UNIVERSITY OF CAMBRIDGE

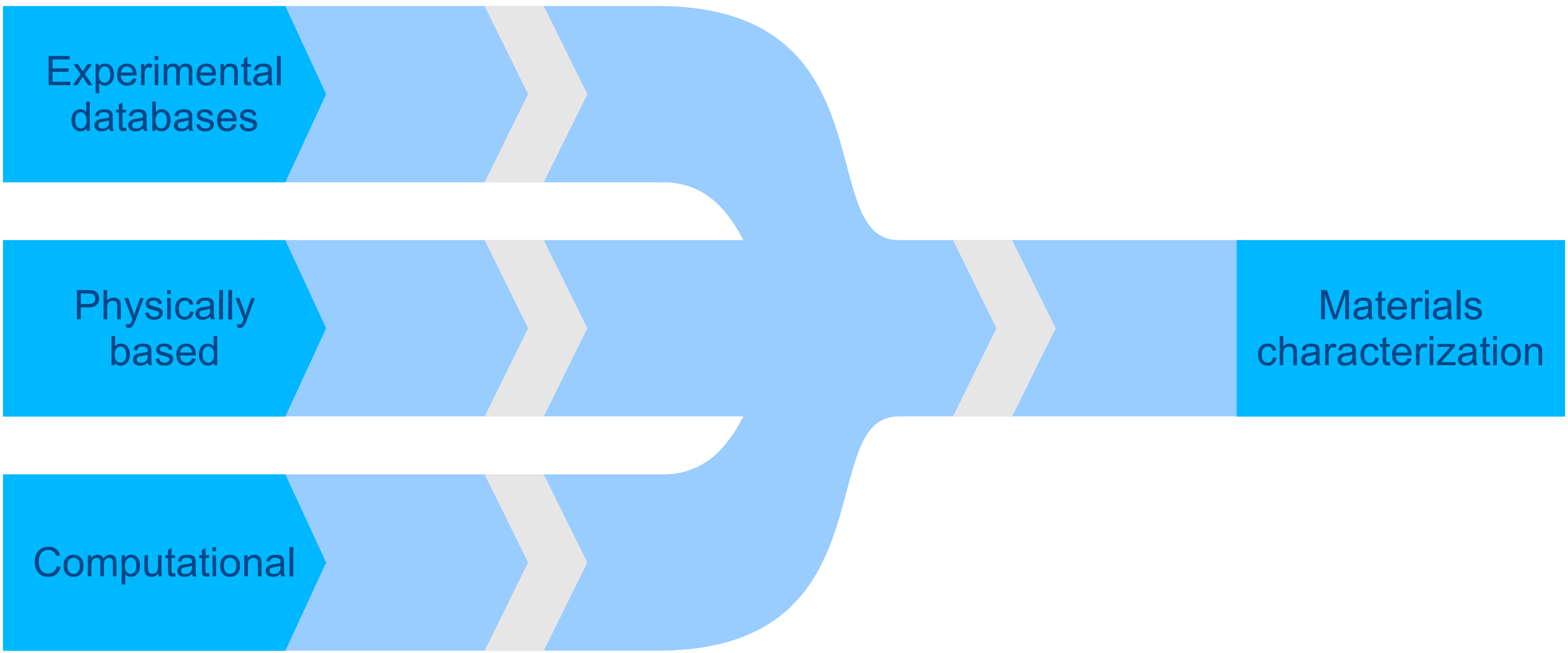
Concurrent materials design

Gareth Conduit

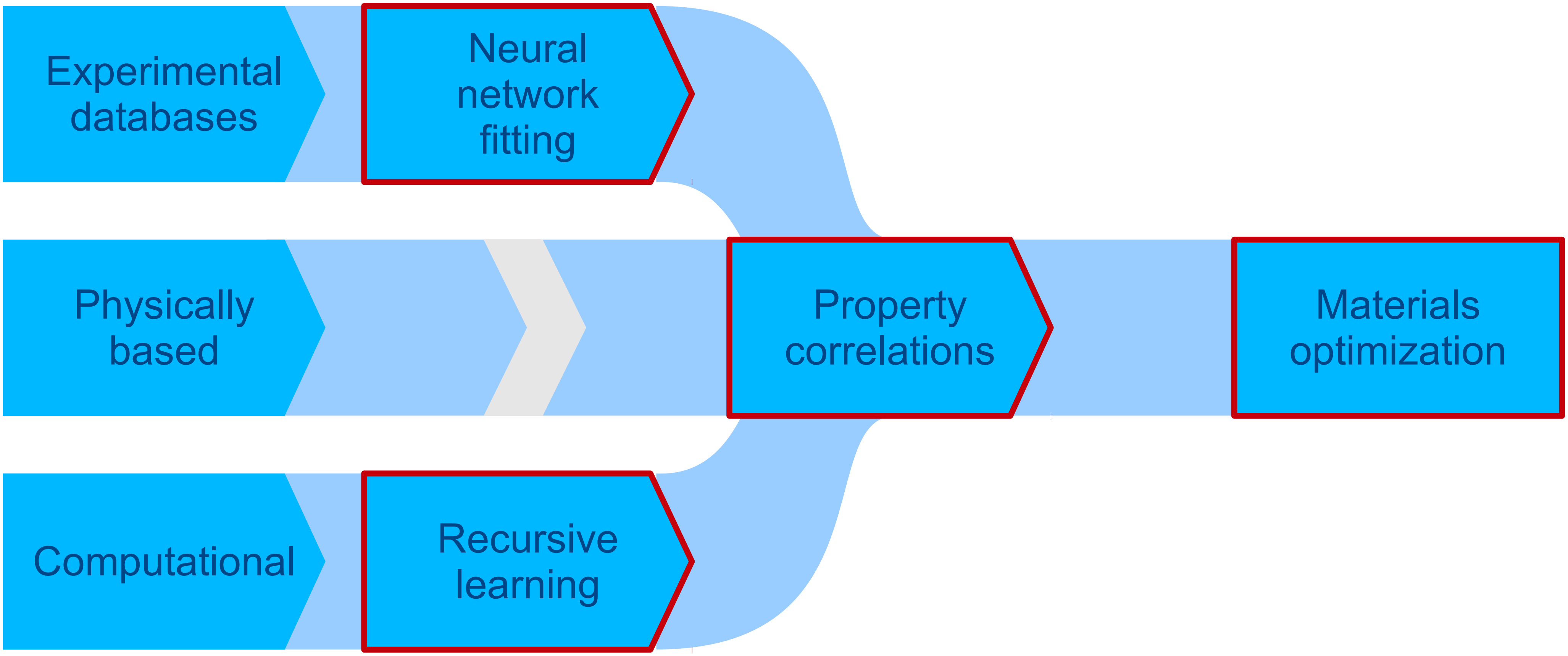
EP14153898.3; US 2014/177578; GB1302743.8
EP14161255.6; US 2014/223465; GB1307533.8
EP14161529.4; GB1307535.3
EP14157622.3; amendment to US 2013/0052077 A1; GB1408536.9
Acta Materialia **61**, 3378 (2013)
Intermetallics **48**, 62 (2014)

