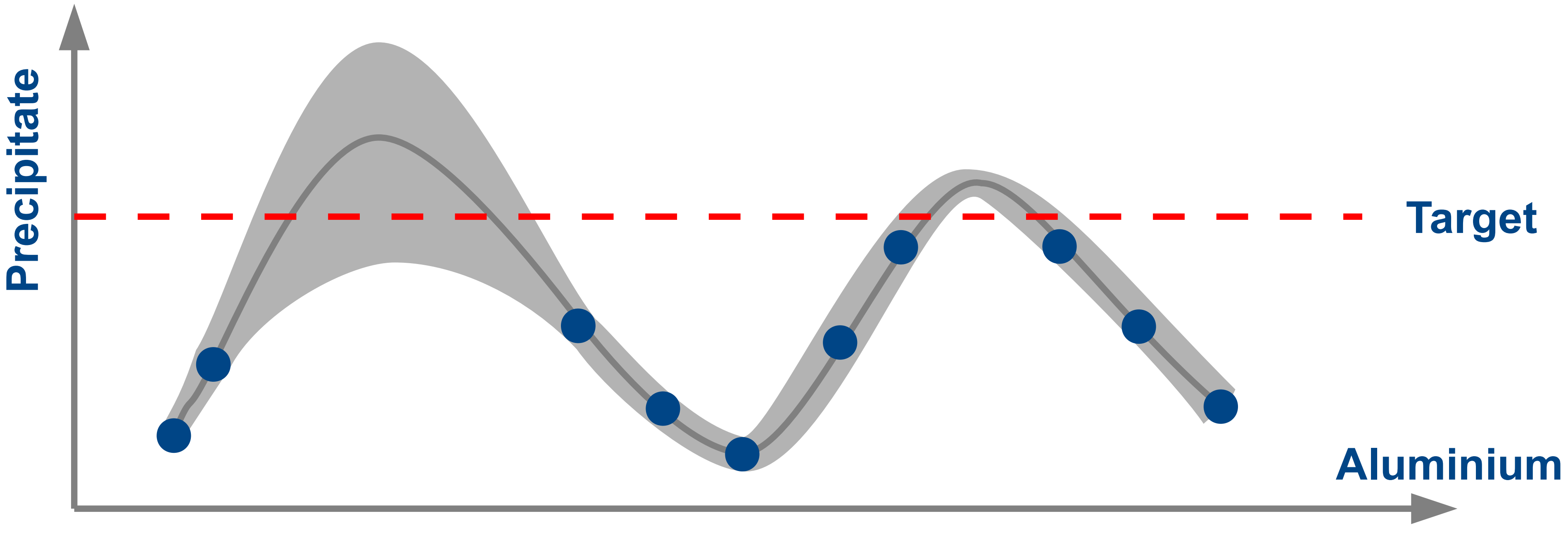
Calculate material property

↓

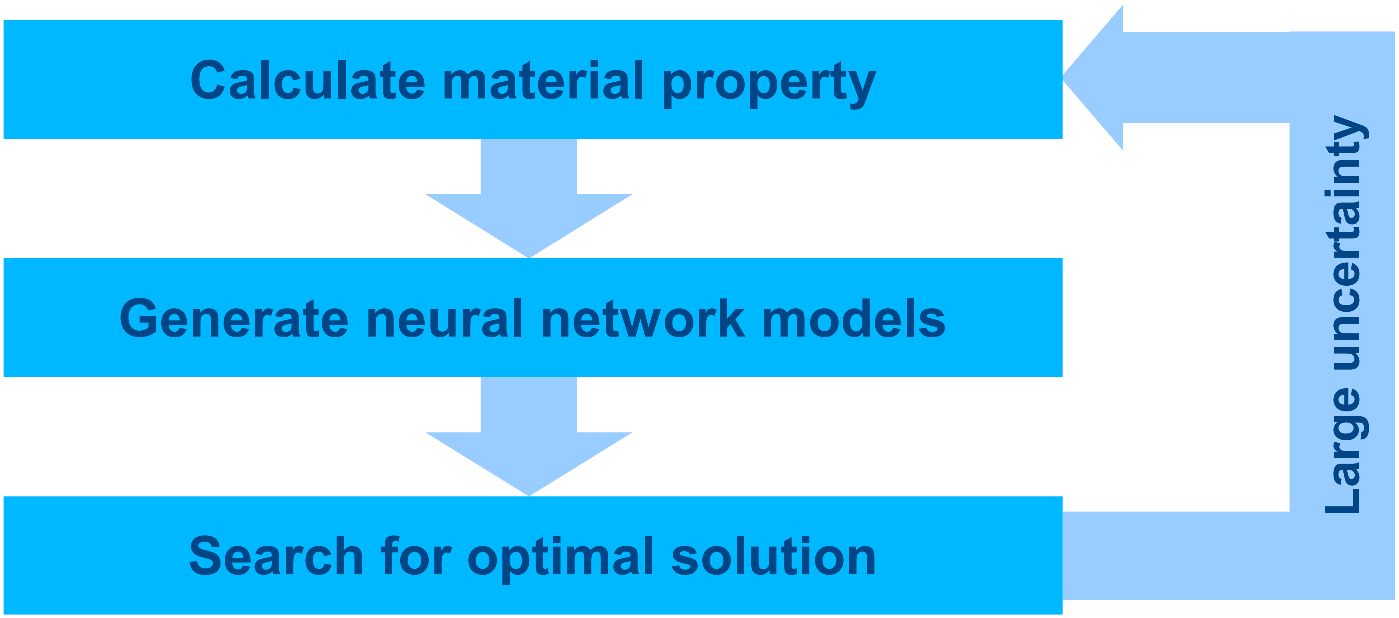
Generate neural network models

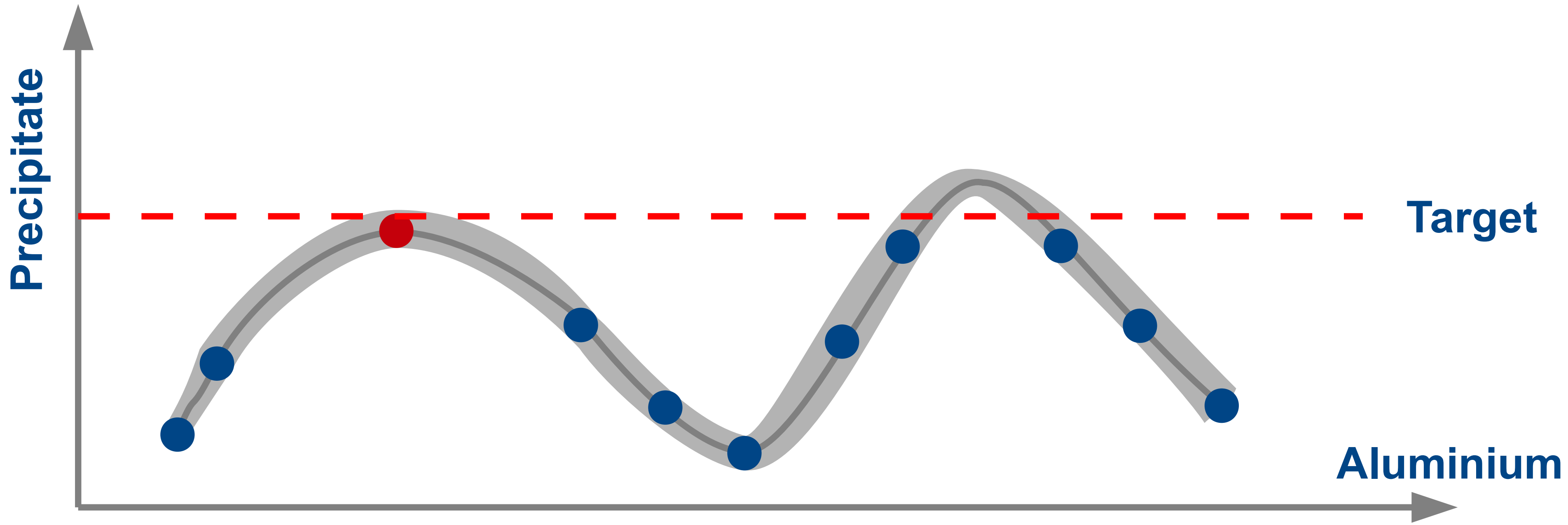
↓

Search for optimal solution

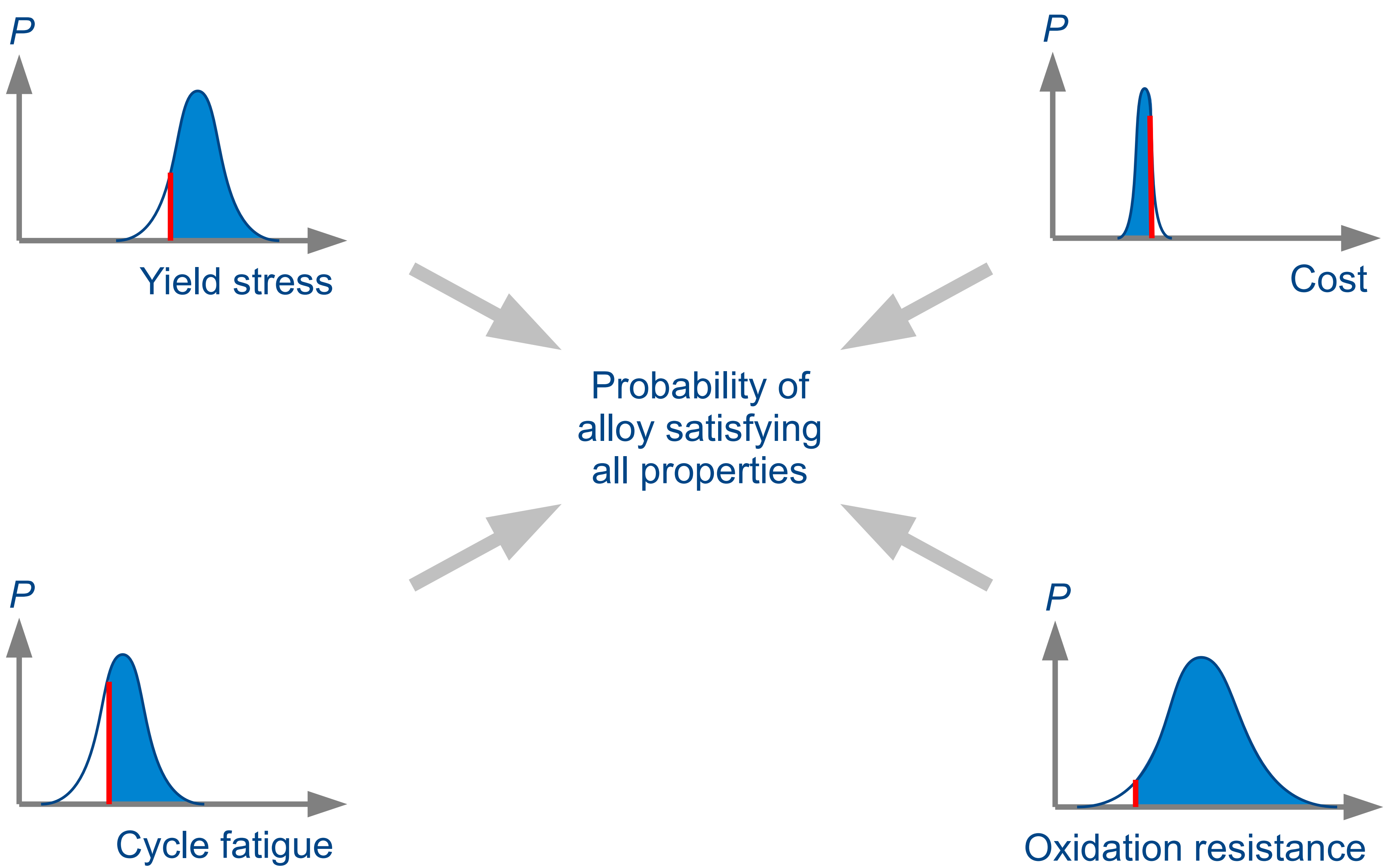


