

Concurrent materials design

Gareth Conduit

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

EP14161255.6; US 2014/223465; GB1307533.8

EP14161529.4; GB1307535.3

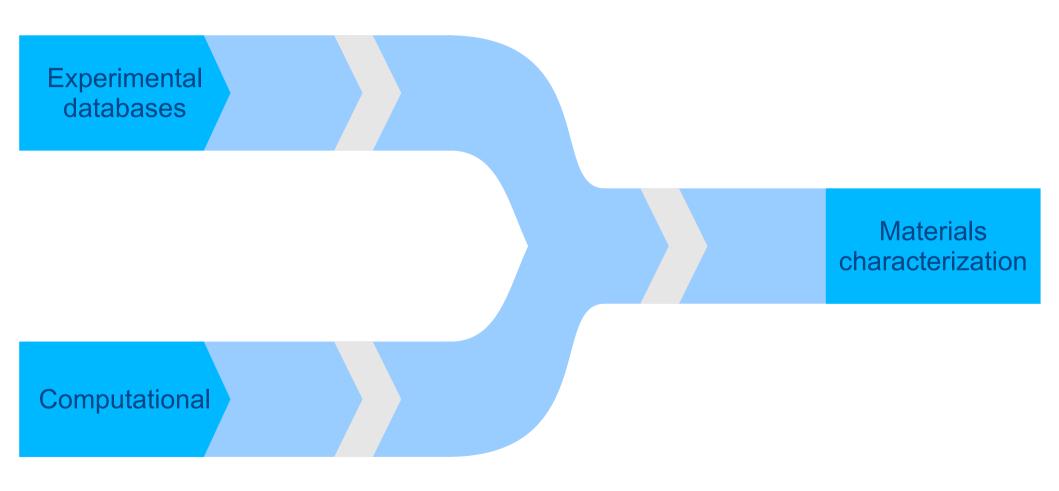
EP14157622.3; amendment to US 2013/0052077 A1; GB1408536.9

Acta Materialia 61, 3378 (2013)

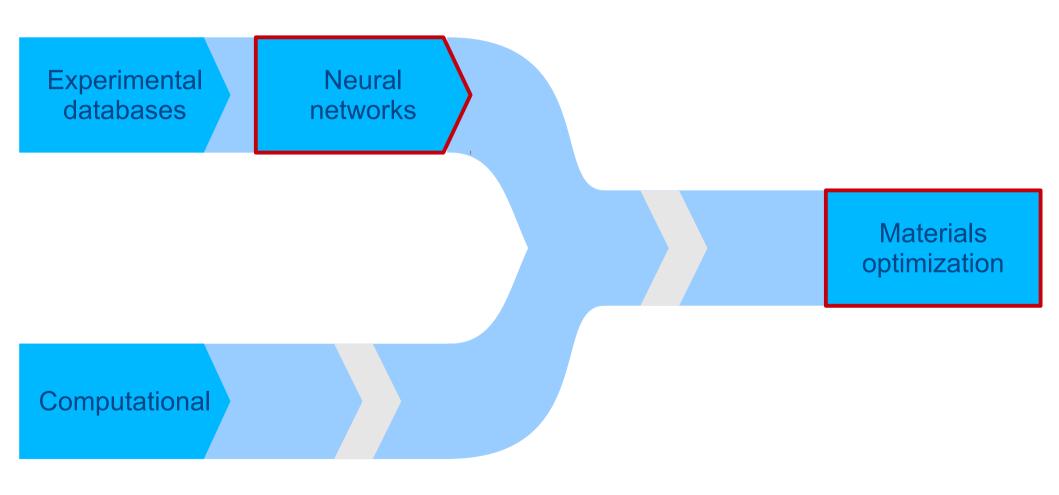
Intermetallics 48, 62 (2014)

