UNIVERSITY OF CAMBRIDGE

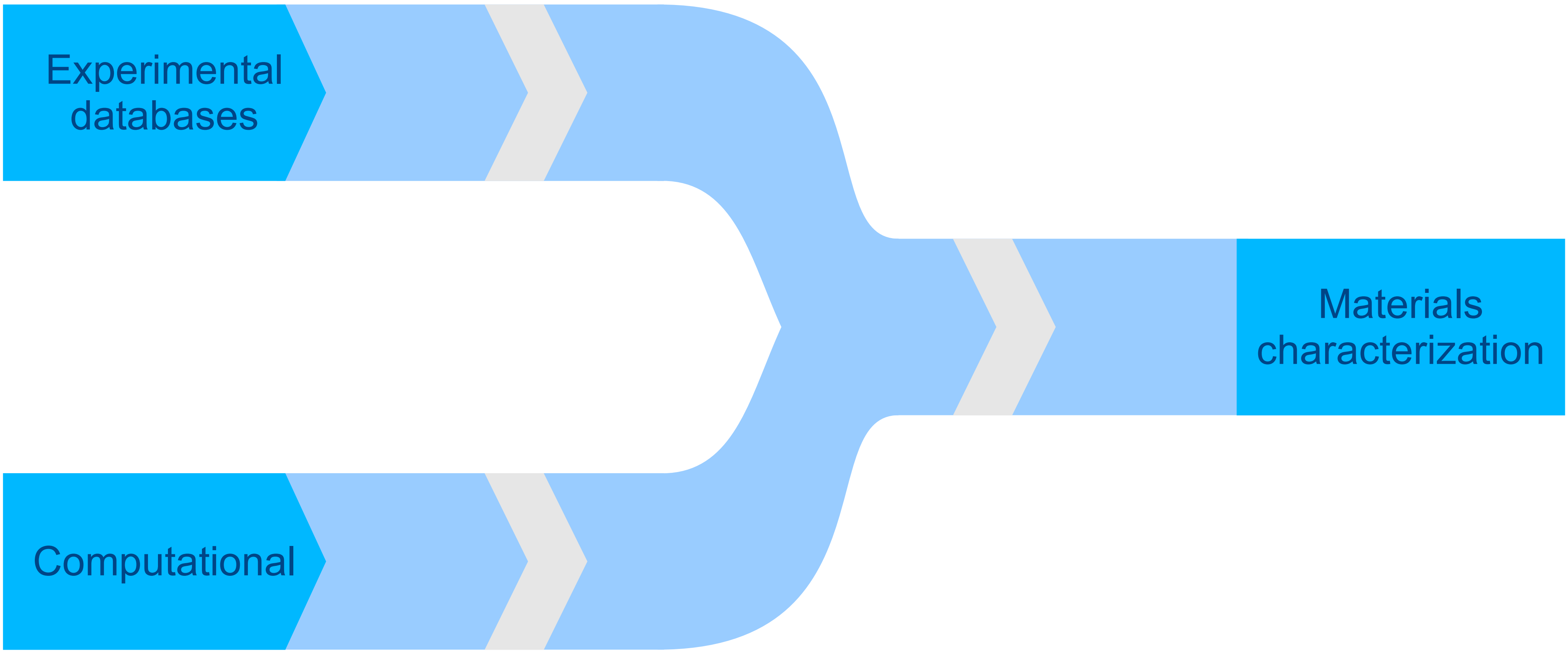
Concurrent materials design

Gareth Conduit

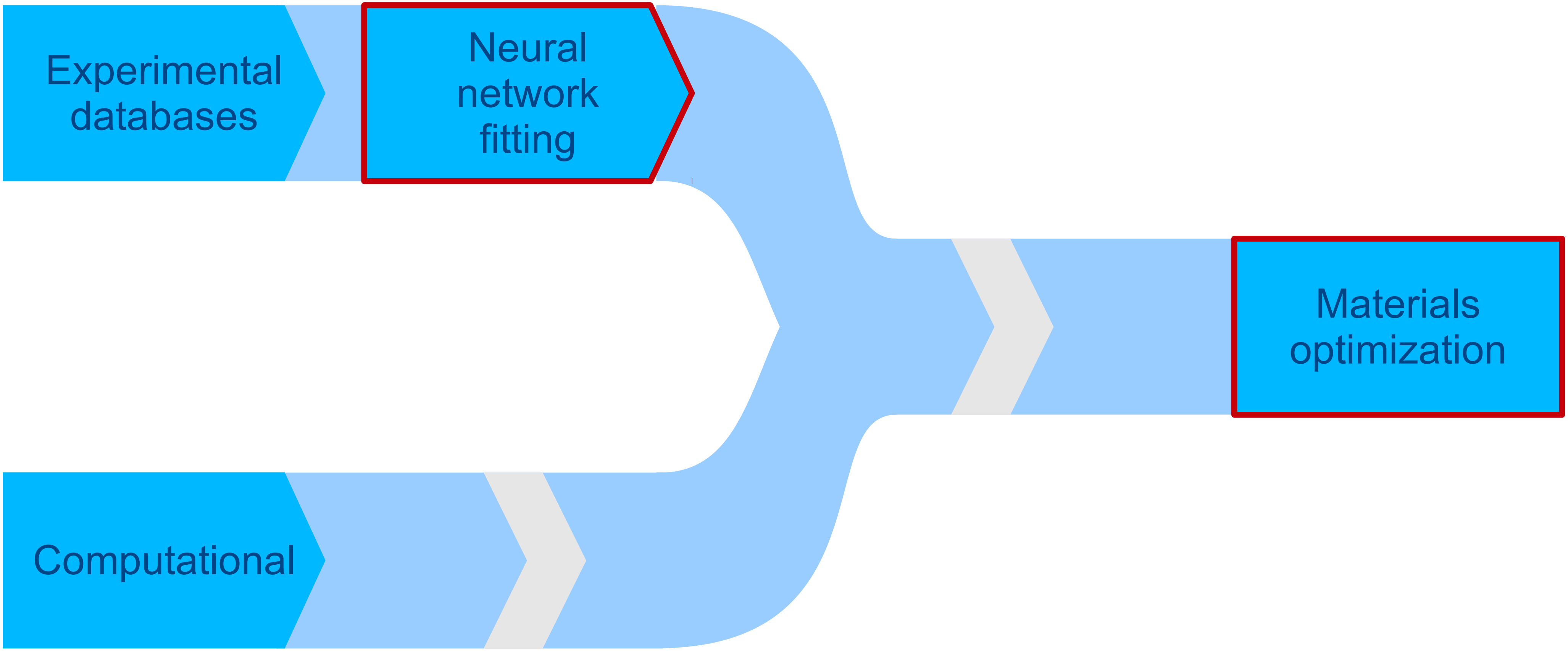
EP14153898.3; US 2014/177578; GB1302743.8
EP14161255.6; US 2014/223465; GB1307533.8
EP14161529.4; GB1307535.3
EP14157622.3; amendment to US 2013/0052077 A1; GB1408536.9
Acta Materialia **61**, 3378 (2013)
Intermetallics **48**, 62 (2014)