Theory of Condensed Matter Group, Department of Physics

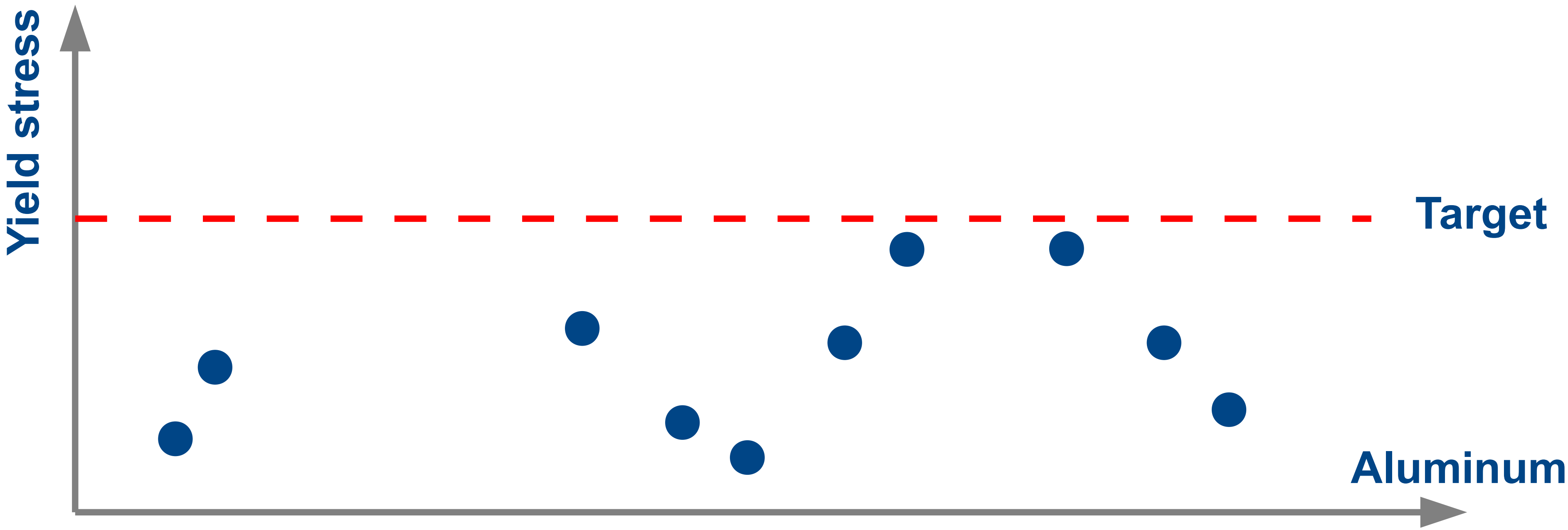
Four new tools



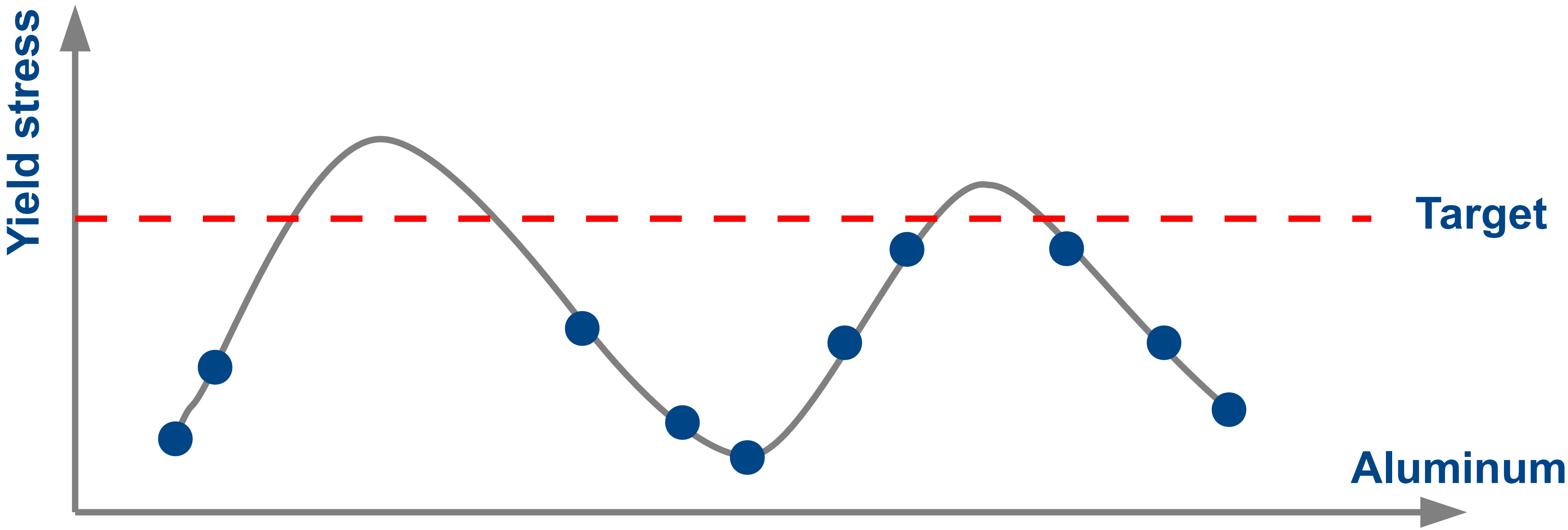
Four new tools



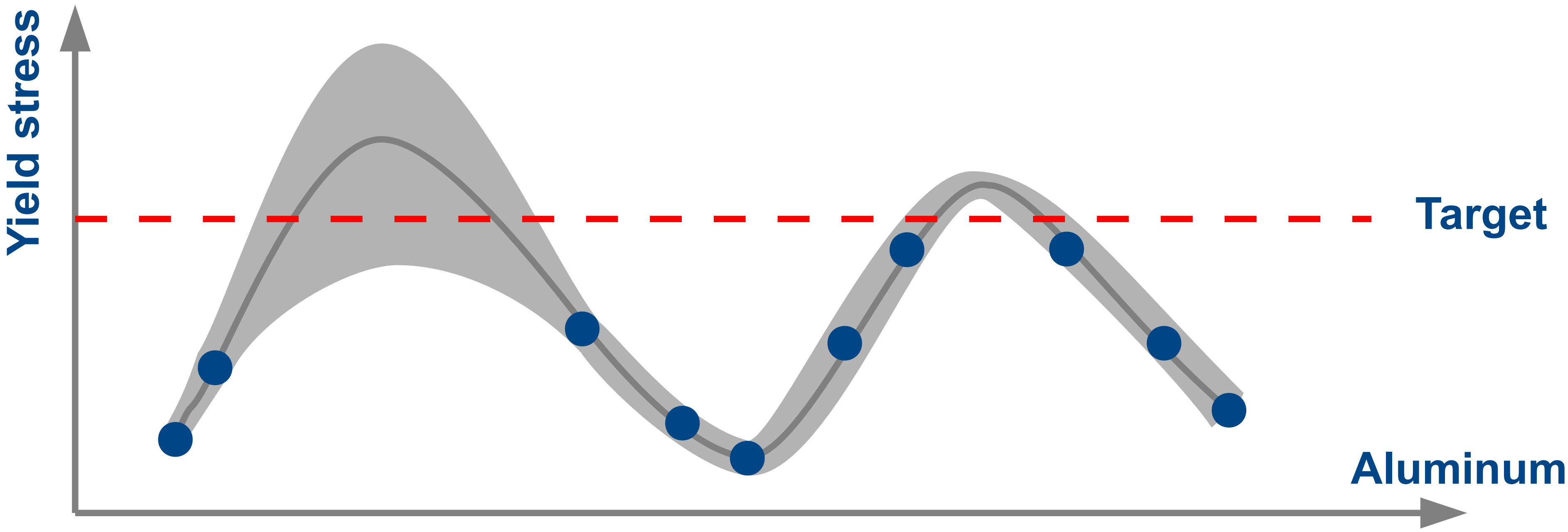
Neural network fitting & optimization



