

Concurrent materials design

Gareth Conduit

Patents GB1302743.8 (2013), EP14153898.3 (2014), US 2014/177578 (2014)

Patents GB1307533.8 (2013), EP14161255.6 (2014), US 2014/223465 (2014)

Patent GB1307535.3 (2013)

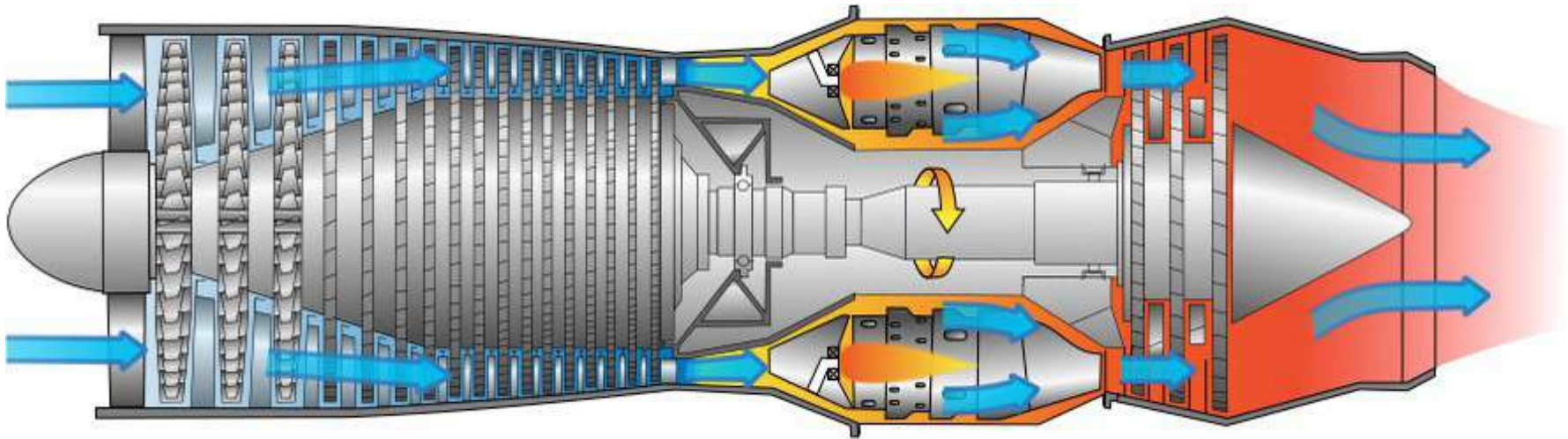
Patent US 2013/0052077 A1 (2013)

Acta Materialia, **61**, 3378 (2013)

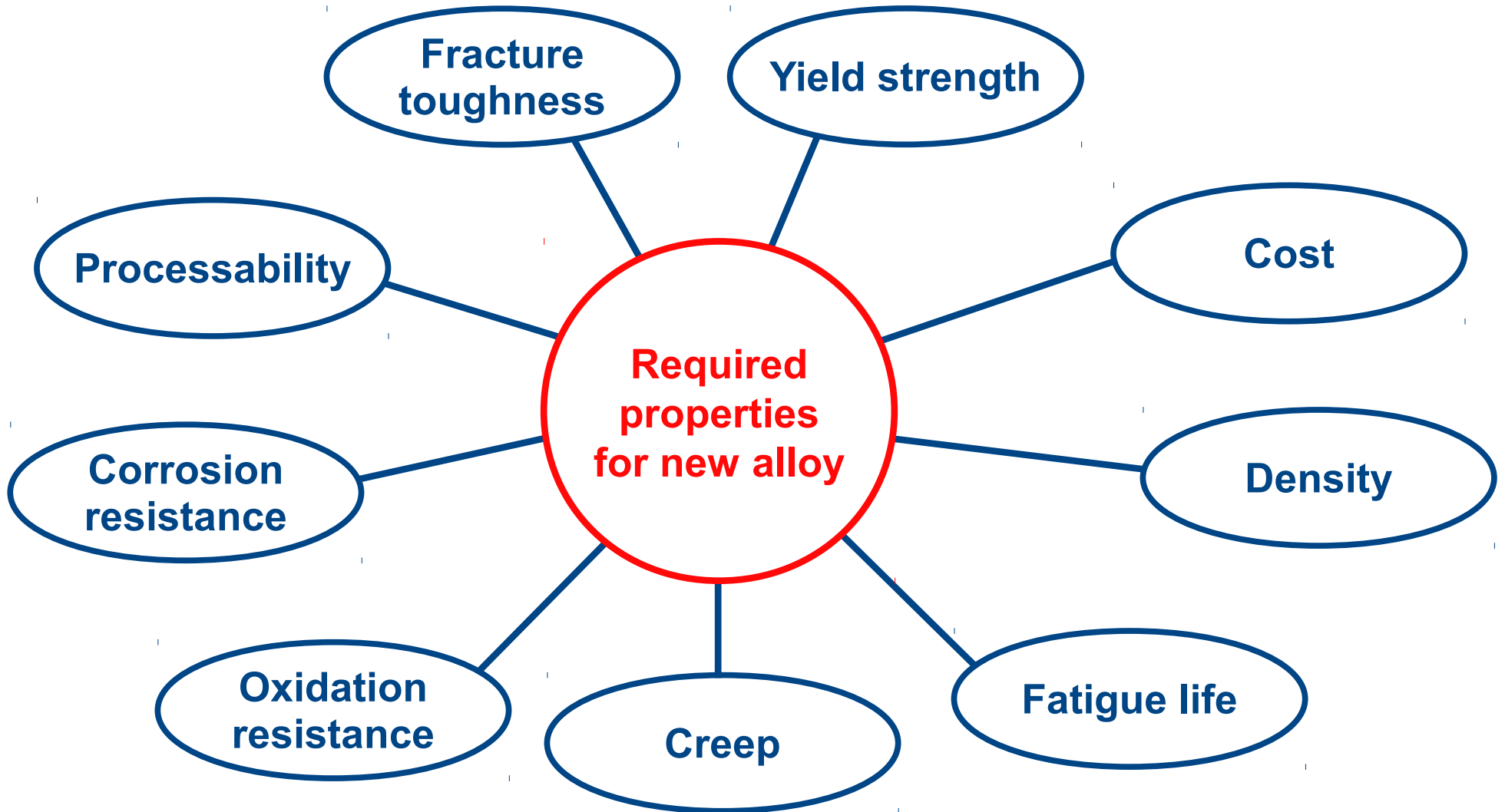
Intermetallics, **48**, 62 (2014)