Theory of Condensed Matter Group, Department of Physics

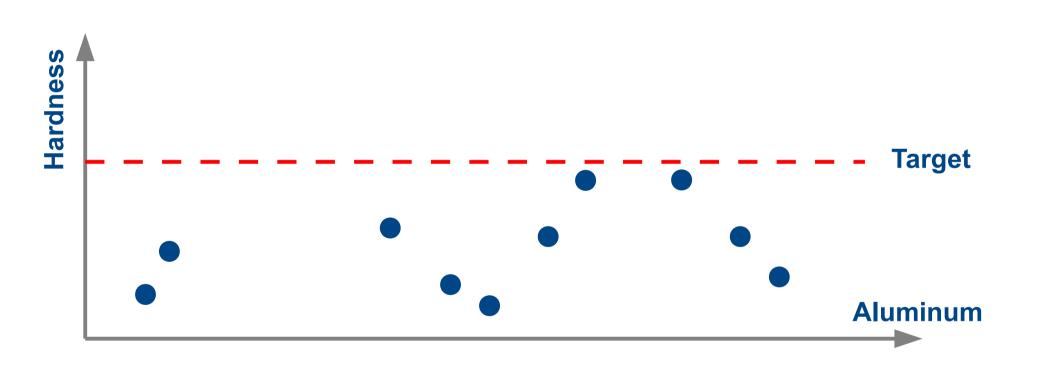
Materials pipeline



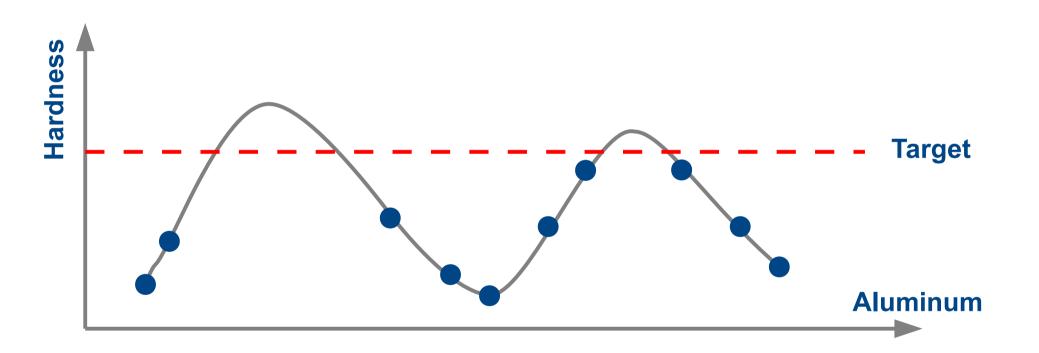
Two new tools



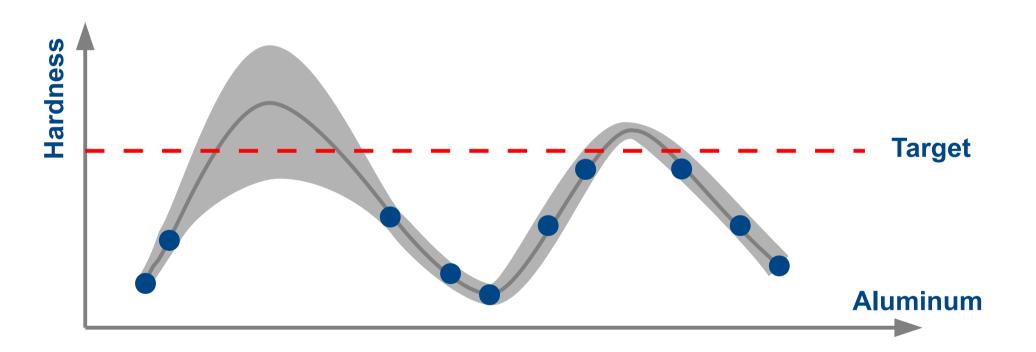
Neural network fitting & optimization



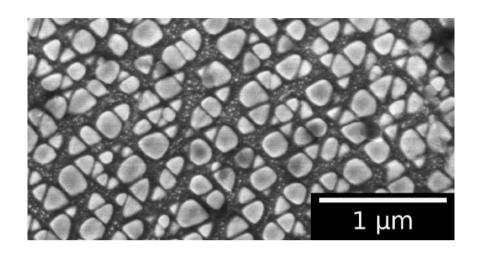
Neural network fitting & optimization

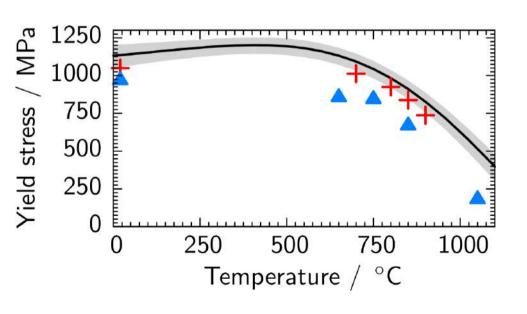


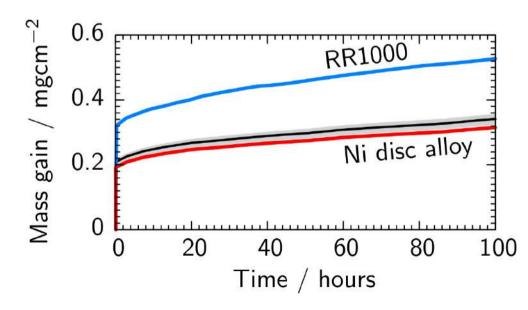
Neural network fitting & optimization



Ni-base superalloy

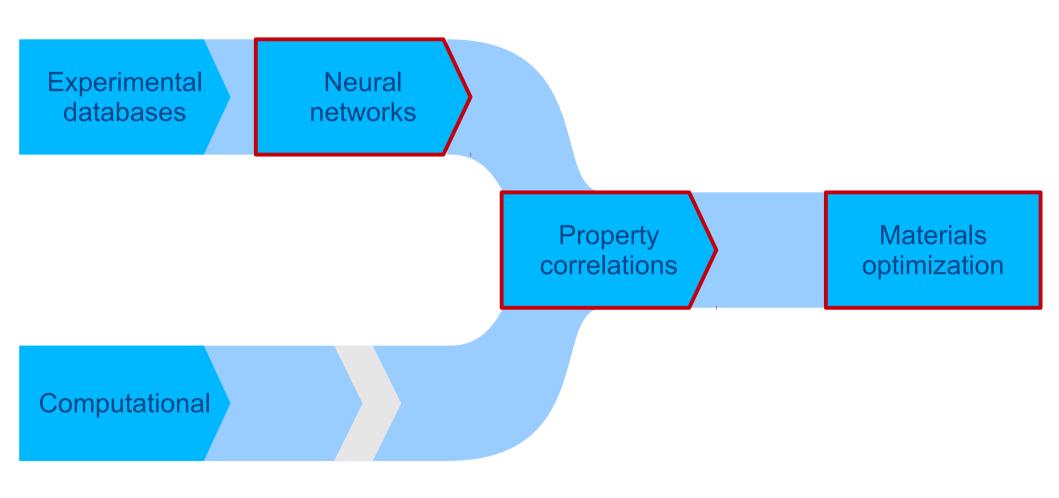




