UNIVERSITY OF CAMBRIDGE

DFT modeling research

Gareth Conduit

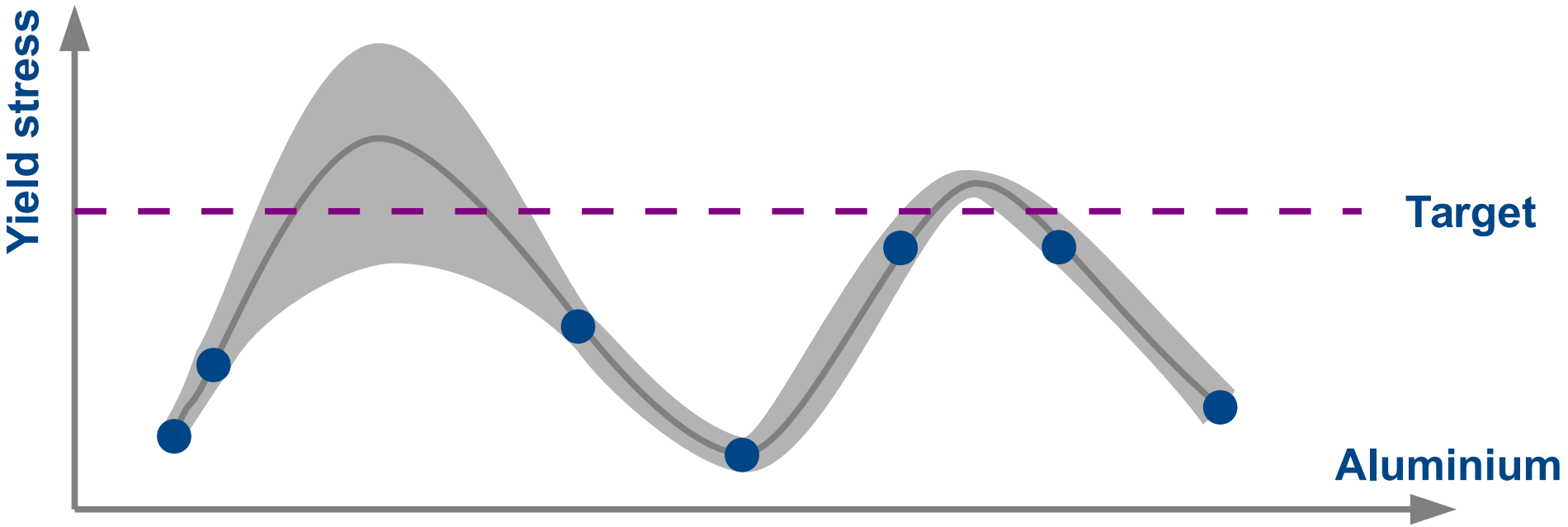
Patent GB1302743.8 (2013)
Patent GB1307533.8 (2013)
Patent GB1307535.3 (2013)
Acta Materialia, **61**, 3378 (2013)
Intermetallics, advanced online publication (2013)
Rolls-Royce Group plc invention submission NC12261 (2012)
Rolls-Royce Group plc invention submission NC13006 (2013)