Recursive learning





Probability

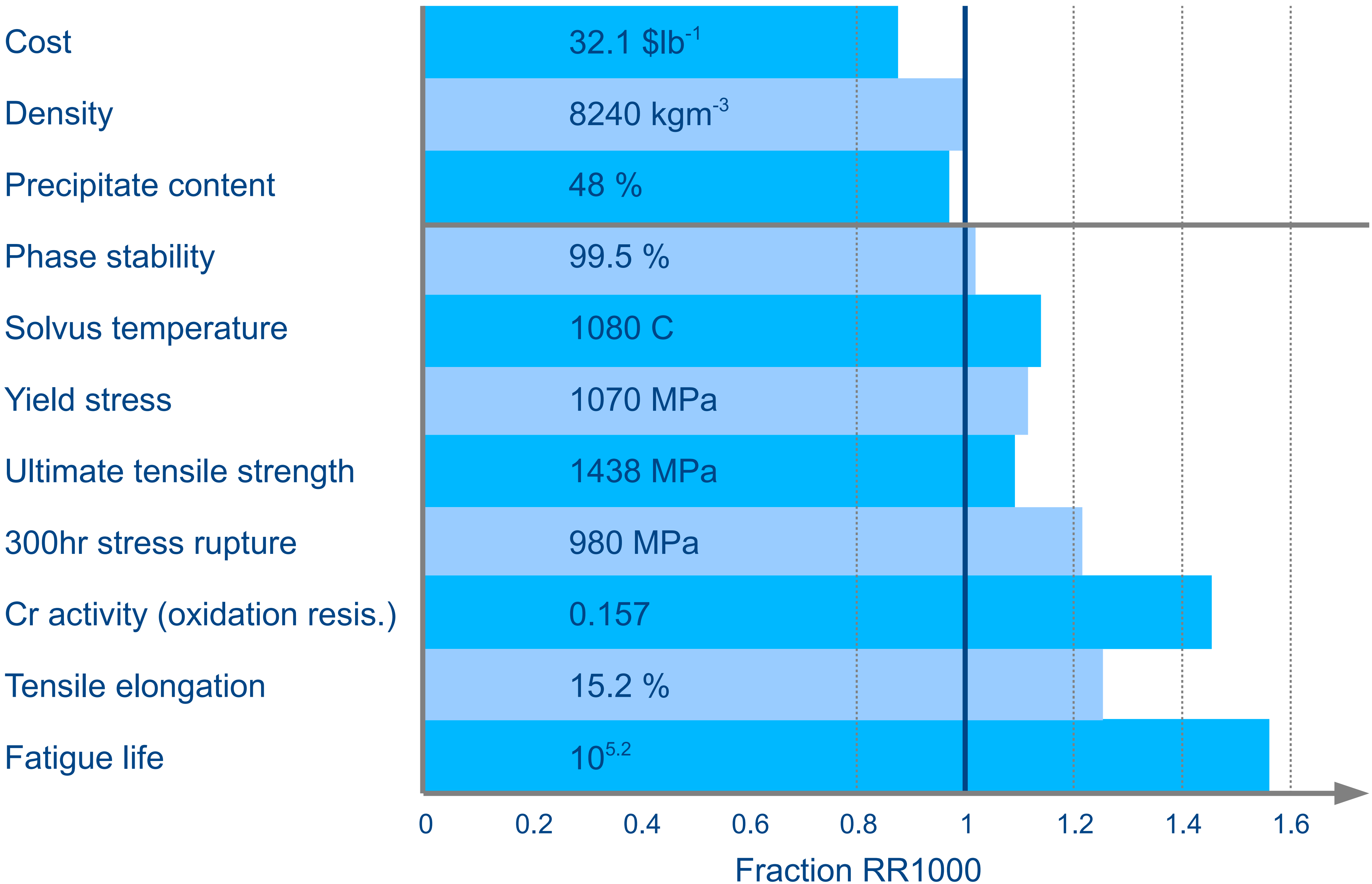


Patent GB1302743.8 (2013)

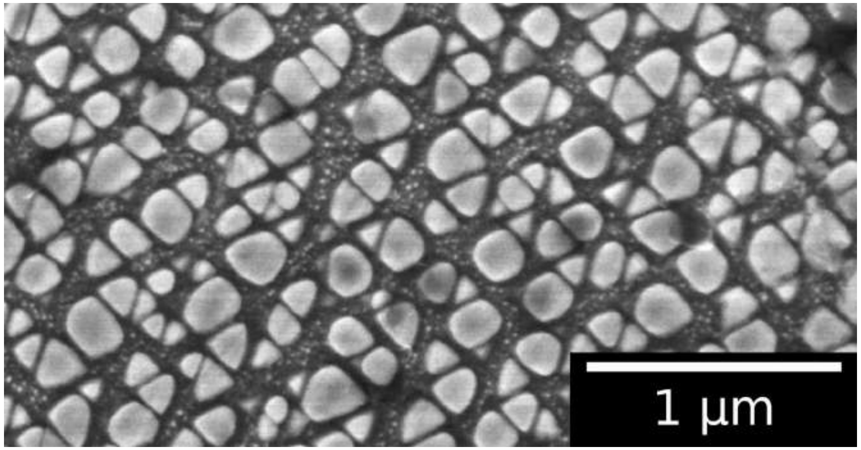
Ni-base superalloy

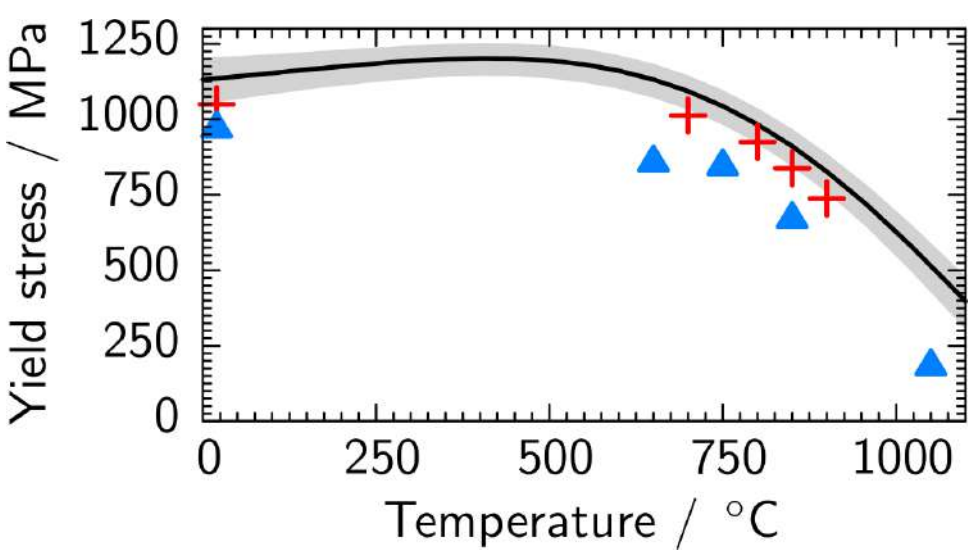
Cost	Physically based	
Density	Physically based	
Precipitate content	CALPHAD (Thermocalc)	
Phase stability	CALPHAD (Thermocalc)	
Solvus temperature	CALPHAD (Thermocalc)	
Yield stress	Neural net over database	6939 points
Ultimate tensile strength	Neural net over database	6127 points
300hr stress rupture	Neural net over database	10860 points
Cr activity (oxidation resis.)	Neural net over database	915 points
Tensile elongation	Neural net over database	2248 points
Fatigue life	Neural net over database	15105 points