Theory of Condensed Matter Group, Department of Physics

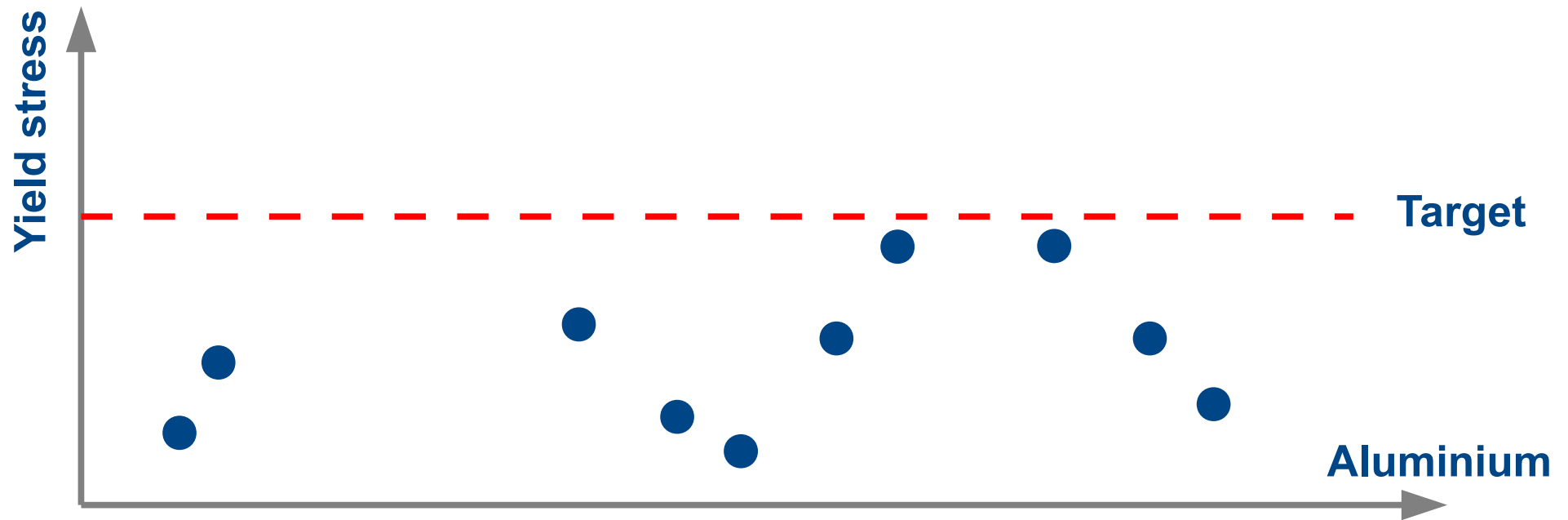
Jet engine: turbine discs



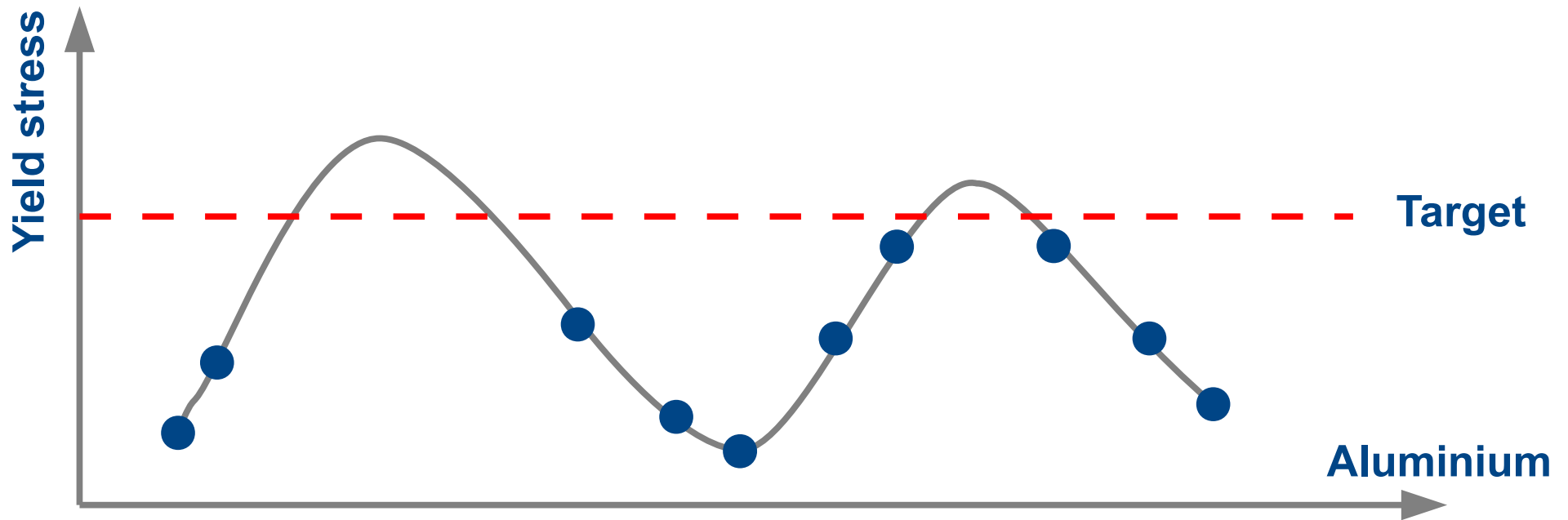
Designing a new alloy – what is required?