Theory of Condensed Matter Group, Department of Physics

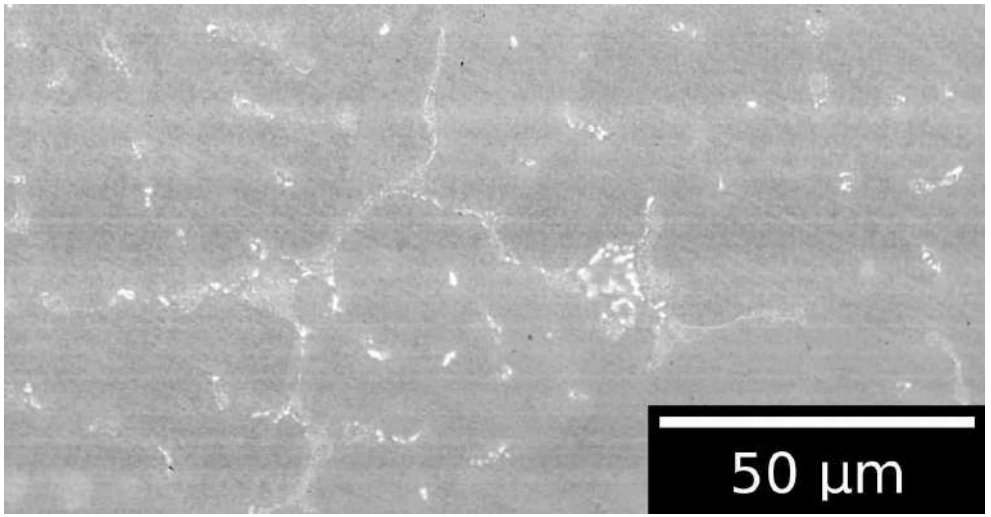
Four new tools

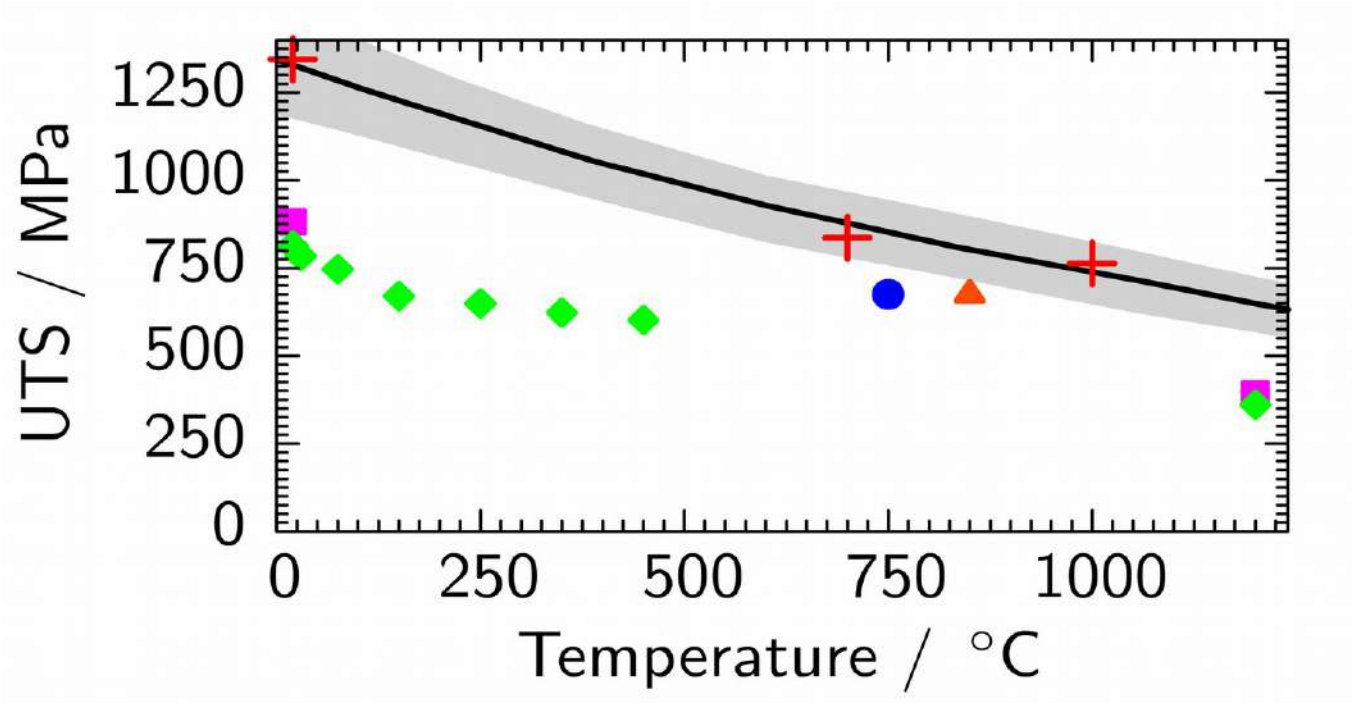
- Neural network fitting & optimization
- Phonons in DFT
- Recursive learning DFT
- Correlations between properties