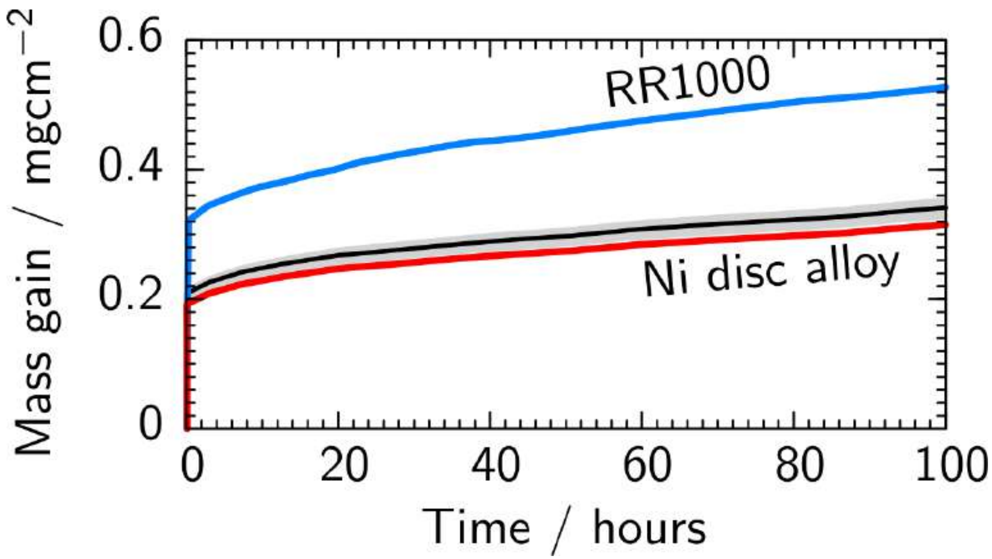
Ni-base superalloy



Ni-base superalloy

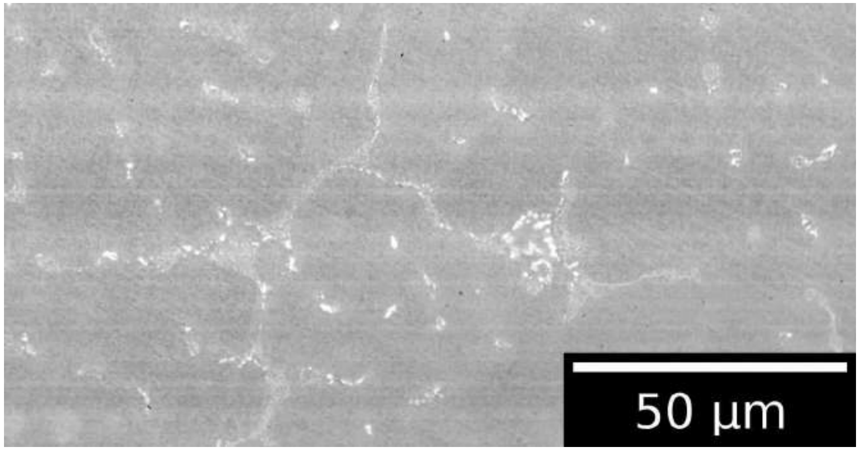


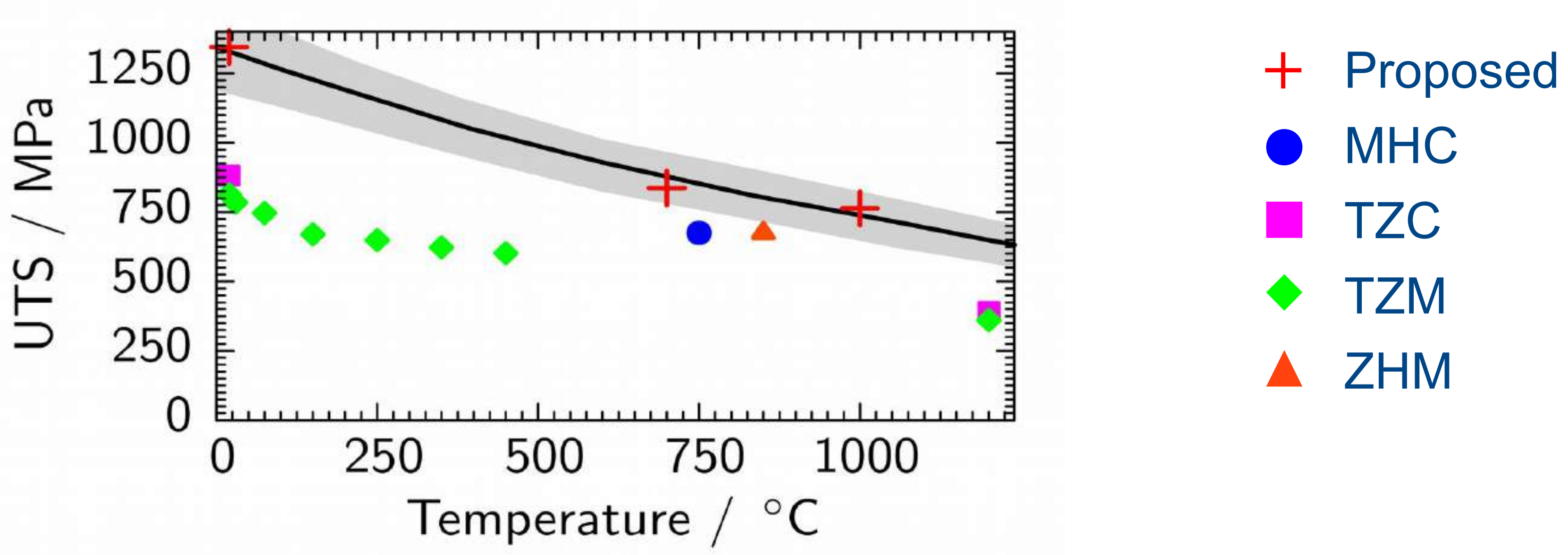




Amendment to patent US 2013/0052077 A1 (2013)