Theory of Condensed Matter Group, Department of Physics

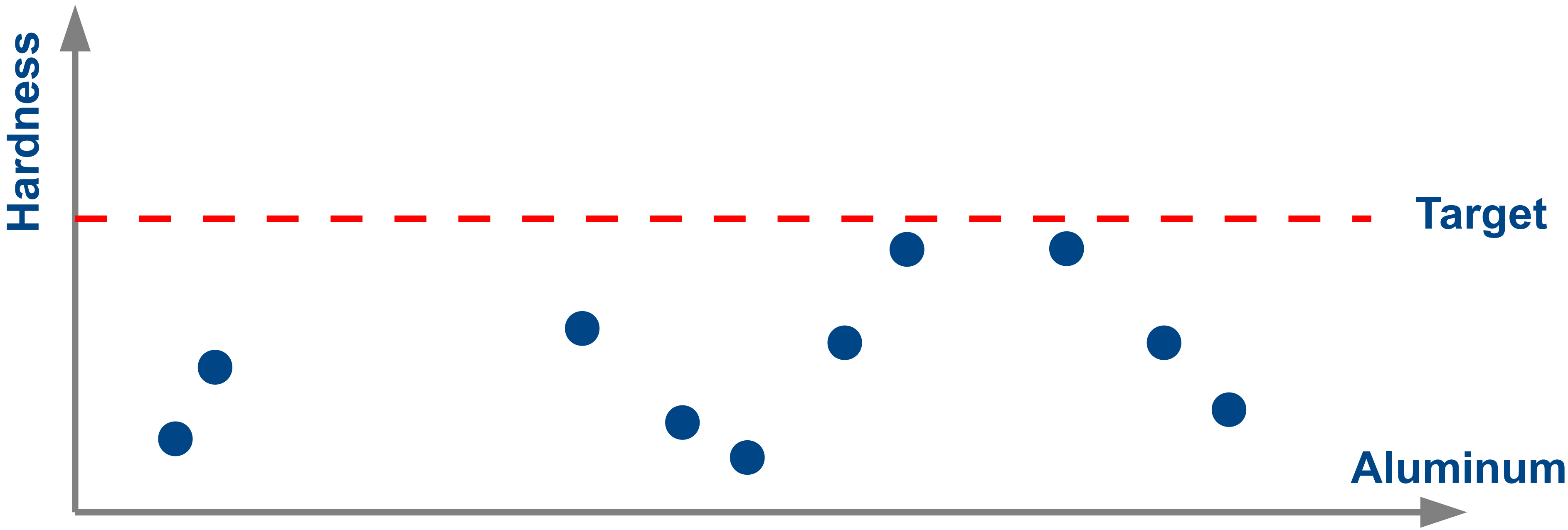
Materials pipeline



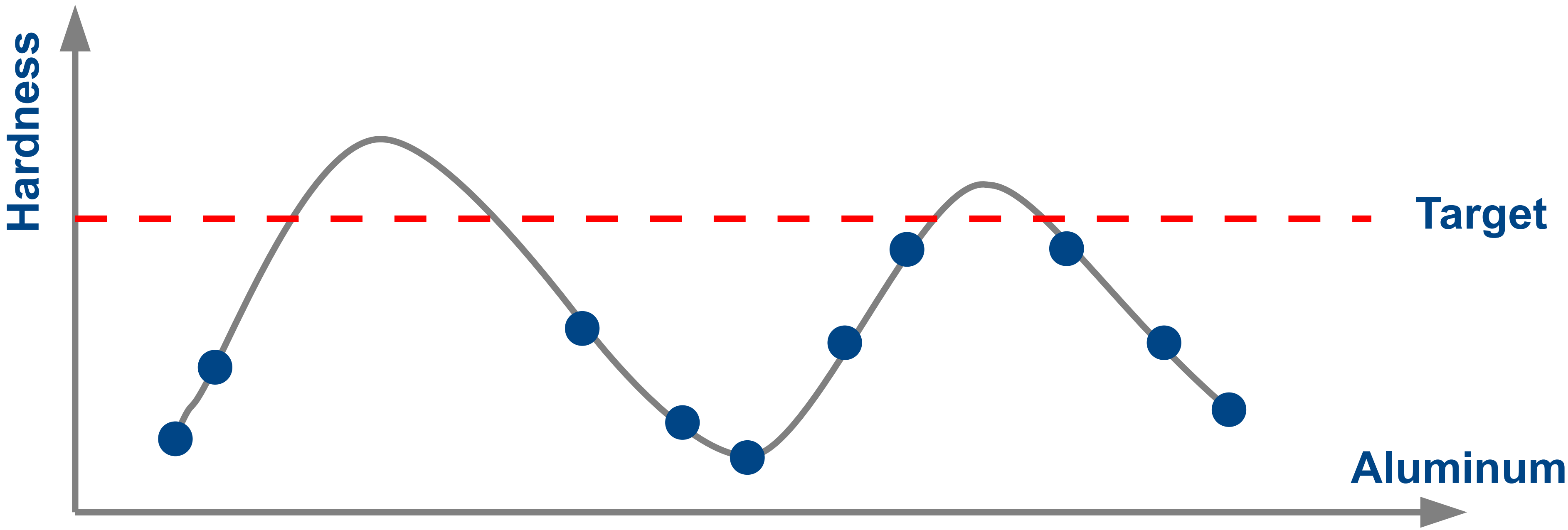
Two new tools



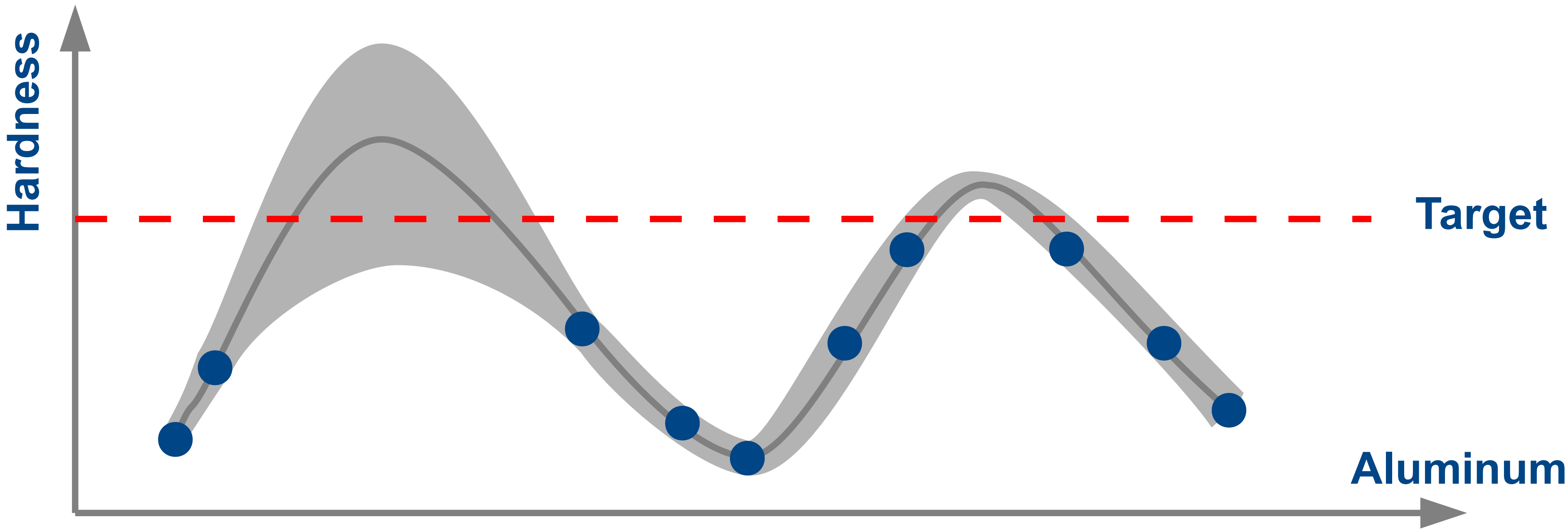
Neural network fitting & optimization



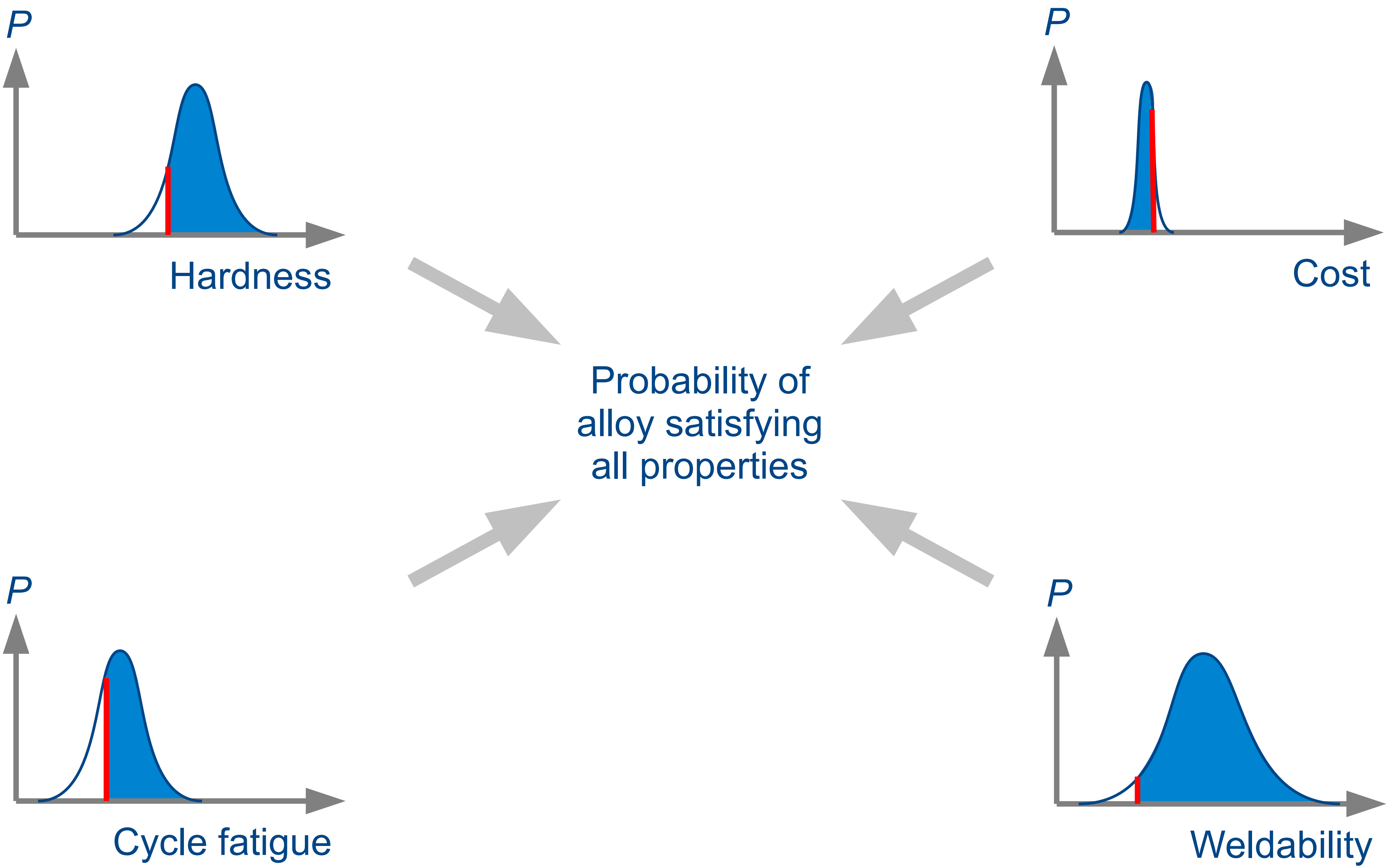