Neural network fitting & optimization

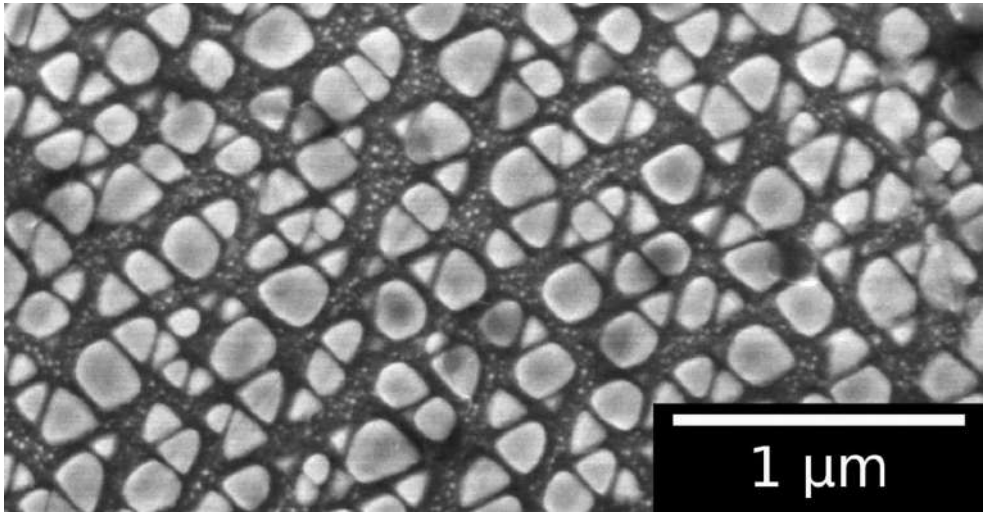


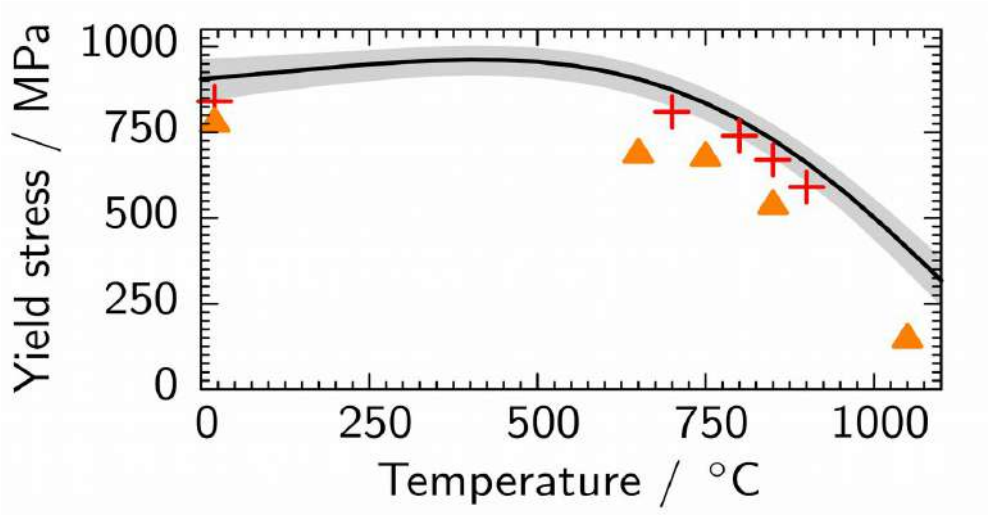
Mo-base alloy

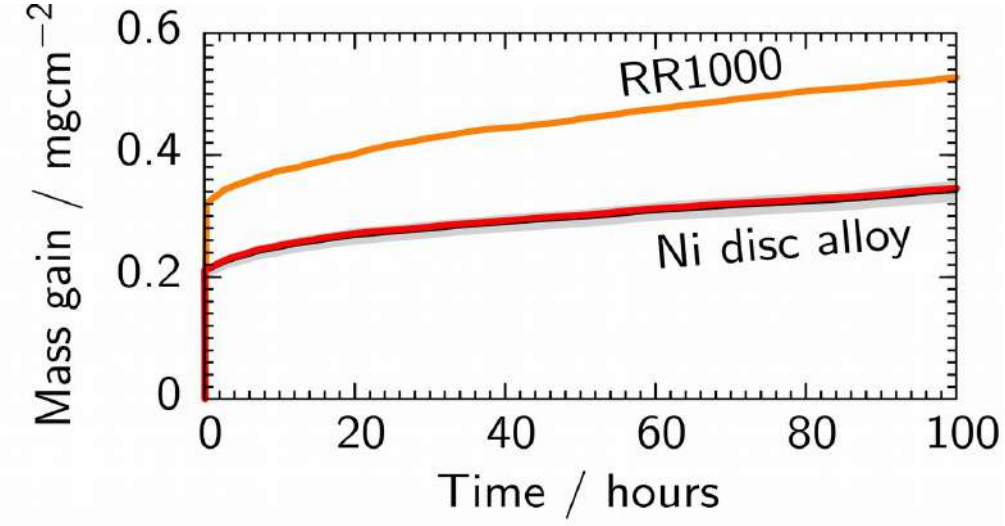