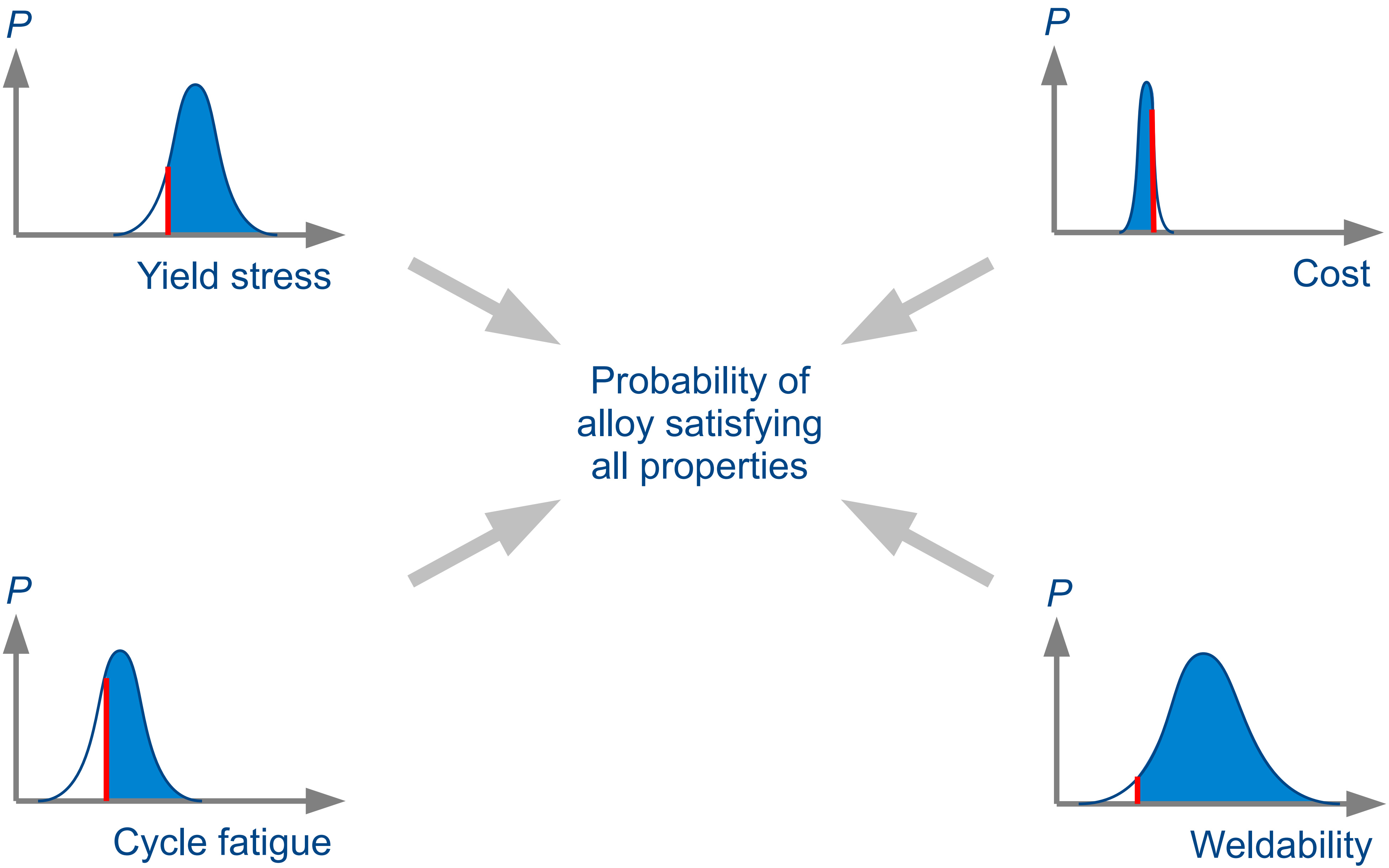
Neural network fitting & optimization



Neural network fitting & optimization

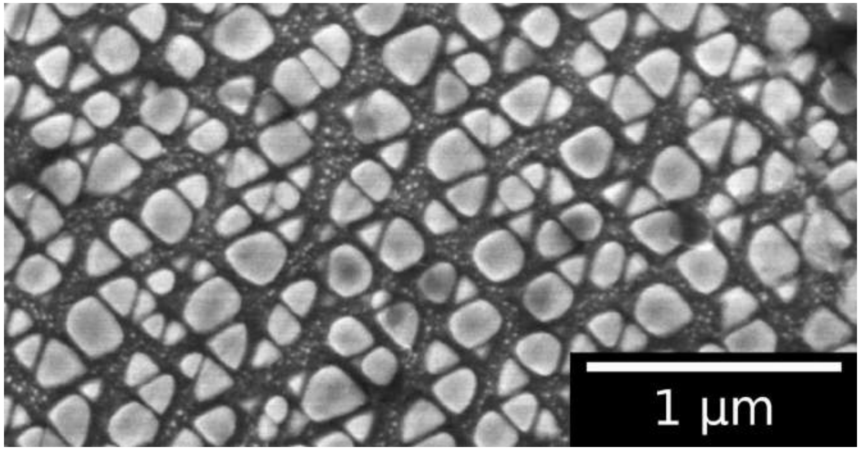


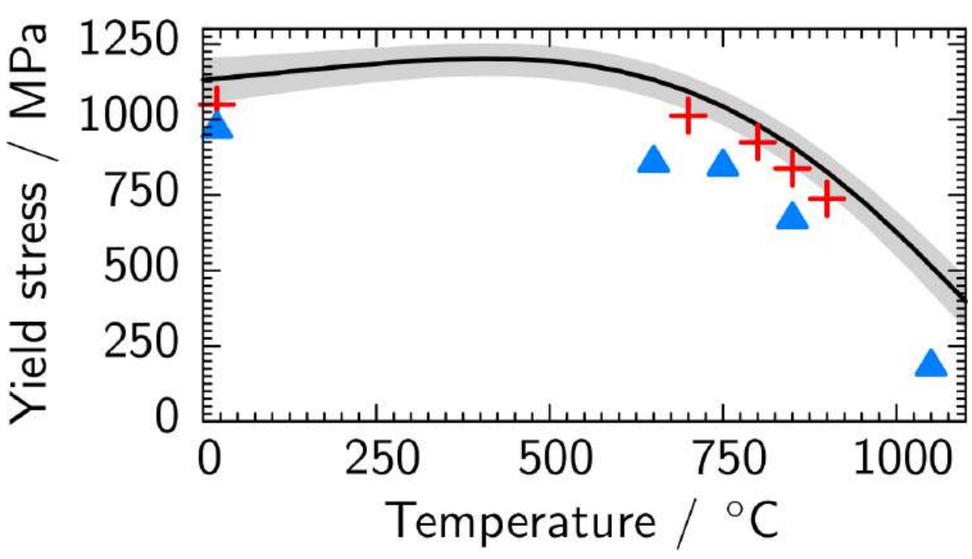
Probability

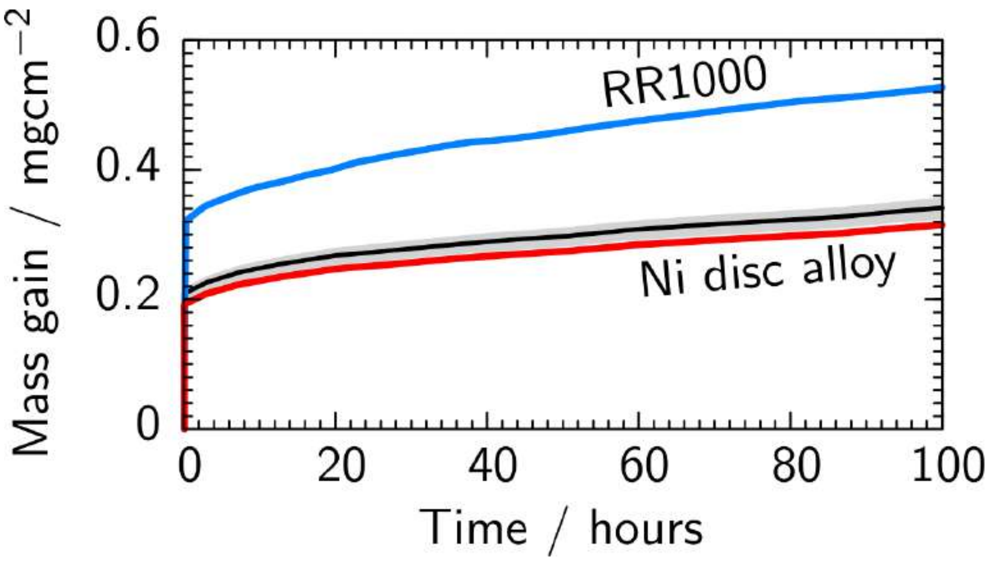


EP14153898.3; US 2014/177578; GB1302743.8