Neural network fitting & optimization



Neural network fitting & optimization

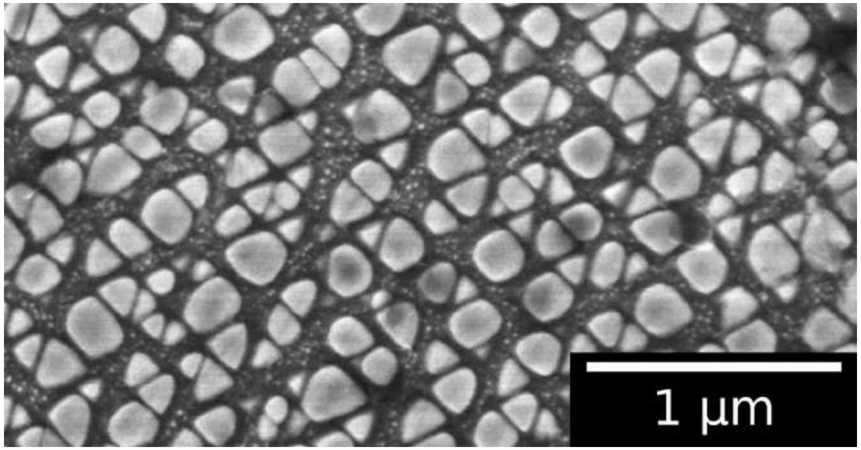


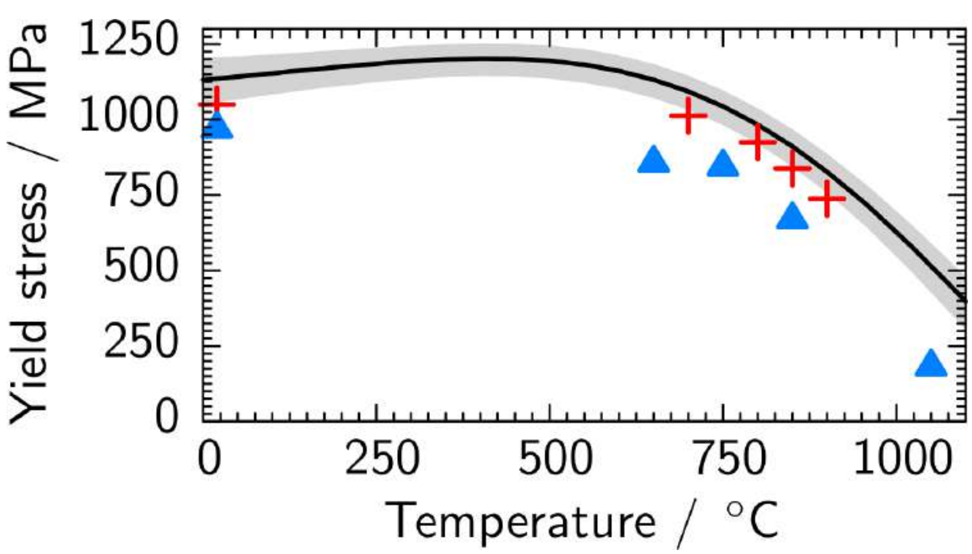
Probability

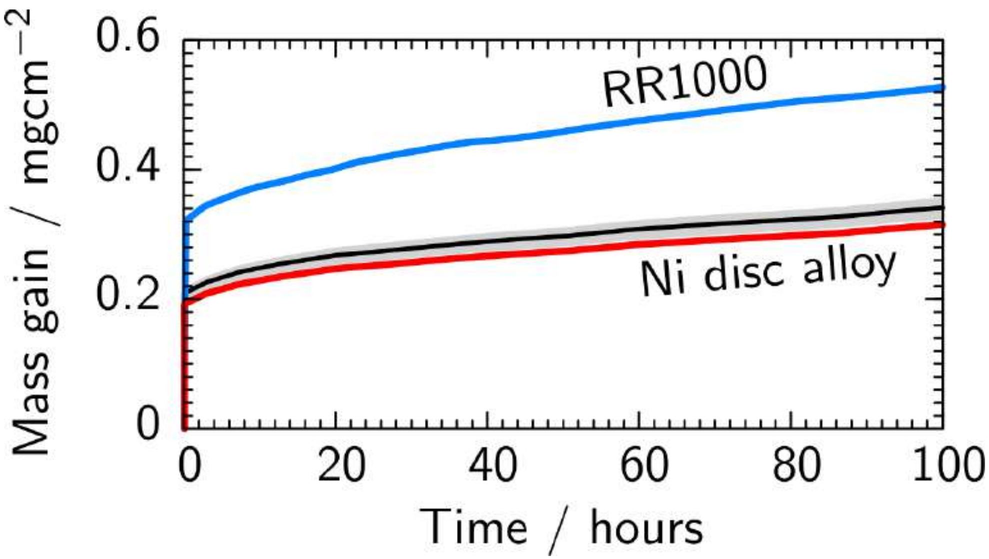


EP14153898.3; US 2014/177578; GB1302743.8

Ni-base superalloy

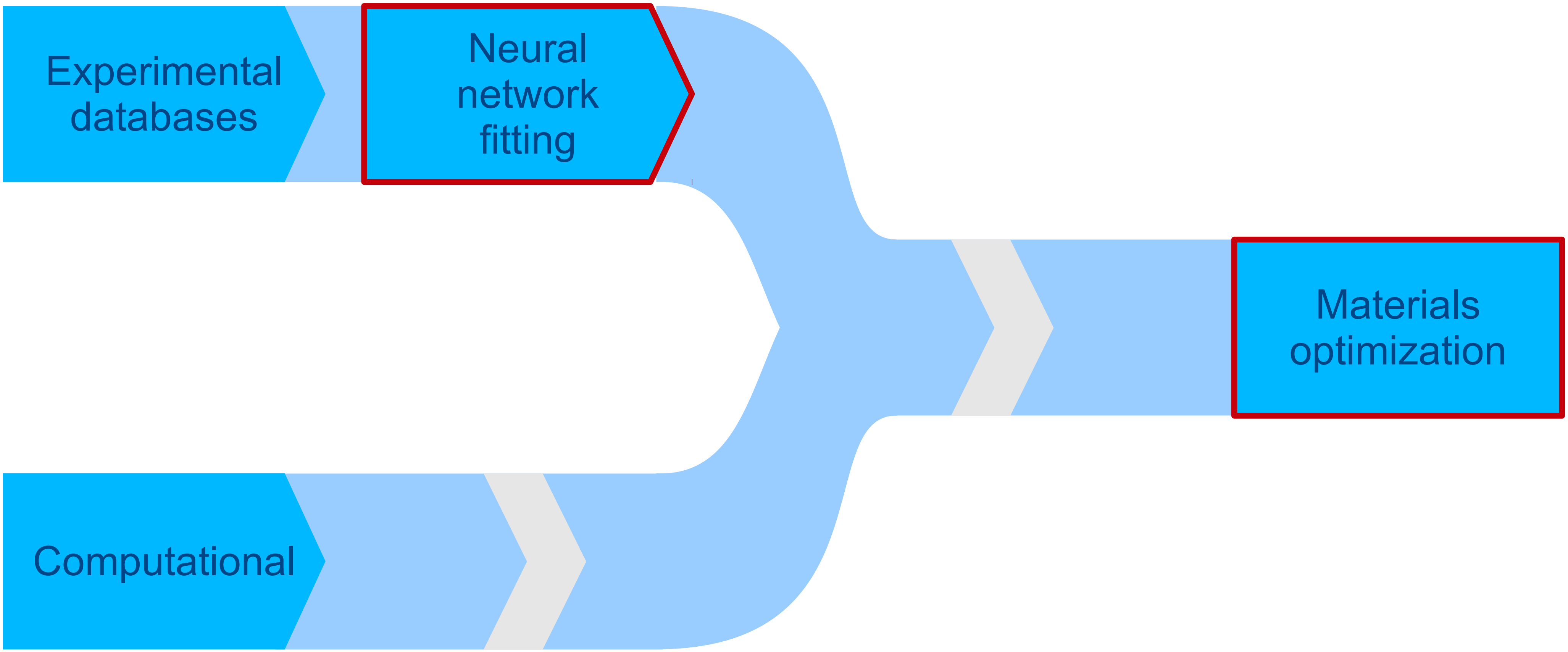