Ni-base superalloy

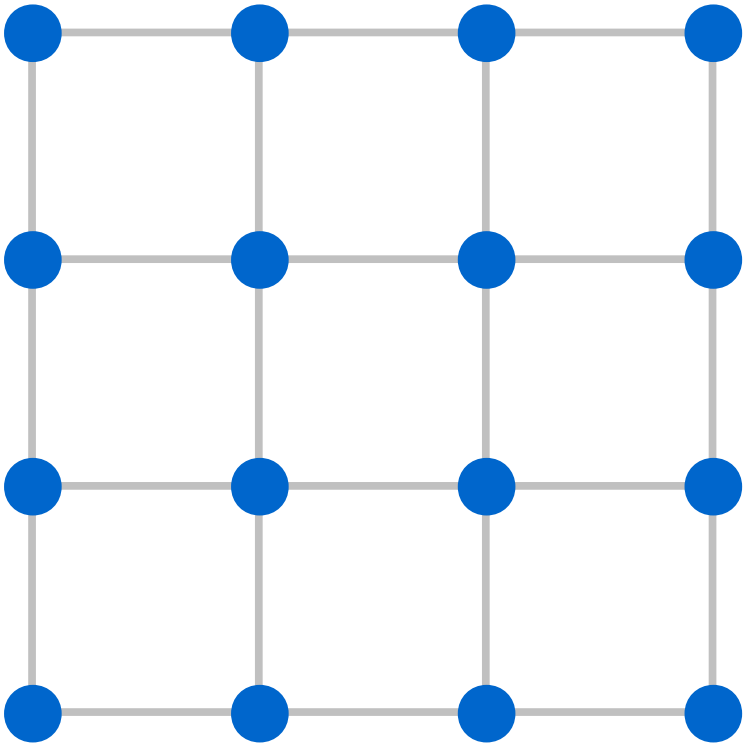






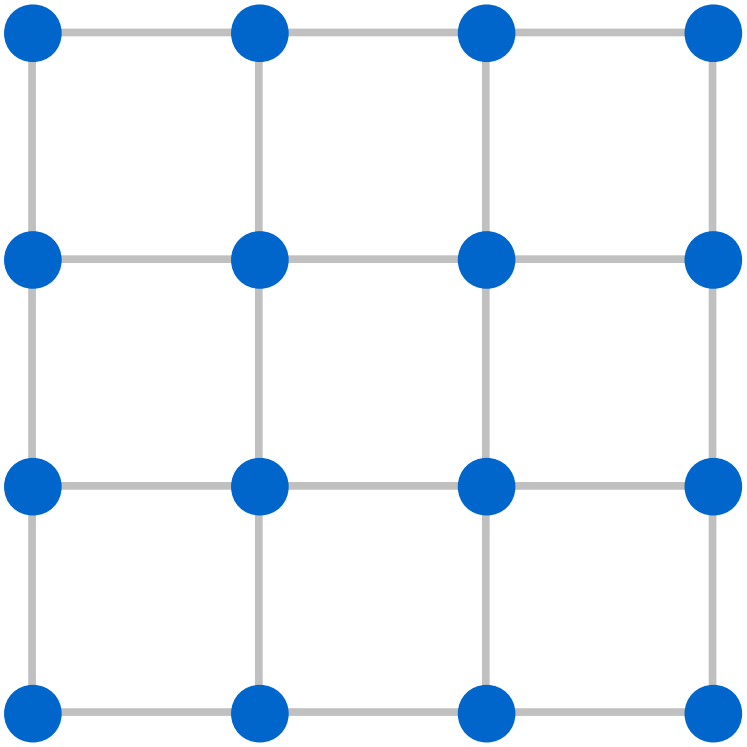
Phonons in DFT

Zero temperature