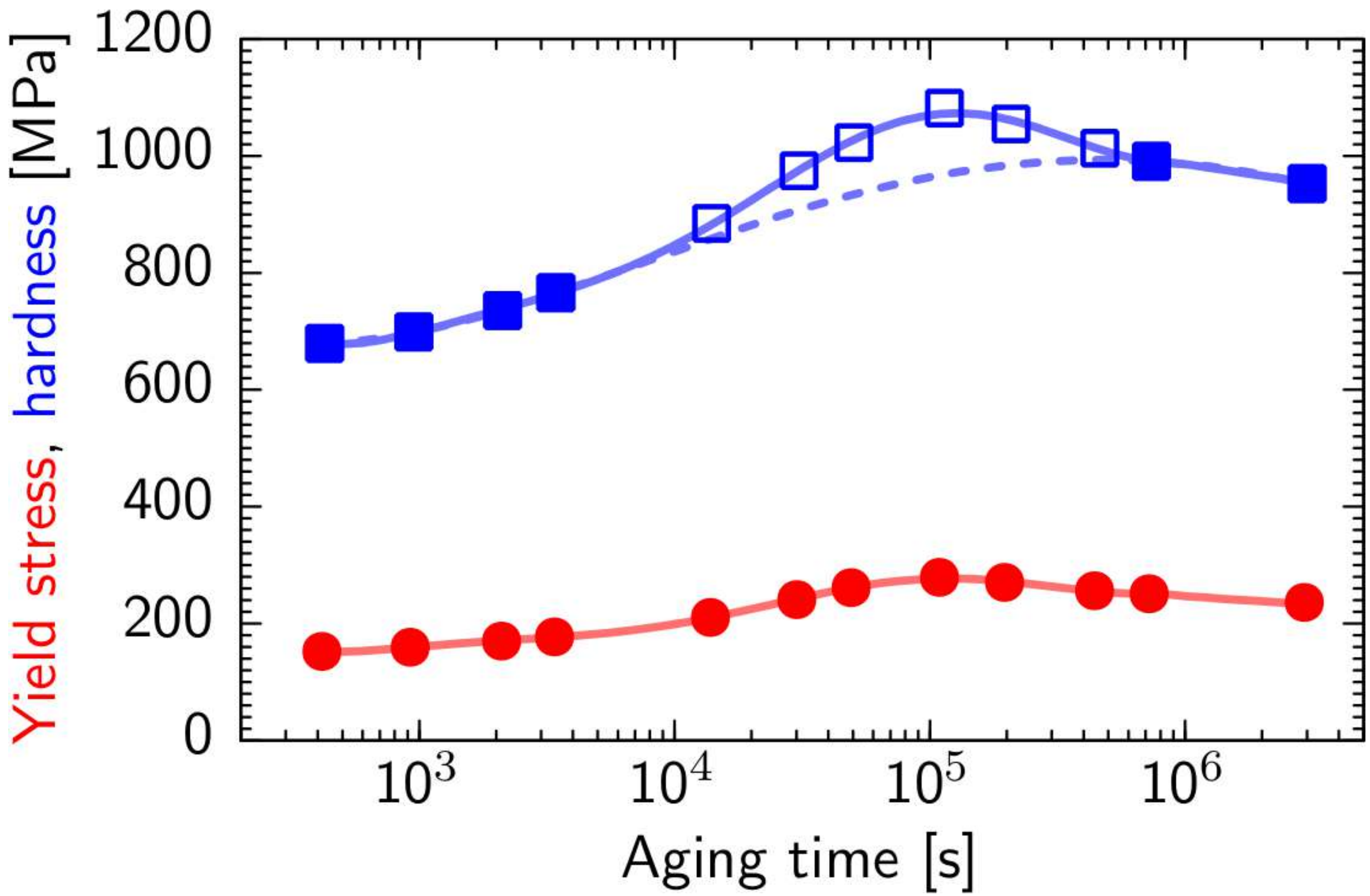
Mo-base alloy





Patents GB1307533.8 (2013), GB1307535.3 (2013)

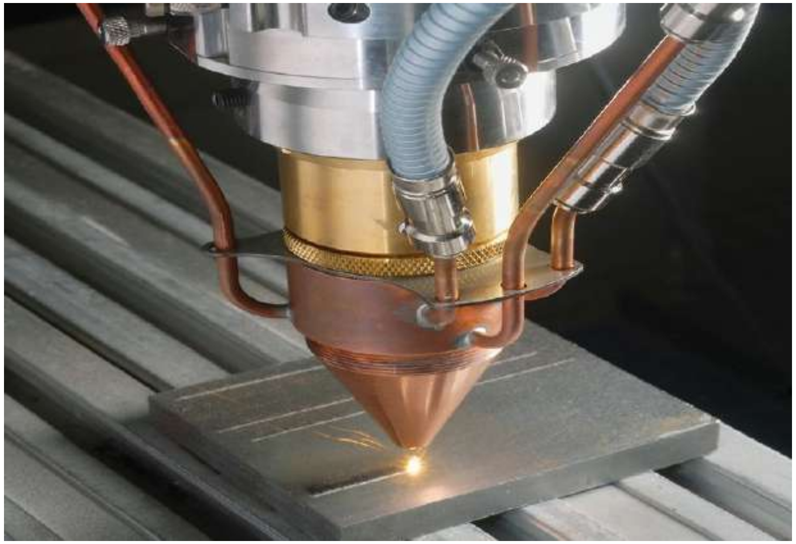
Correlations between properties



Data for Al-Mg-Si alloy from Mat. Sci and Engin. A **443**, 172 (2007)