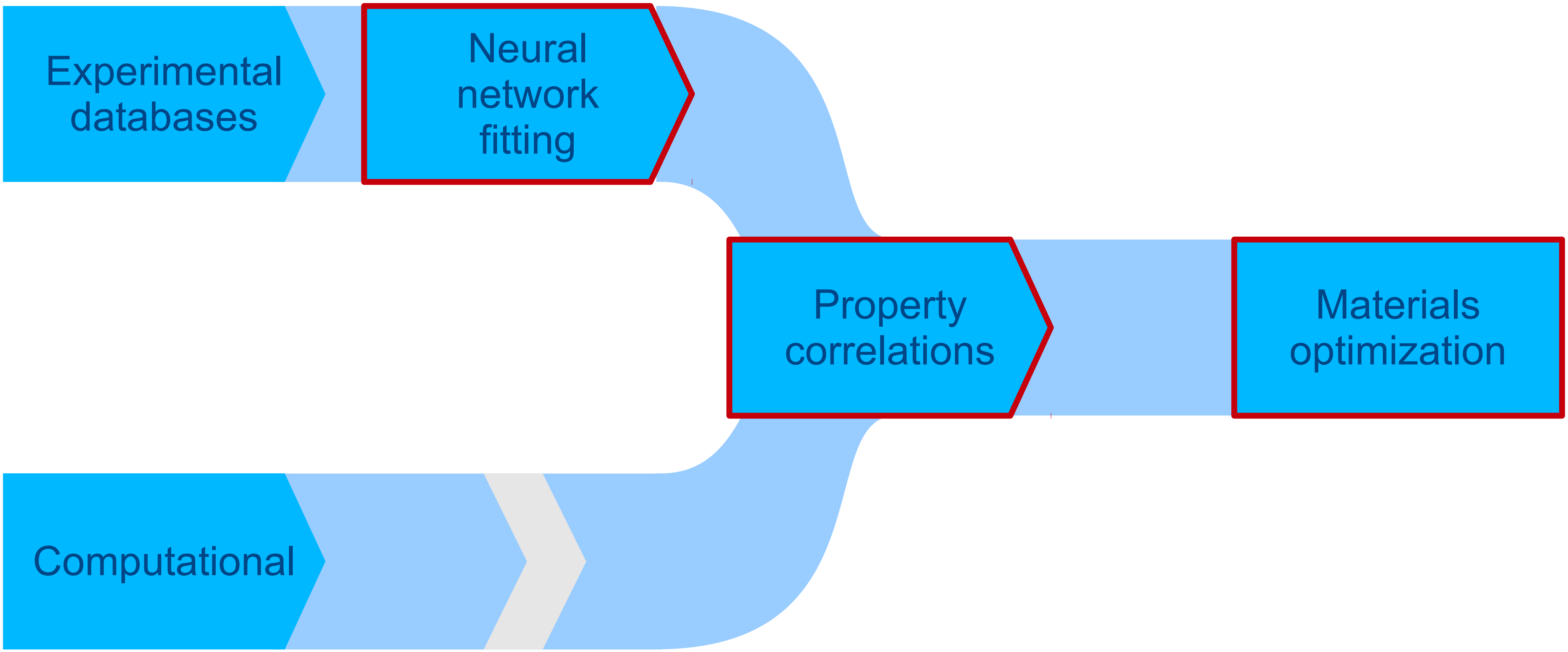


Amendment to US 2013/0052077 A1; EP14157622.3; GB1408536.9

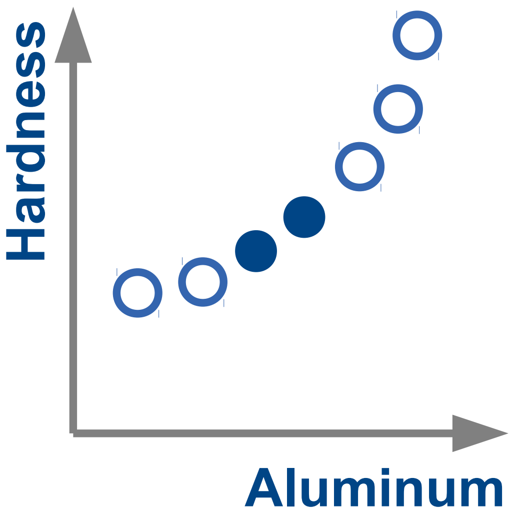
Two new tools



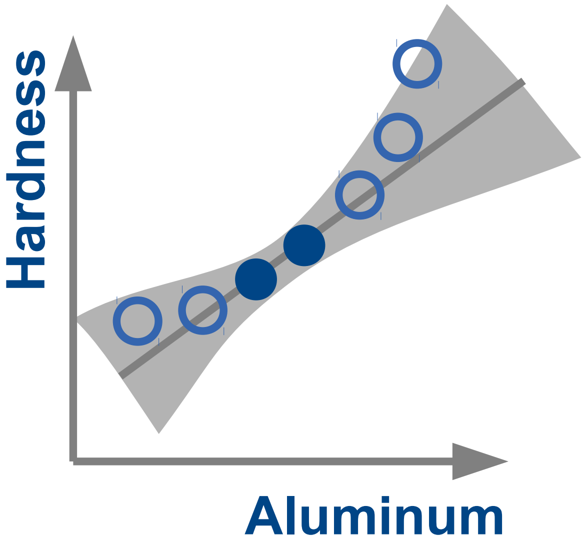
Three new tools



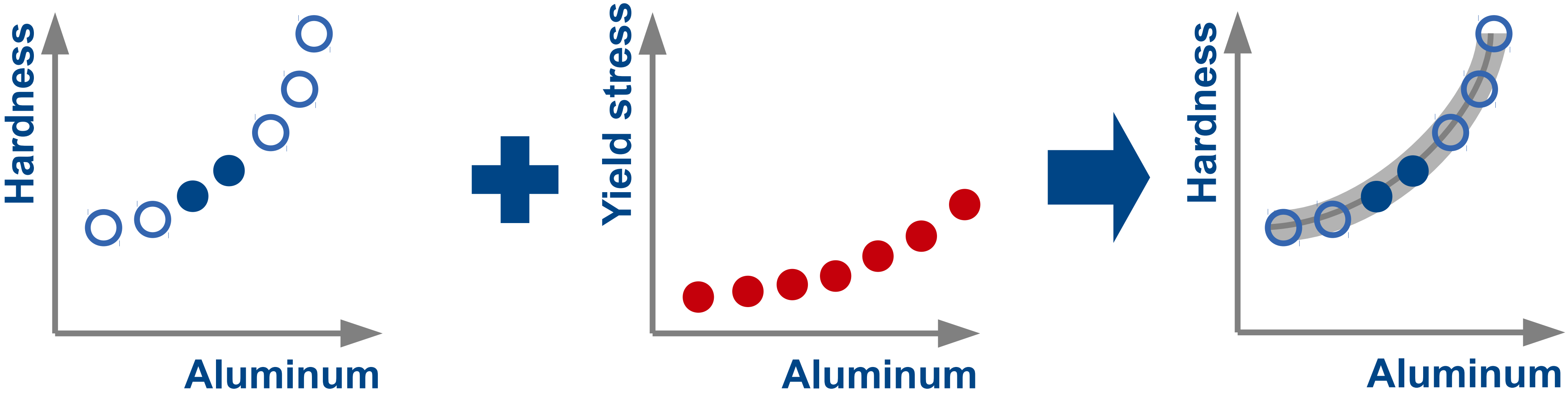
Correlations between properties