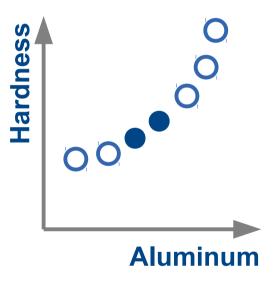


Amendment to US 2013/0052077 A1; EP14157622.3; GB1408536.9

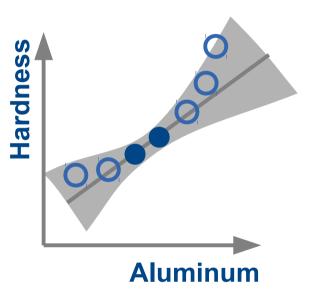
Three new tools



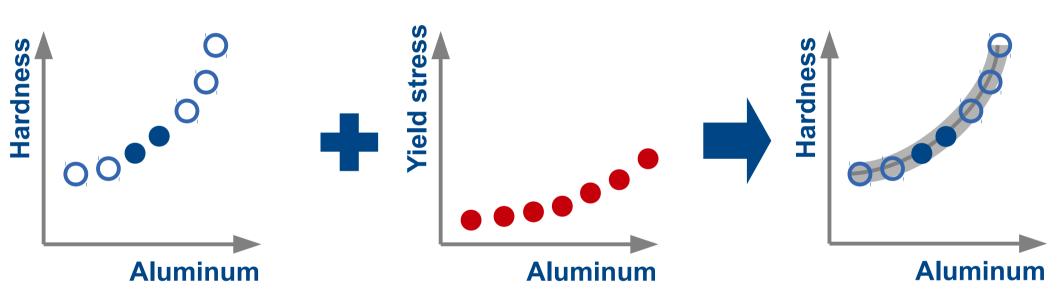
Correlations between properties



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

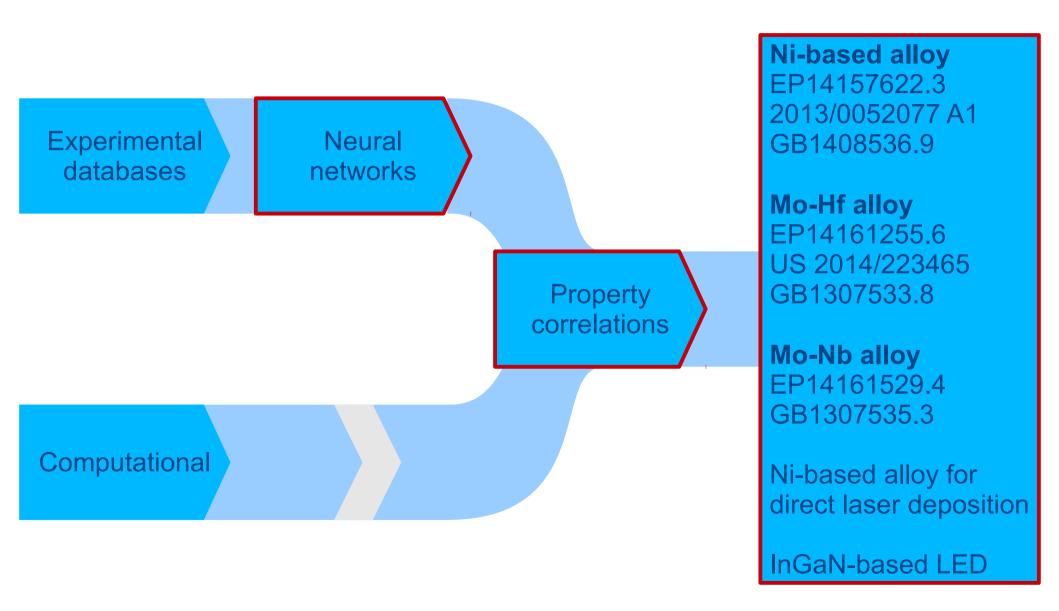


DFT predictions of band gap



Accurate band gaps at all compositions

Three new tools



Prospects in the future

Combine strengths of experimental databases with first principles approaches

Concurrent materials design