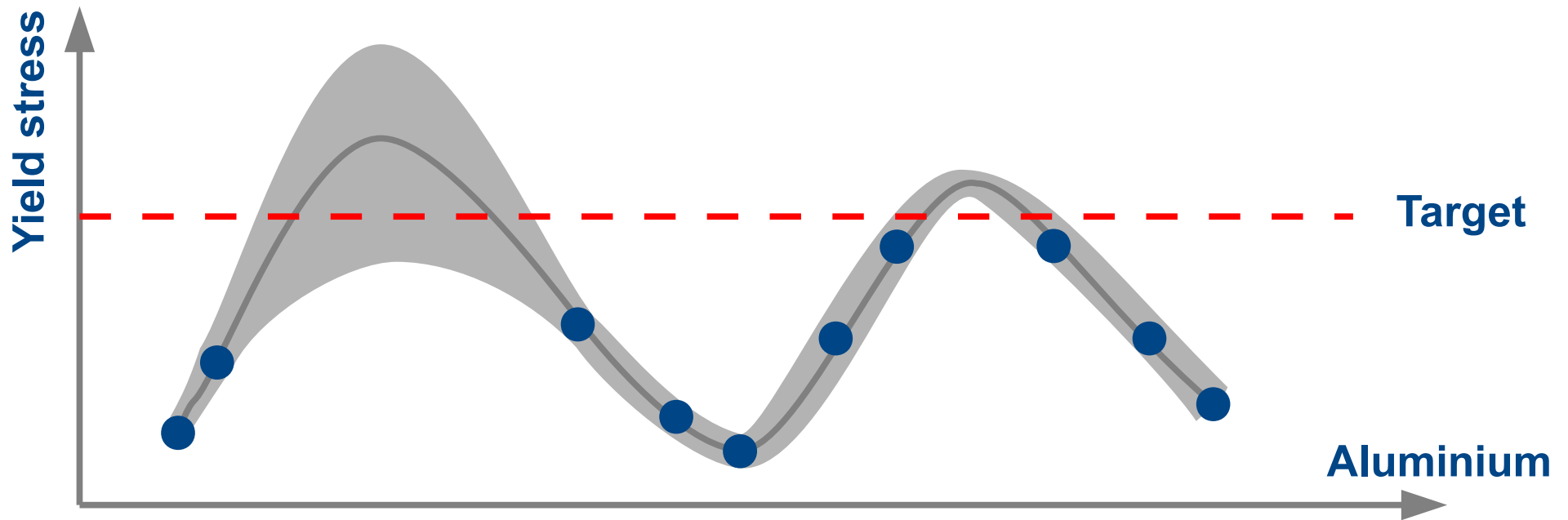
Neural network fitting & optimization



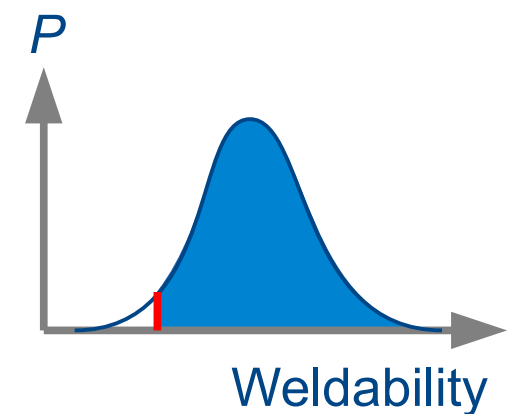
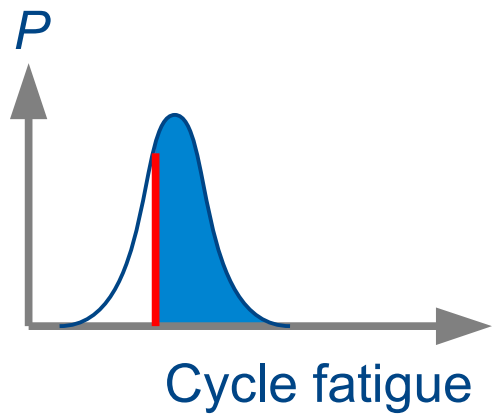
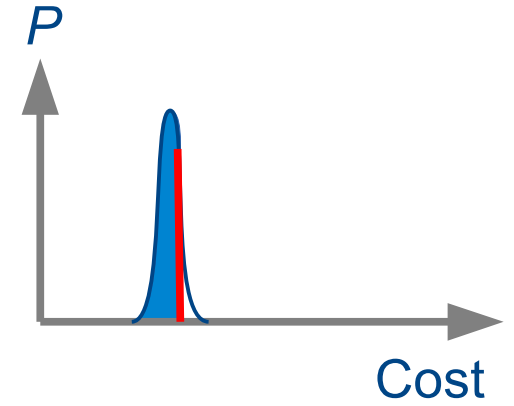
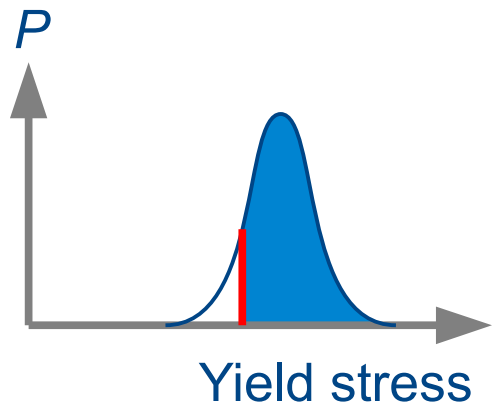
Neural network fitting & optimization