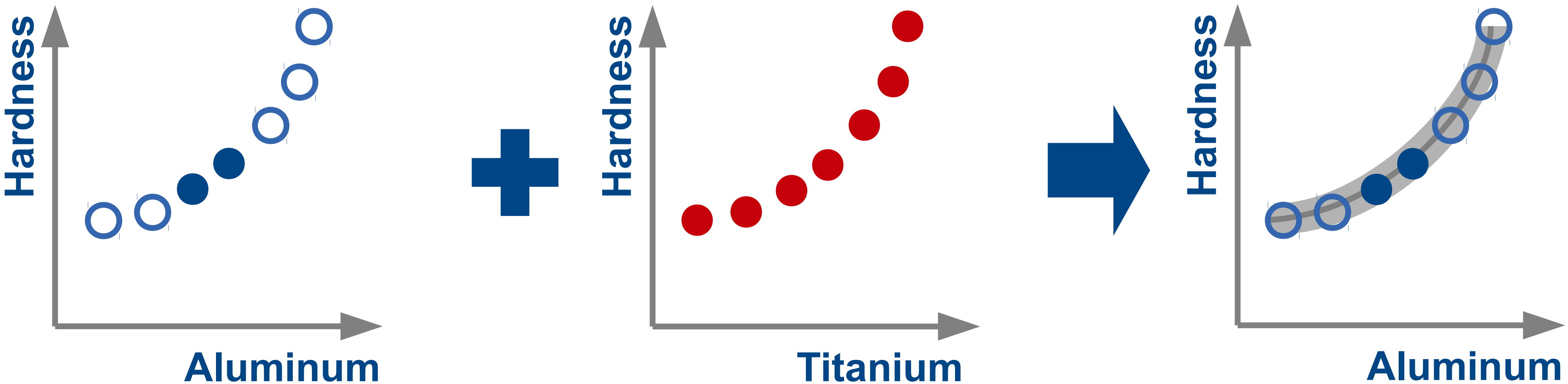
Correlations between properties



Correlations between properties



Correlations between properties



Exploiting correlations: 3D printing

7 points for 3D printability

+

Weldability
Heat capacity
Conductivity
Precipitates

→

Accurate predictions for 3D printability