Ni-base superalloy

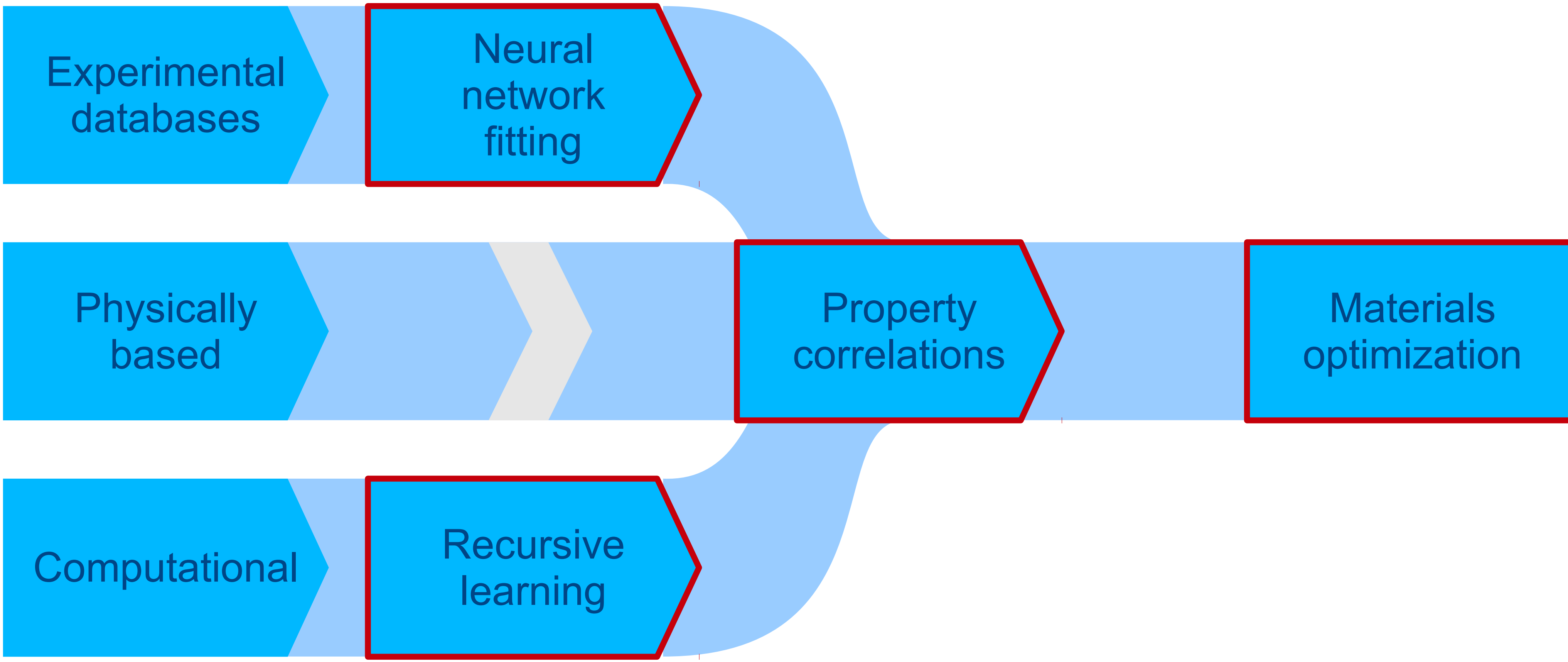




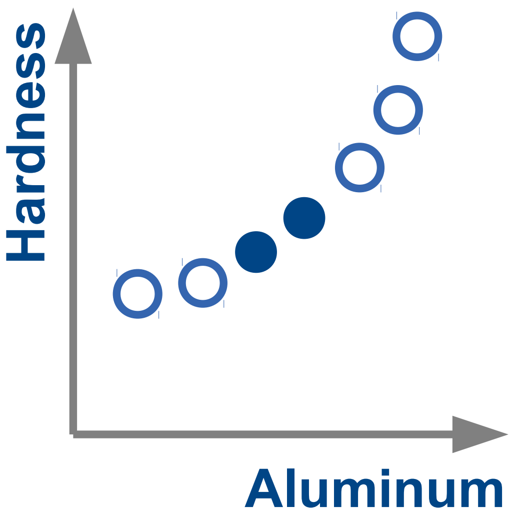


Amendment to US 2013/0052077 A1; EP14157622.3; GB1408536.9

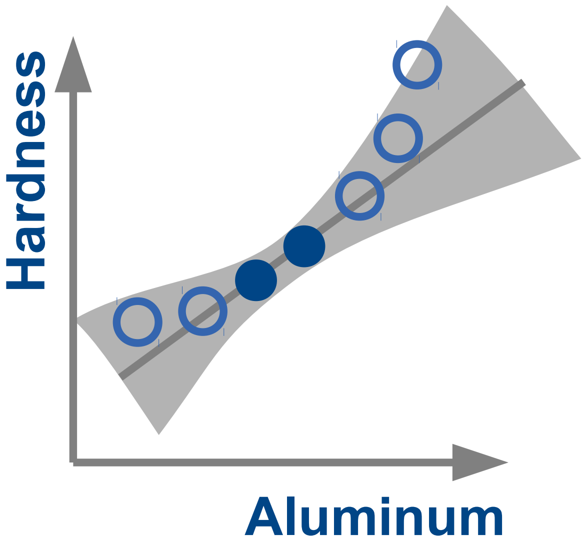
Four new tools



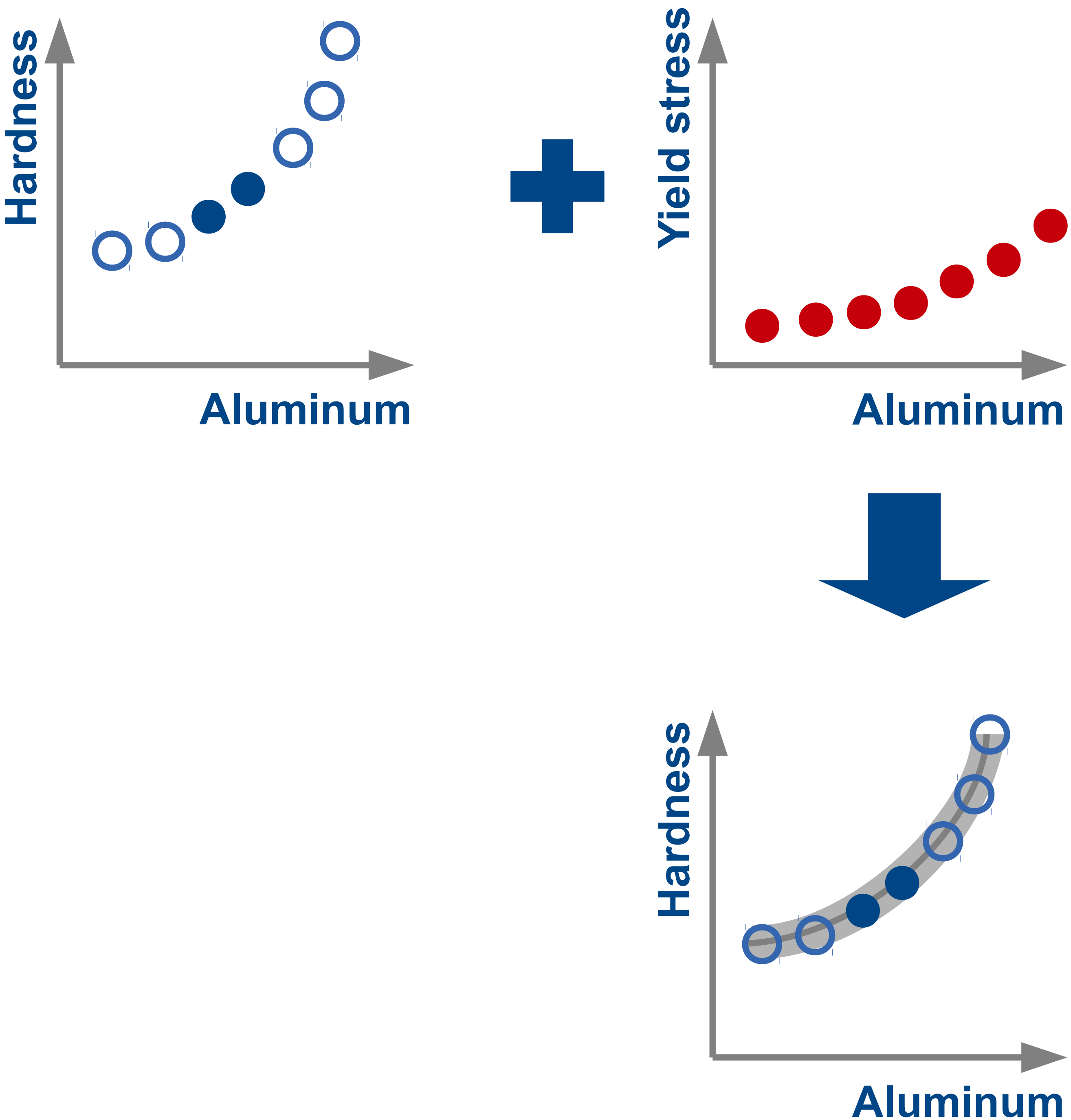