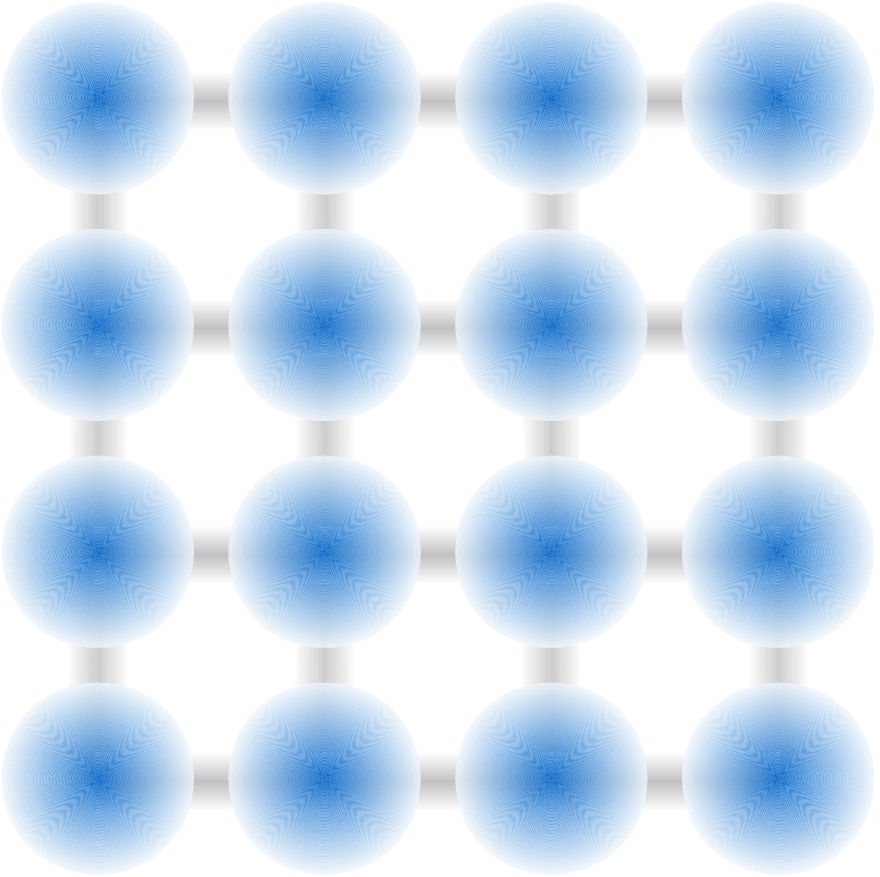


Phonons in DFT

Zero temperature

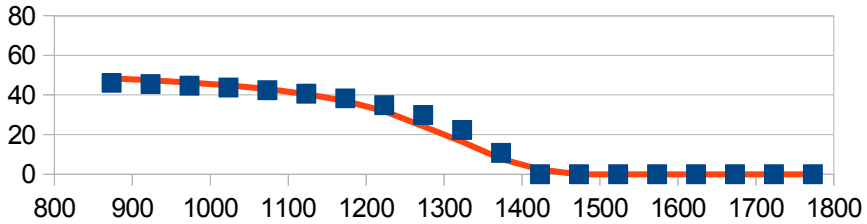


High temperature

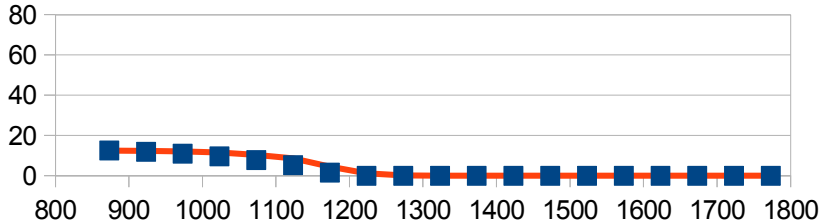