Exploiting correlations: LEDs

Band gap from experiment

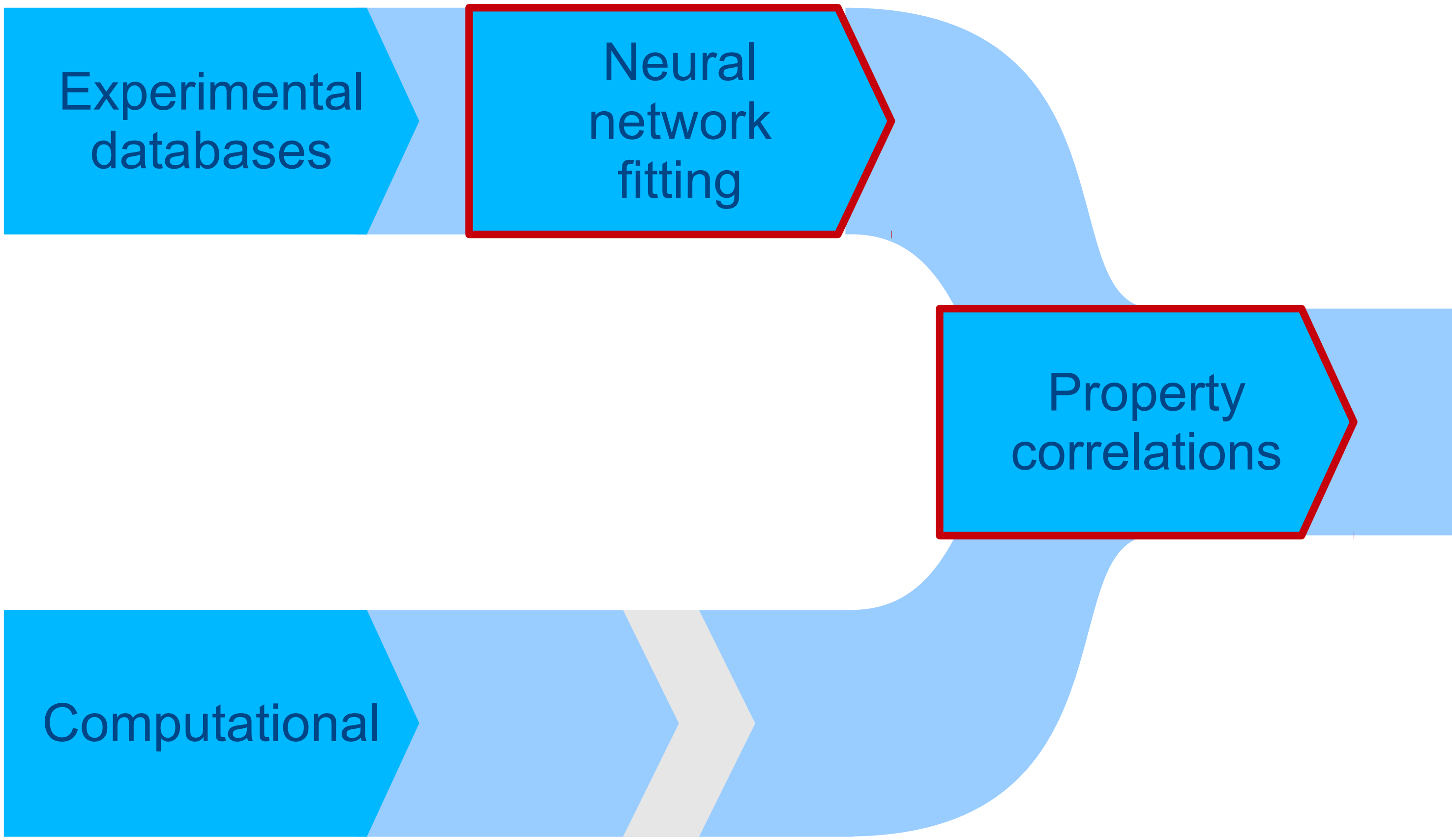
+

DFT predictions of band gap

→

Accurate band gaps at all compositions

Three new tools



Ni-based alloy
EP14157622.3
2013/0052077 A1
GB1408536.9

Mo-Hf alloy
EP14161255.6
US 2014/223465
GB1307533.8