Correlations between properties



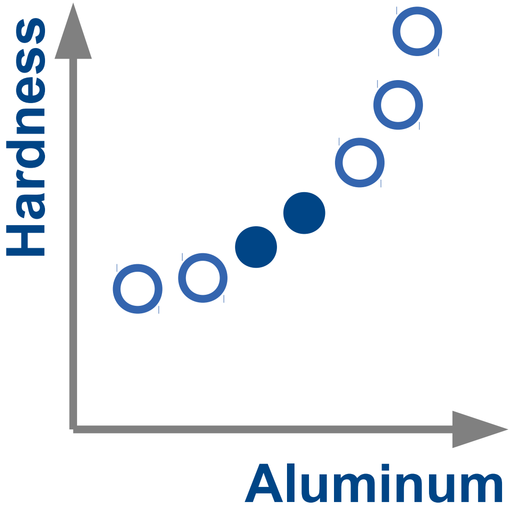
Correlations between properties

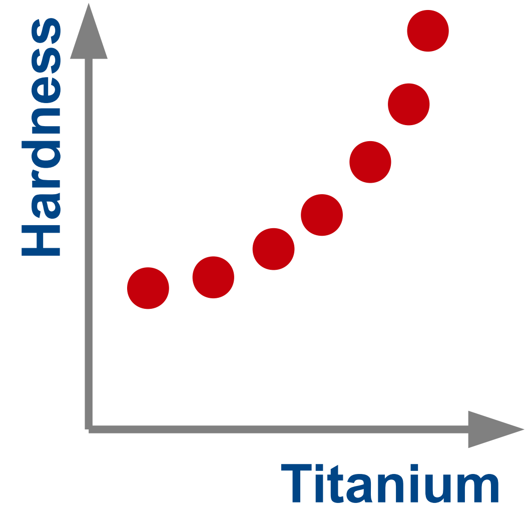


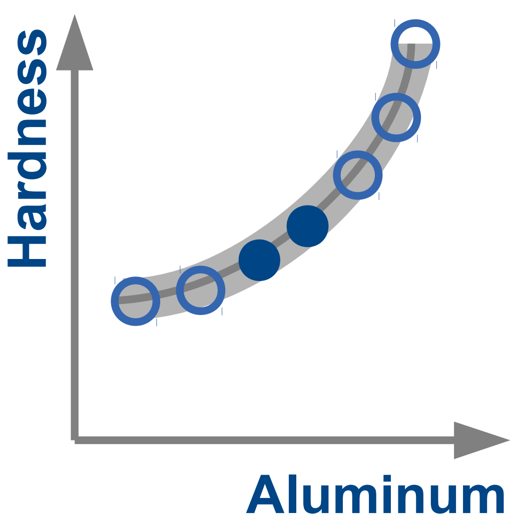
Correlations between properties



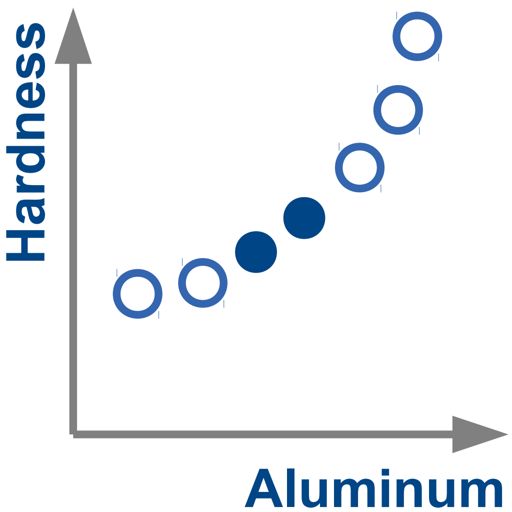