Phonons in DFT to predict phase behavior

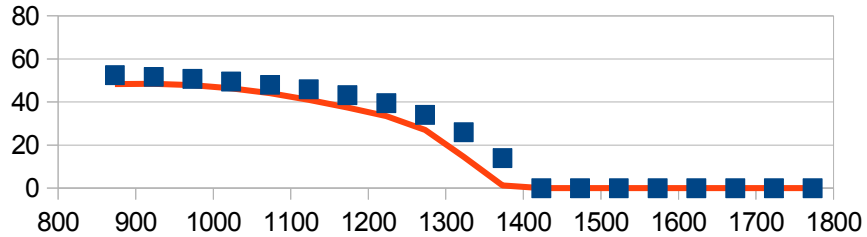
RR1000



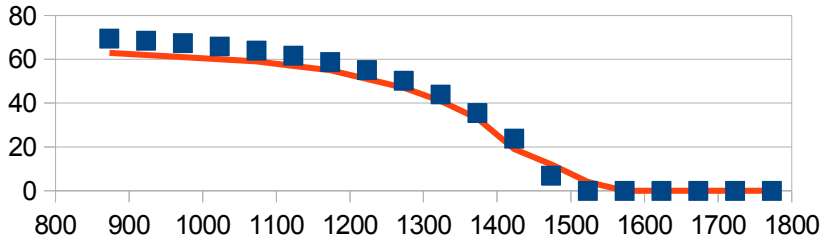
Nimonic263



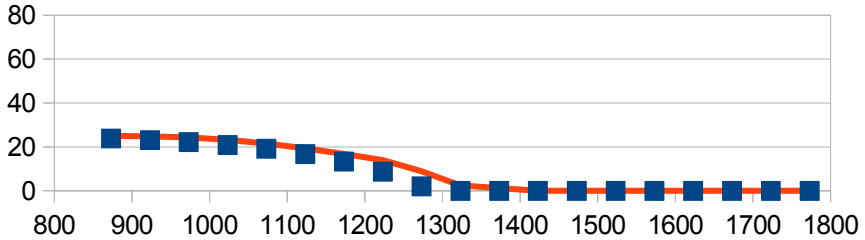