Mo-Nb alloy
EP14161529.4
GB1307535.3

Ni-based alloy for direct laser deposition

InGaN-based LED

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

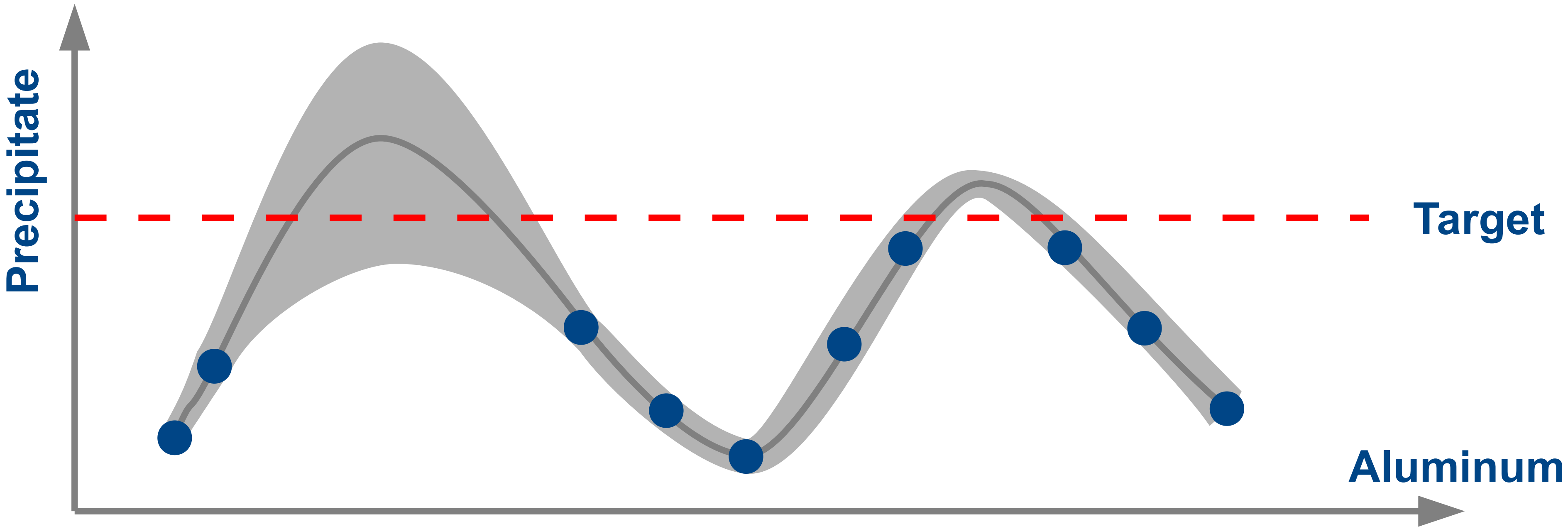
Concurrent materials design

Recursive learning

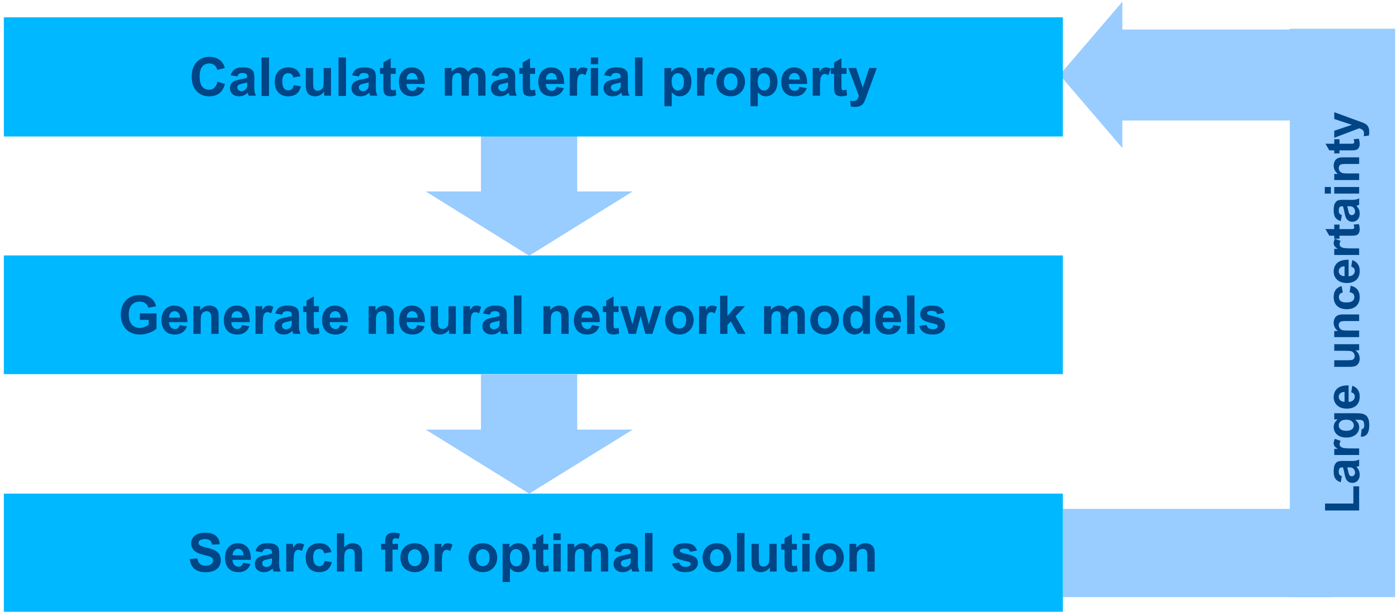
Calculate material property