Correlations between properties

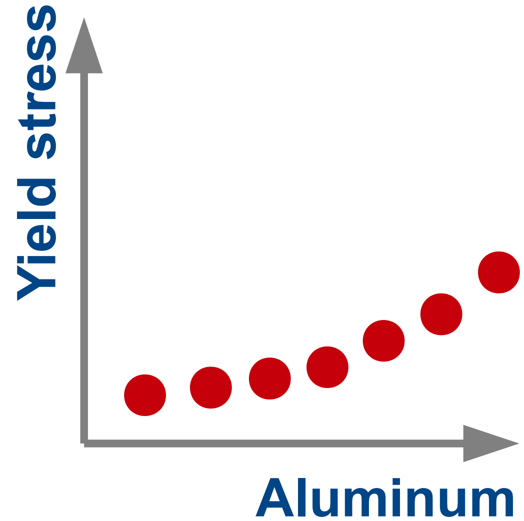


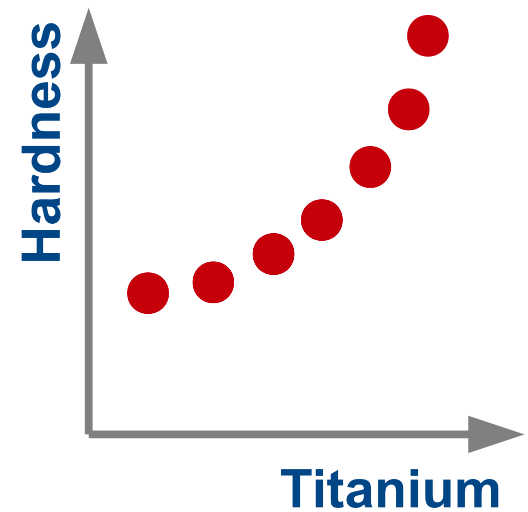




Correlations between properties







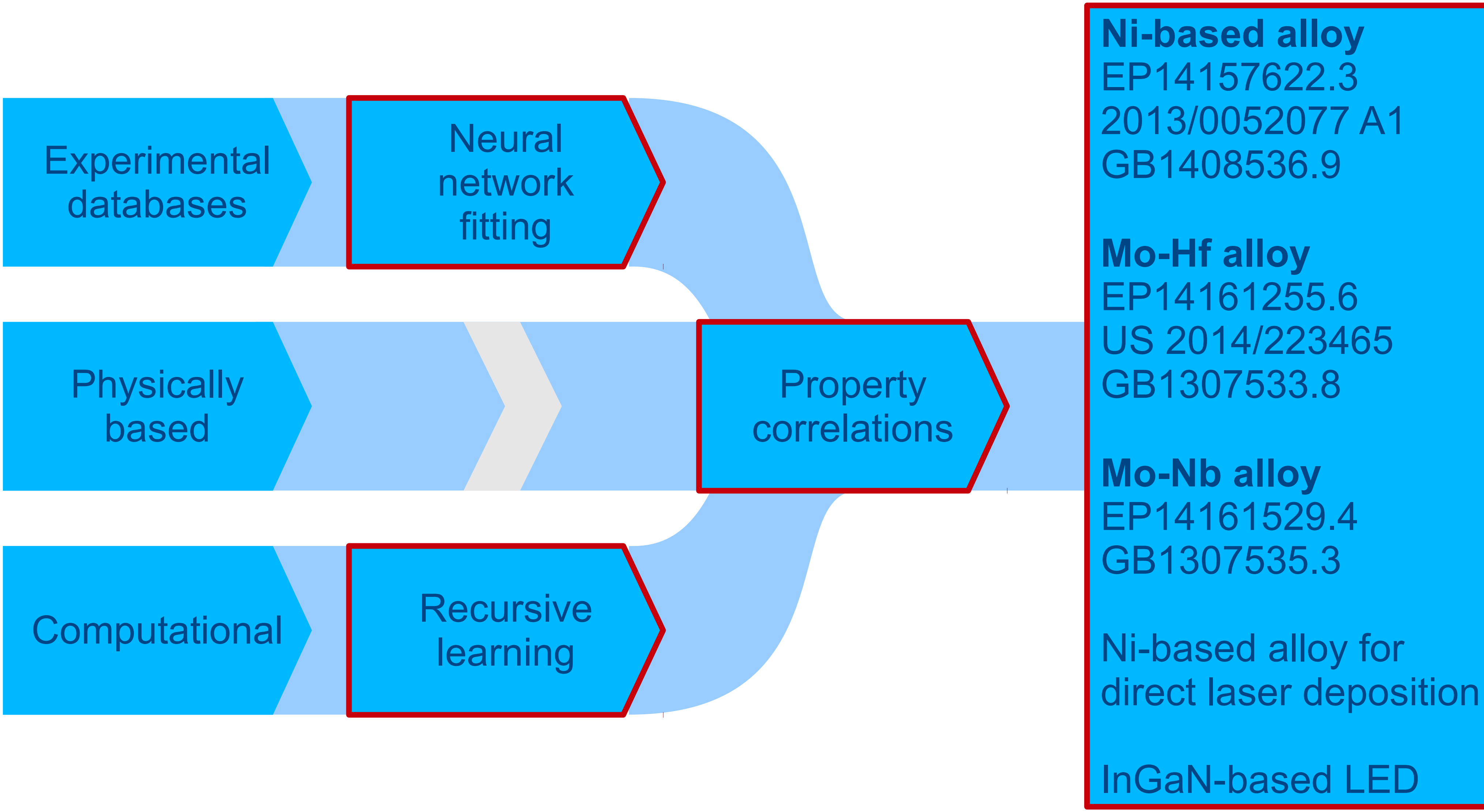
Relationships between material properties & computer simulations