Rene95



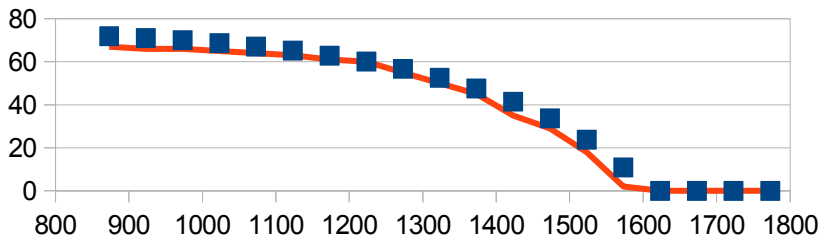
Mar-M200



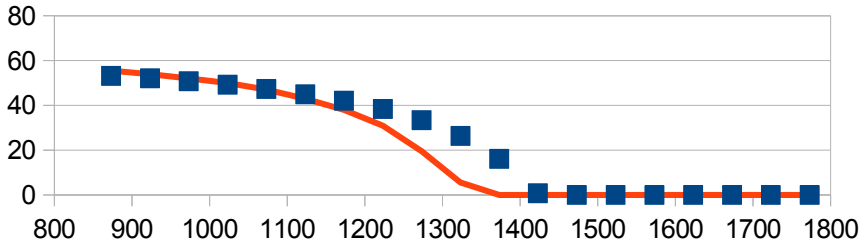
Waspaloy



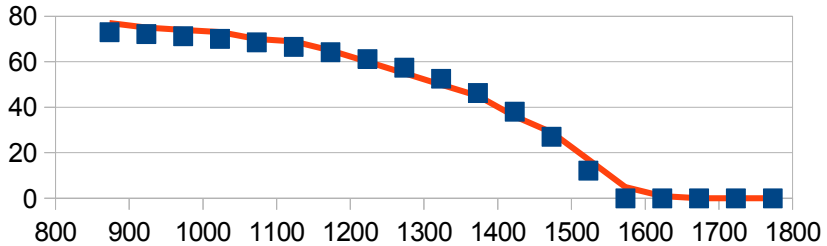