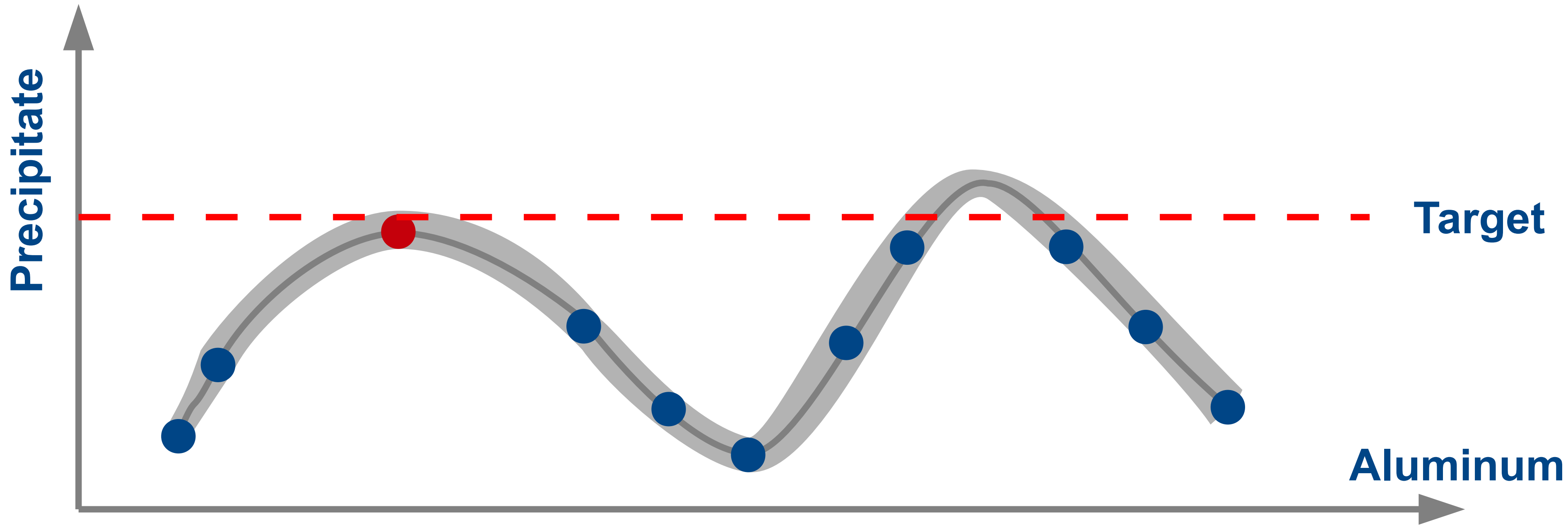
Generate neural network models

Search for optimal solution

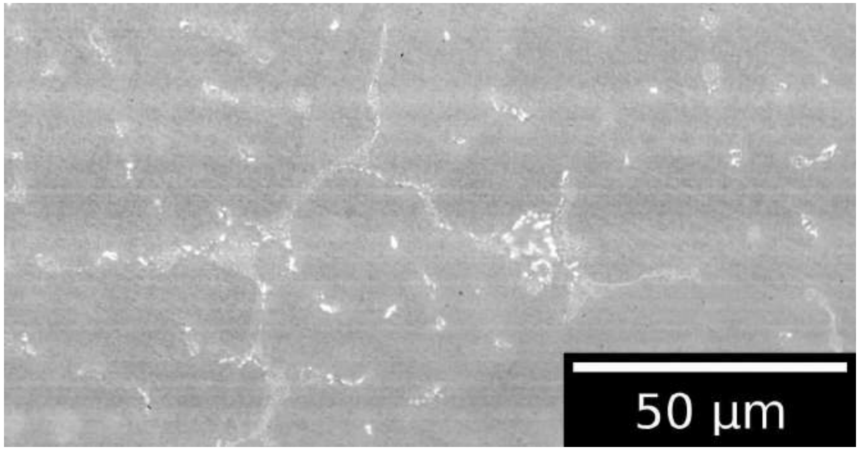


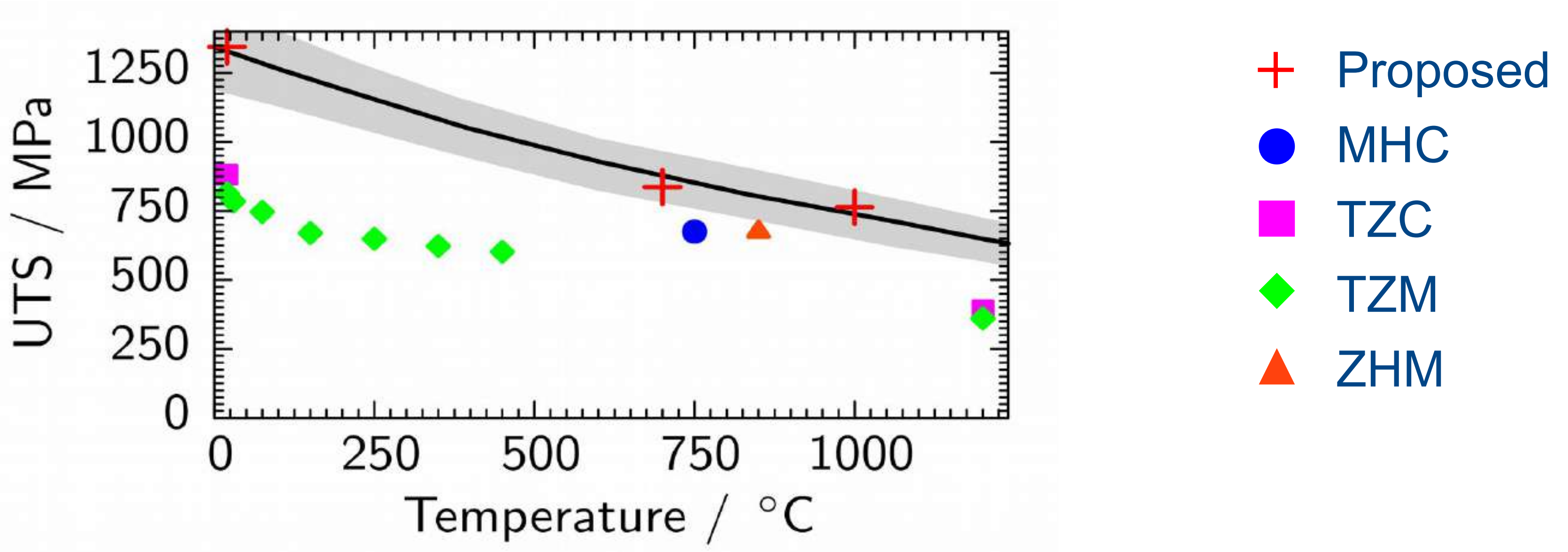
Recursive learning





Mo-base alloy





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

Mo-base alloy