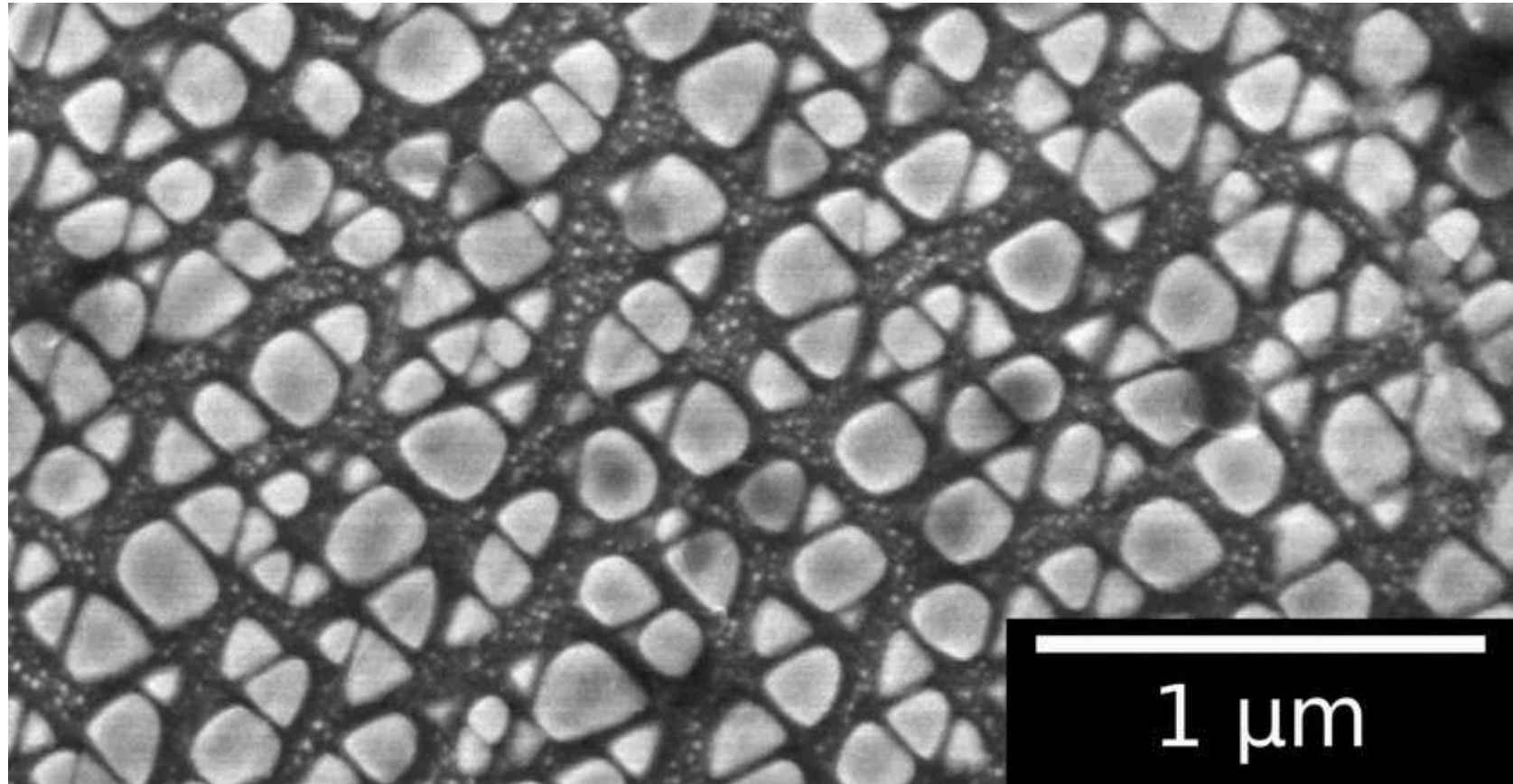
Neural network fitting & optimization



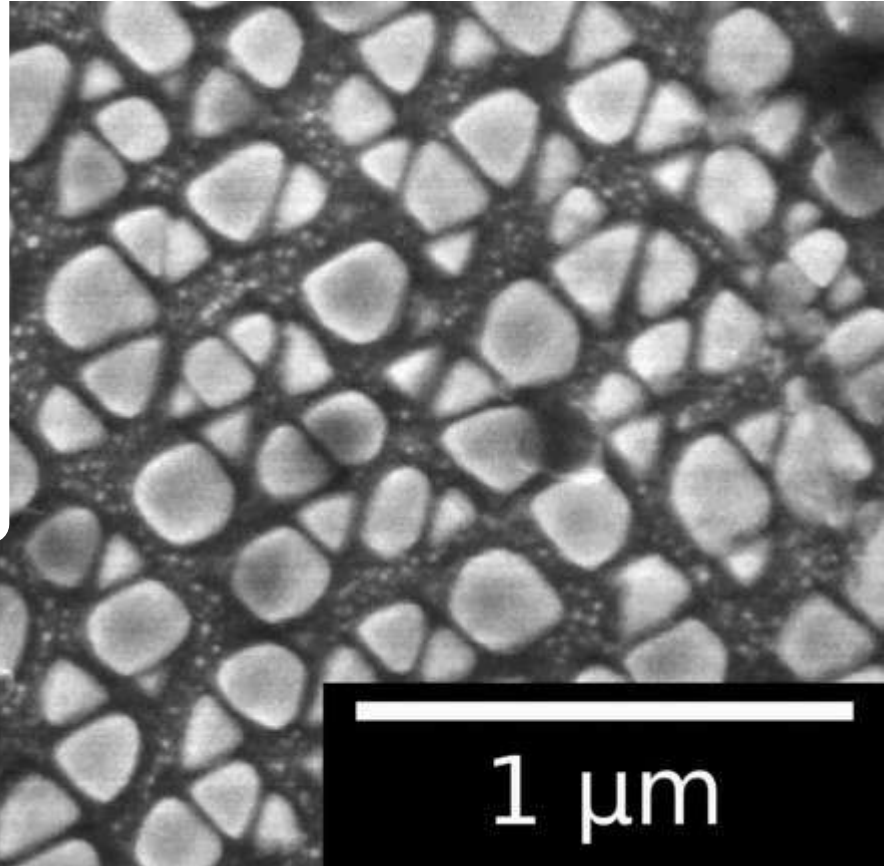
Probability



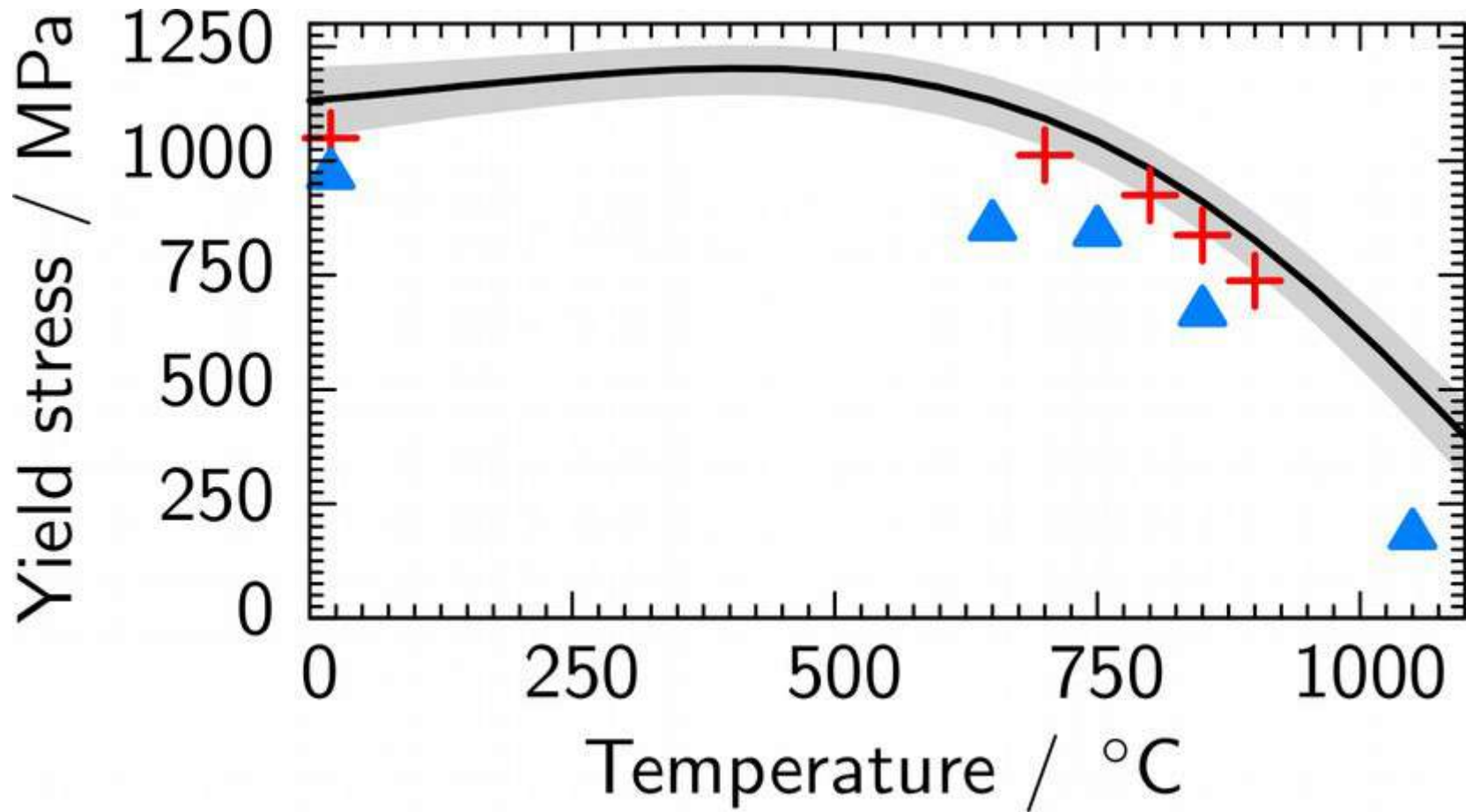
Ni-base superalloy



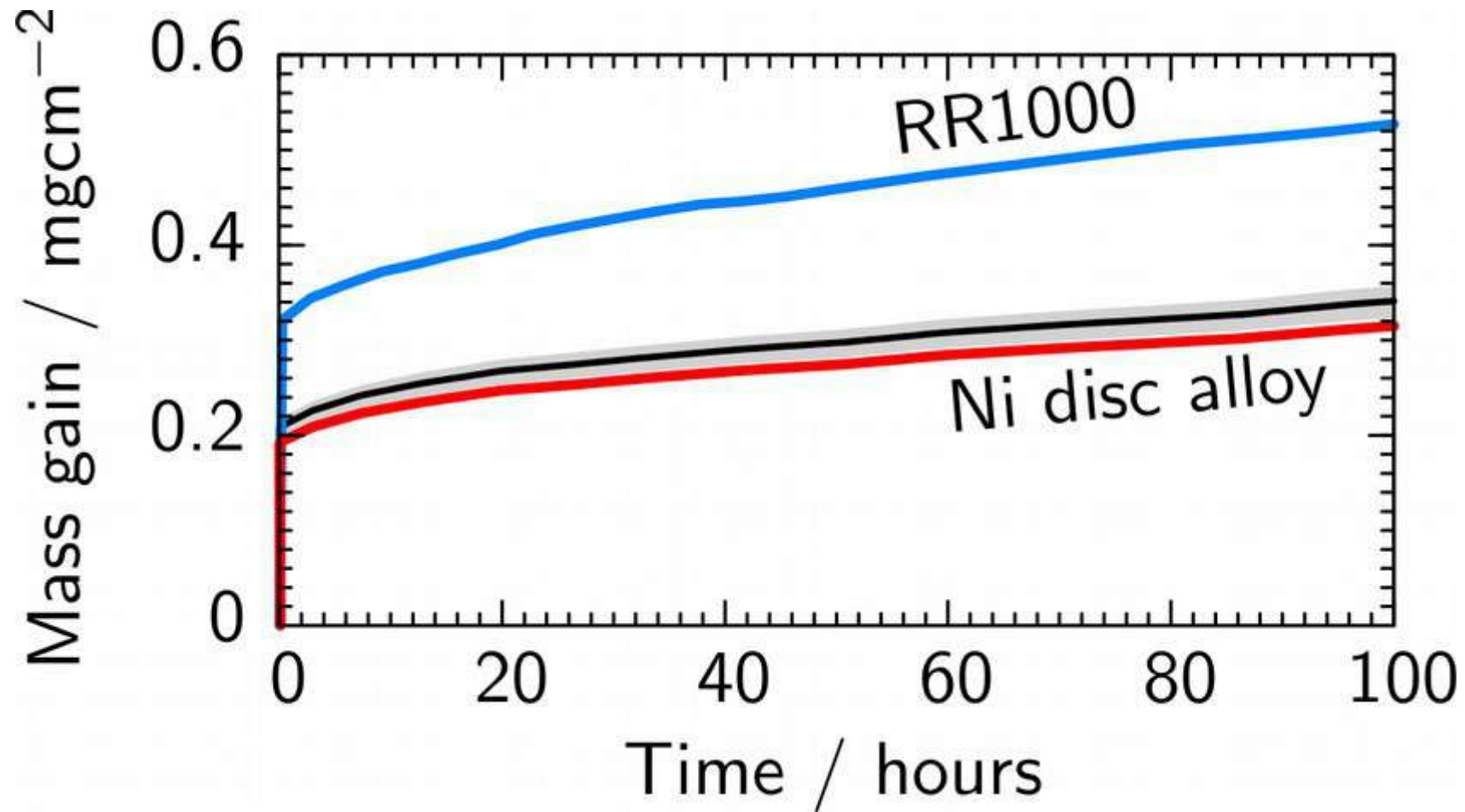
Ni-base superalloy