Correlations between properties

Alloy for
direct laser deposition

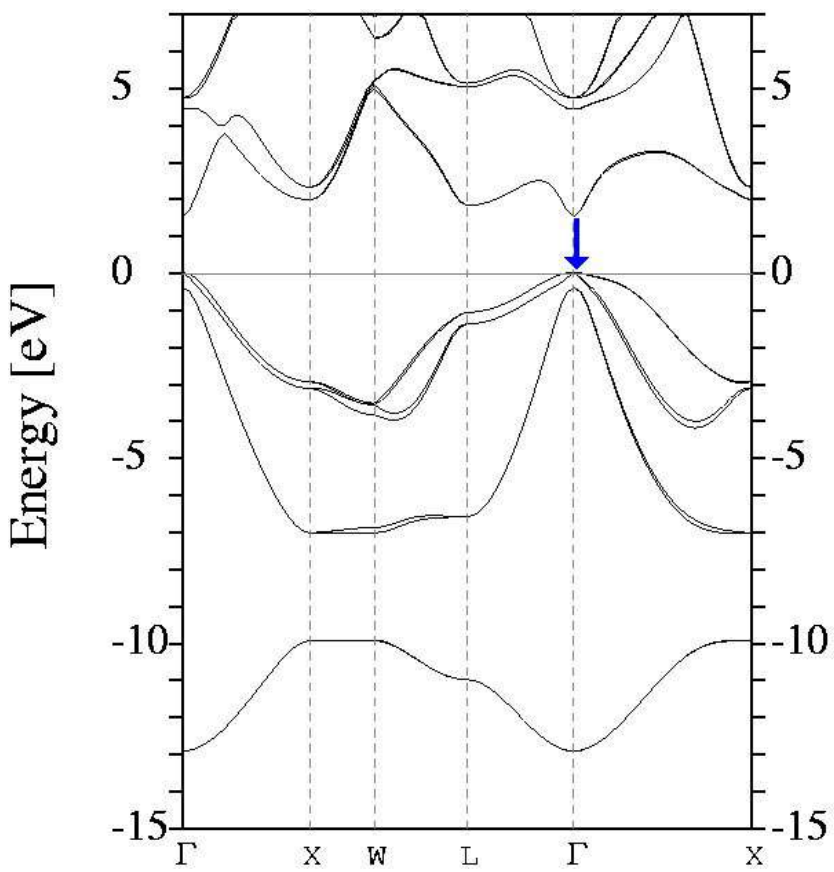


10 points for
quality of deposition

Property
correlations

Weldability, thermal conductivity, thermal expansivity, precipitate fraction

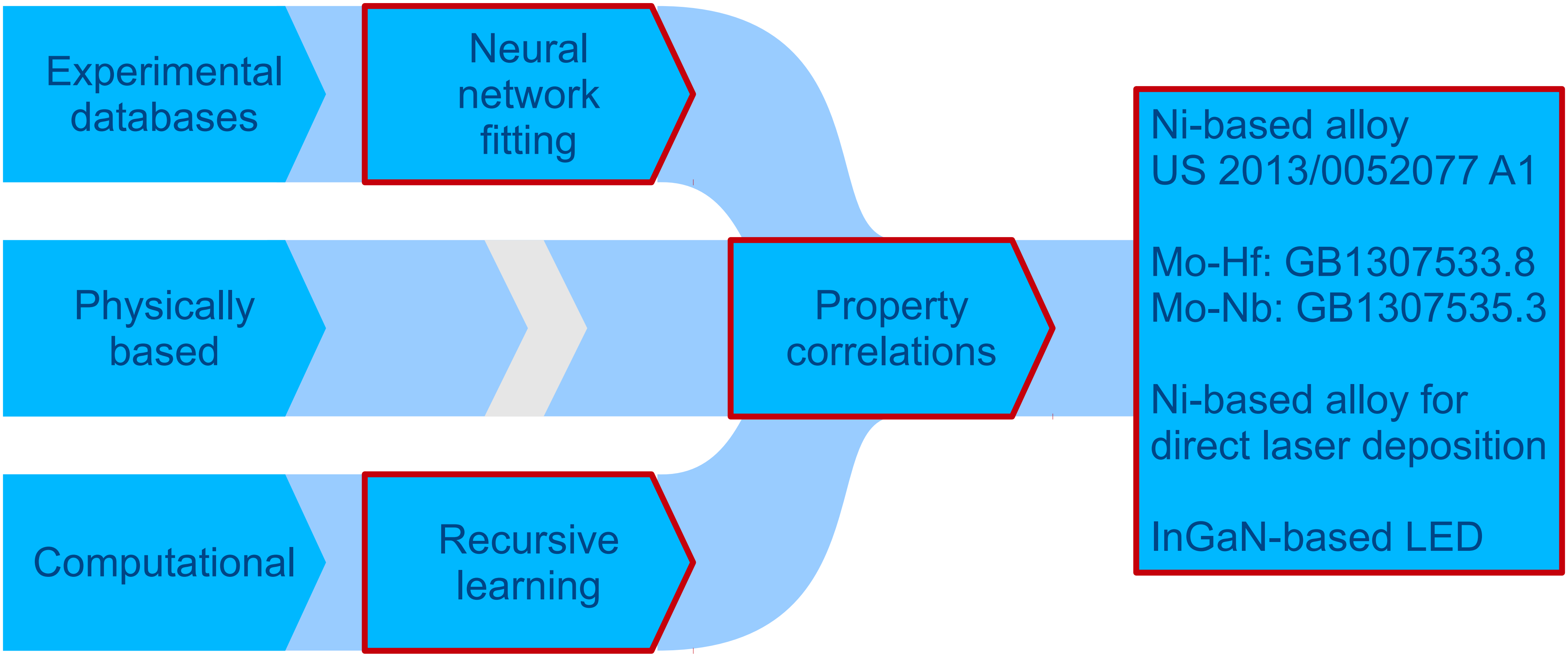
Semiconductors



100 points for band gap, luminous efficacy, efficiency

Band structure: band gap, density of states, effective mass

Four new tools



Prospects in the future

Include other experimental & computational databases

Combine further first principles approaches: DFT, molecular dynamics, phase field models

Conformance testing, retirement-for-cause

Concurrent materials design

Mo-base alloy