Relationships between material families

Search for LEDs with Samsung Electronics

Alloy for direct laser deposition with Rolls-Royce

Four new tools



Prospects in the future

Exploit correlations between material properties, compositions, and families to design four new alloys

Combine strengths of experimental databases with first principles approaches

Concurrent materials design

Recursive learning

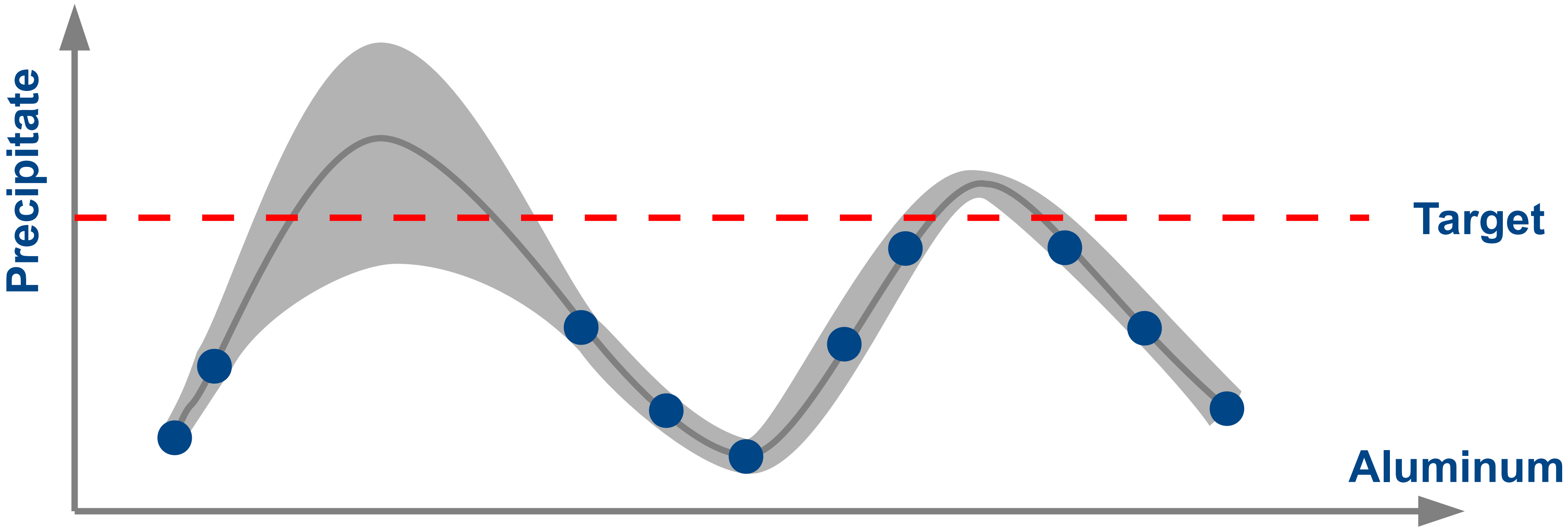
Calculate material property

↓

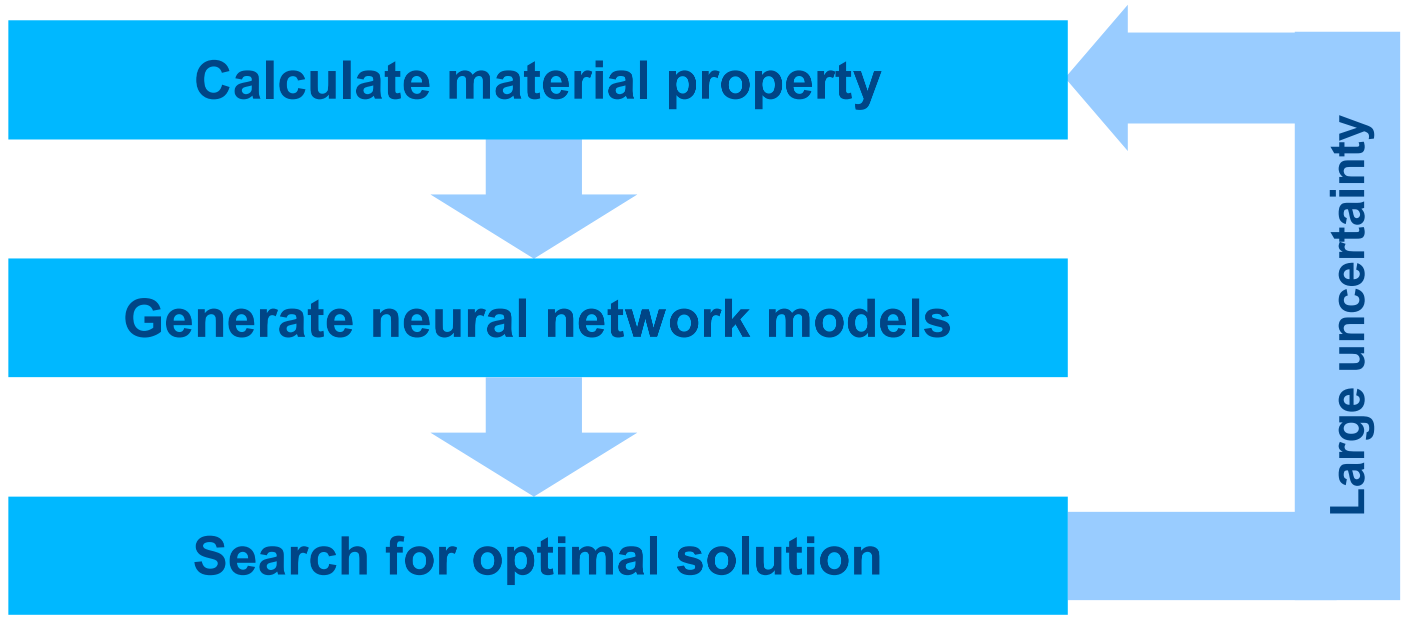
Generate neural network models

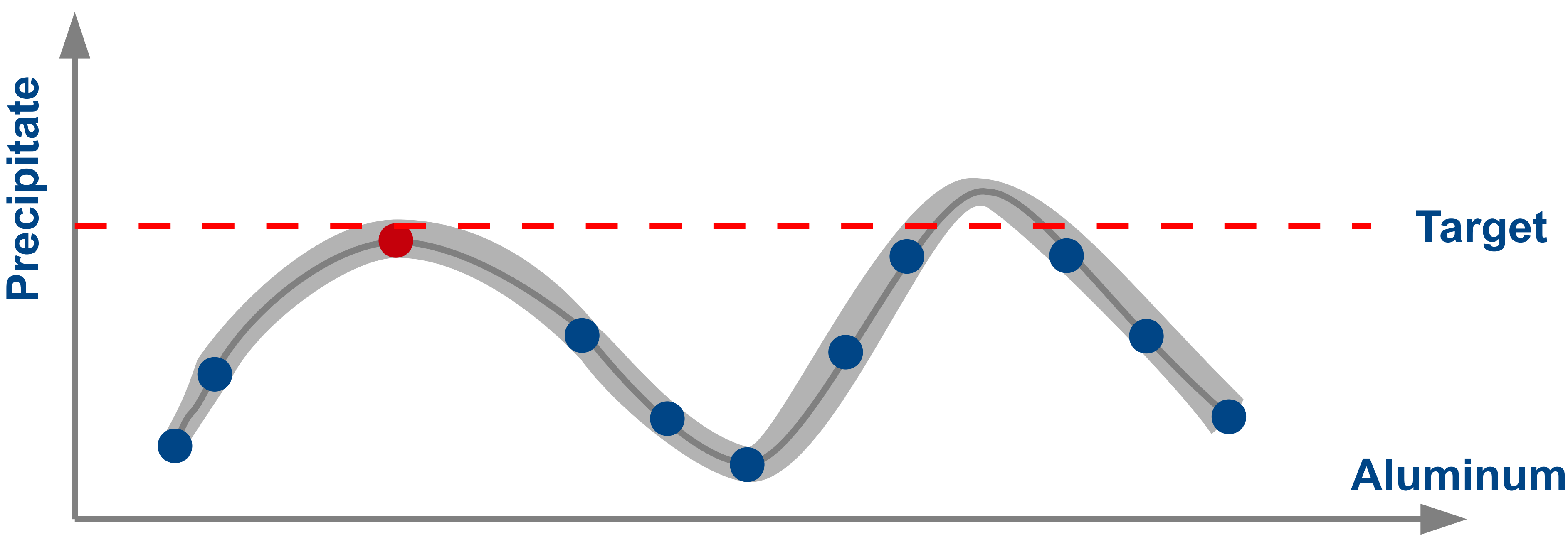
↓

Search for optimal solution

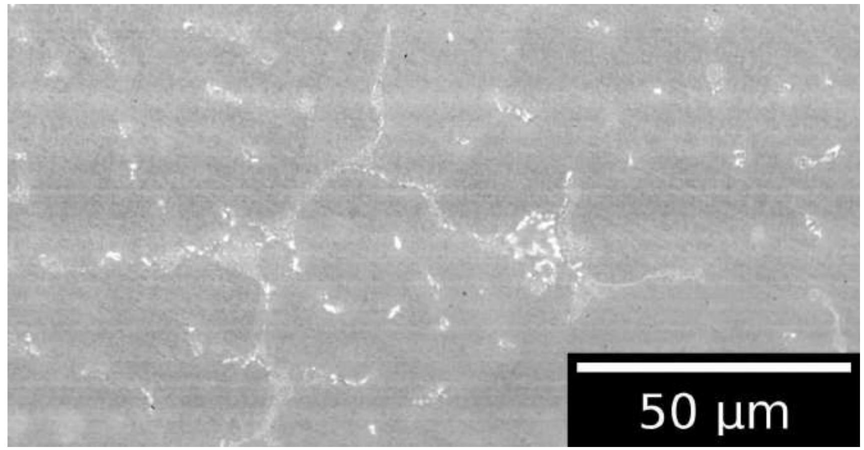


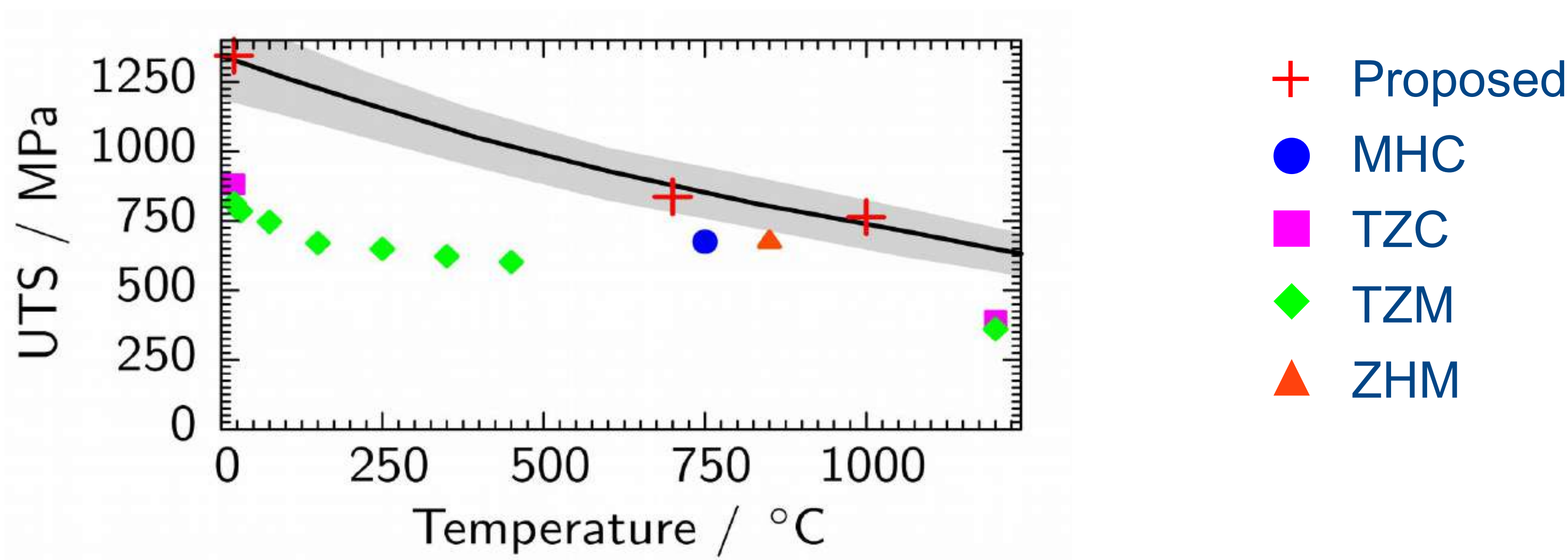
Recursive learning





Mo-base alloy





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

Mo-base alloy