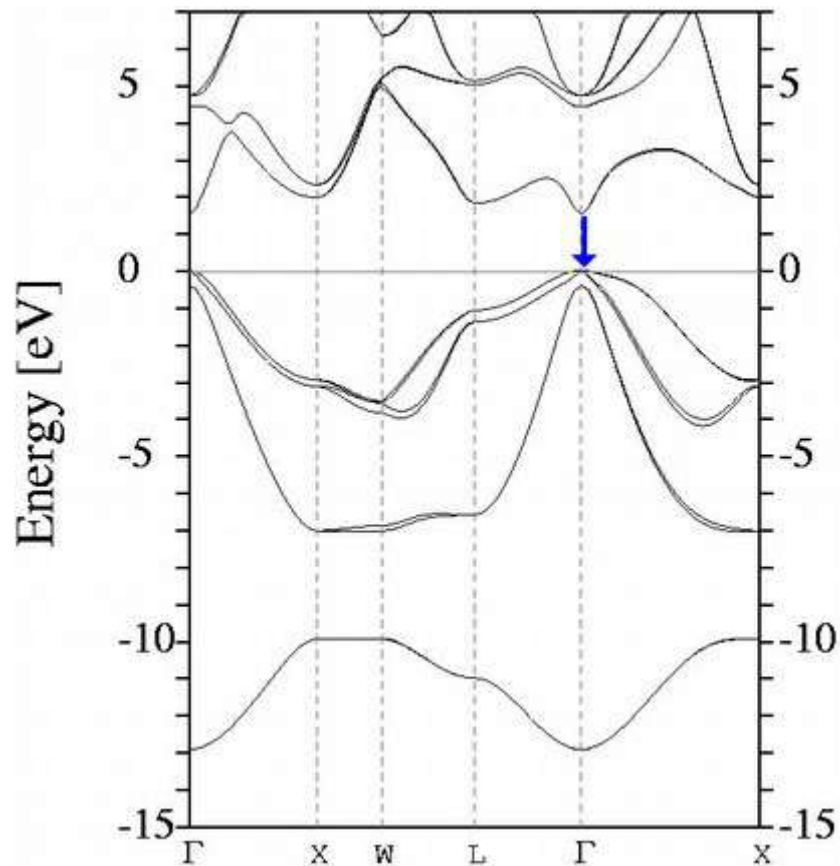
Ni-base superalloy



Ni-base superalloy



Semiconductors

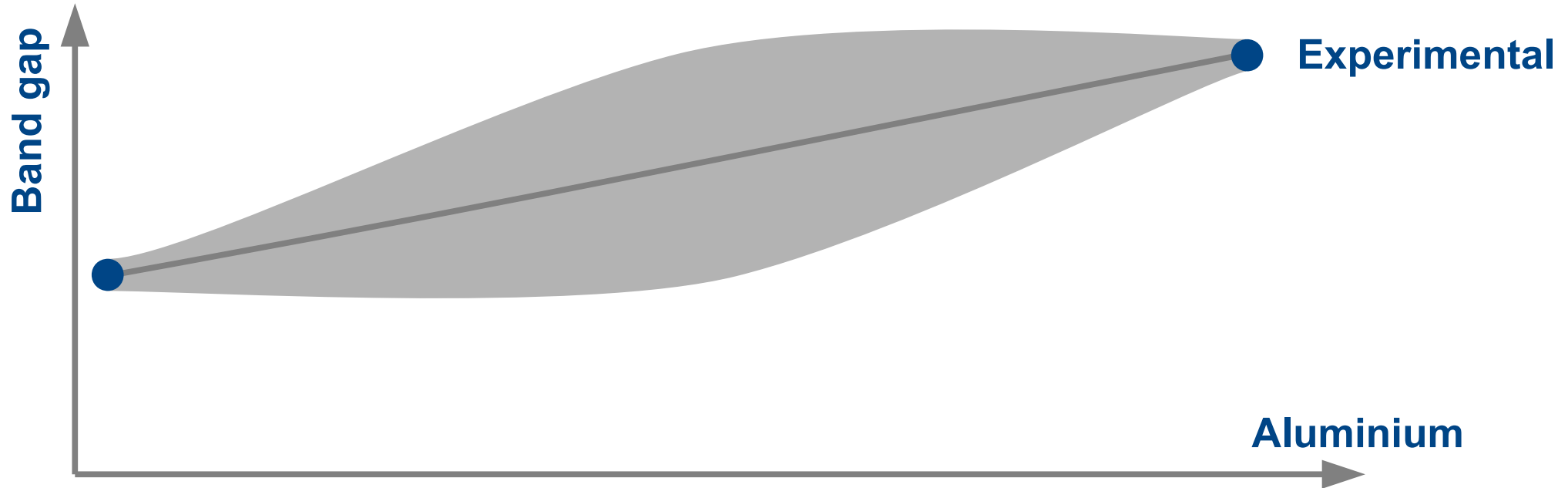


100 points for band gap, efficacy



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

Semiconductors

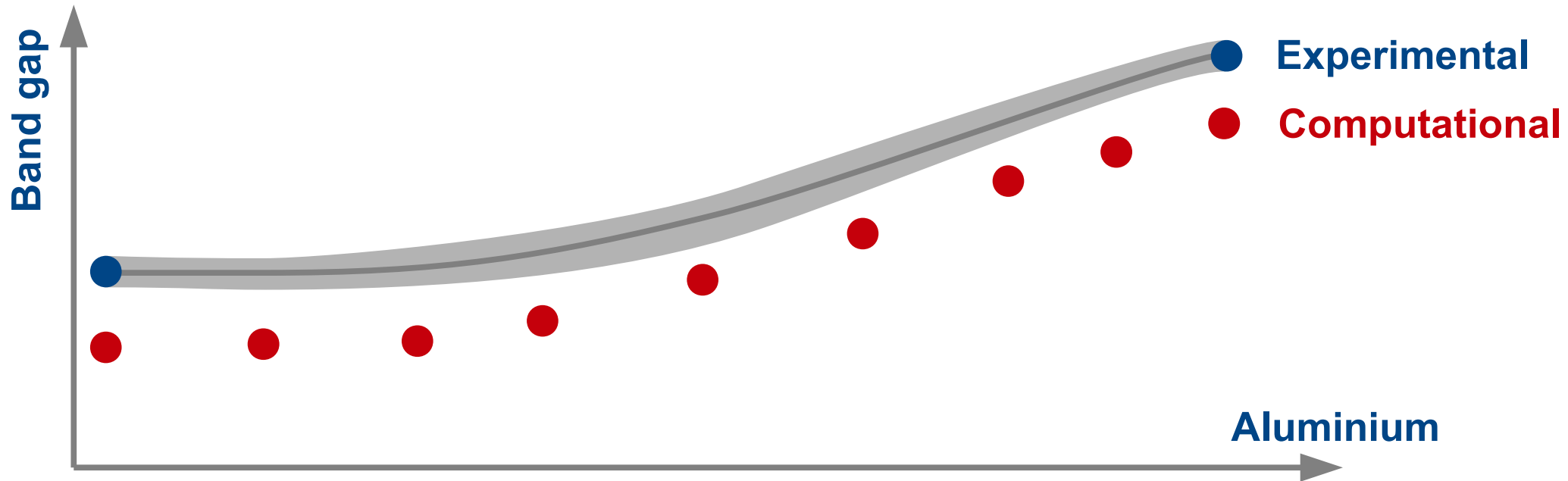


100 points for band gap, efficacy



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

Semiconductors



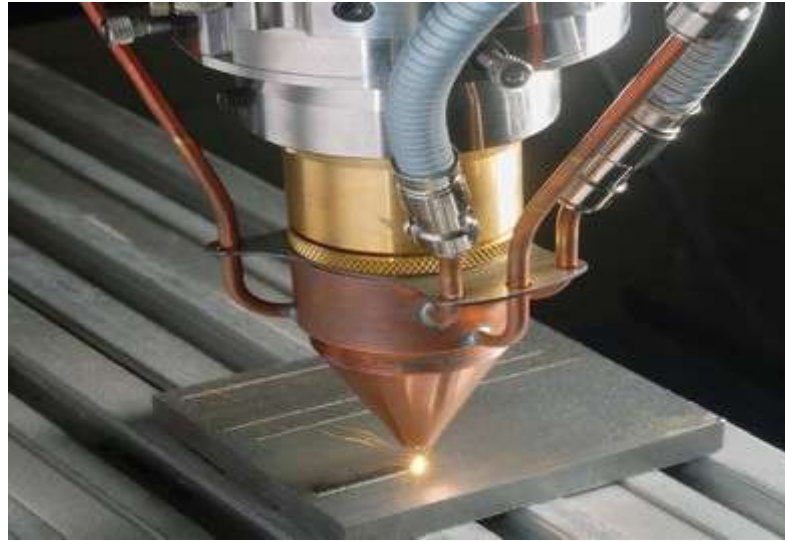
100 points for band gap, efficacy



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

Correlations between properties

Alloy for
direct laser deposition



7 points for
quality of deposition



Weldability, thermal
conductivity, thermal
expansivity, precipitate
fraction

Prospects in the future

Take advantage of experimental databases to develop Ni and Mo-based alloys

Combine further first principles approaches to build new databases and guide extrapolation

Projects with Rolls Royce, Samsung, Royal Society Brian Mercer Feasibility award

Long-term goal of concurrent materials design