CMSX10



Astroloy



PWA1484

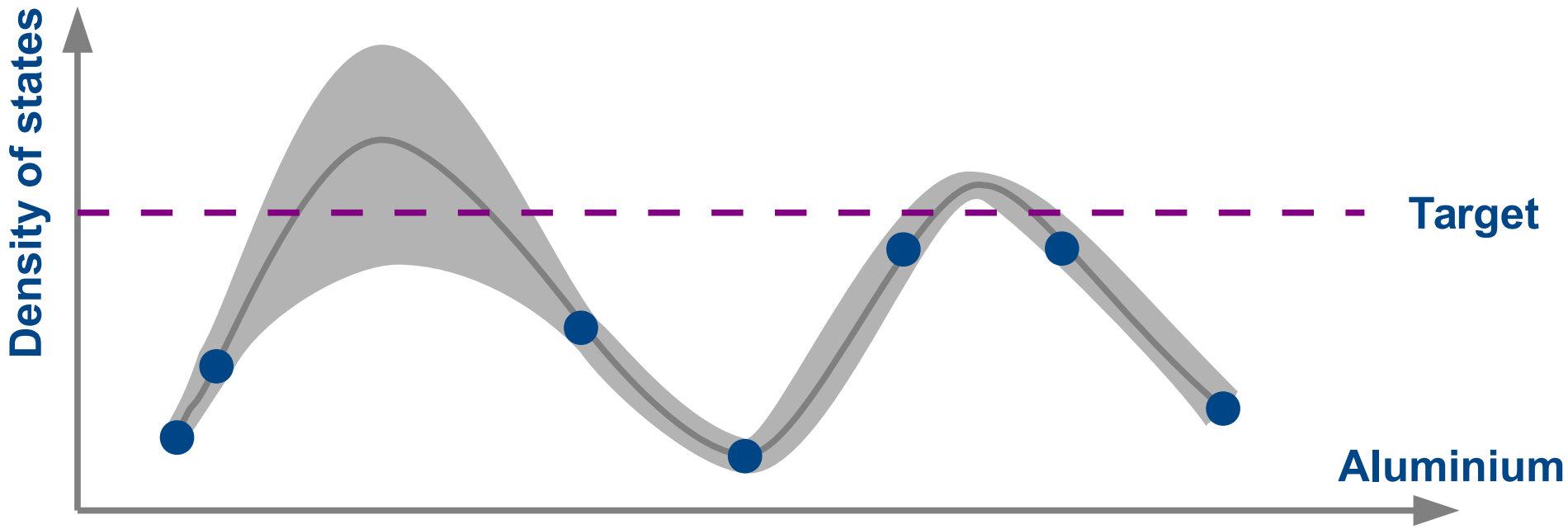


Recursive learning DFT

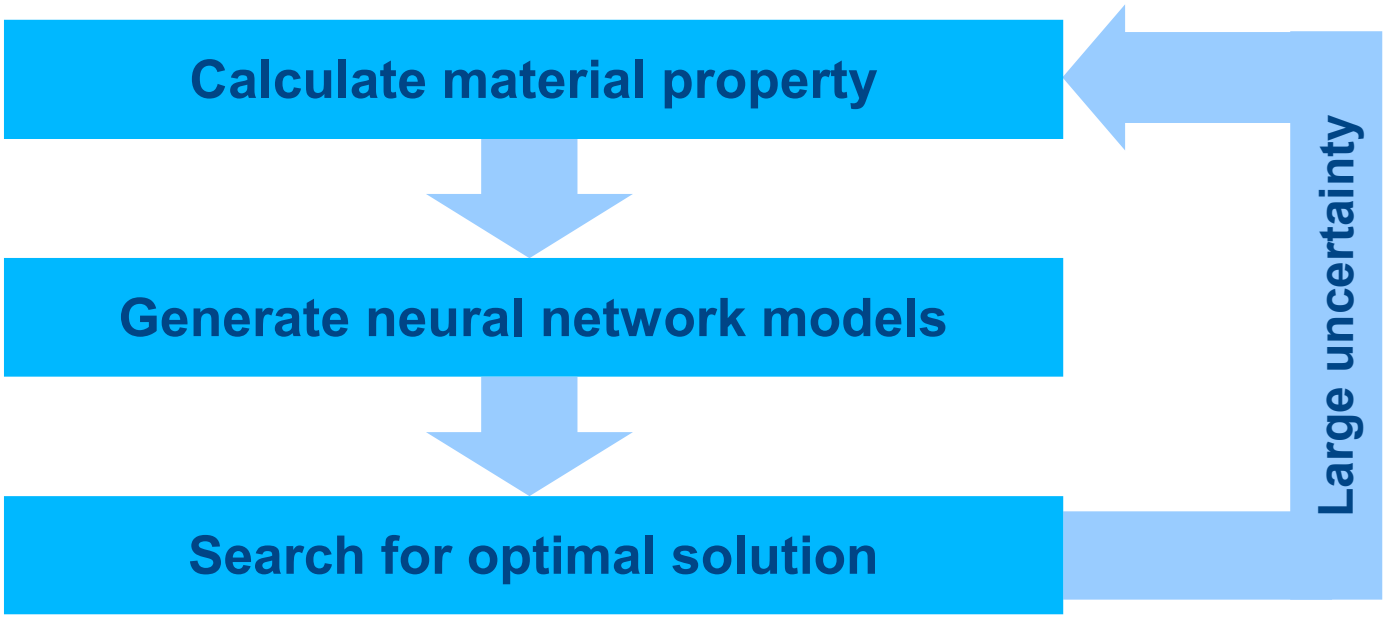
Calculate material property

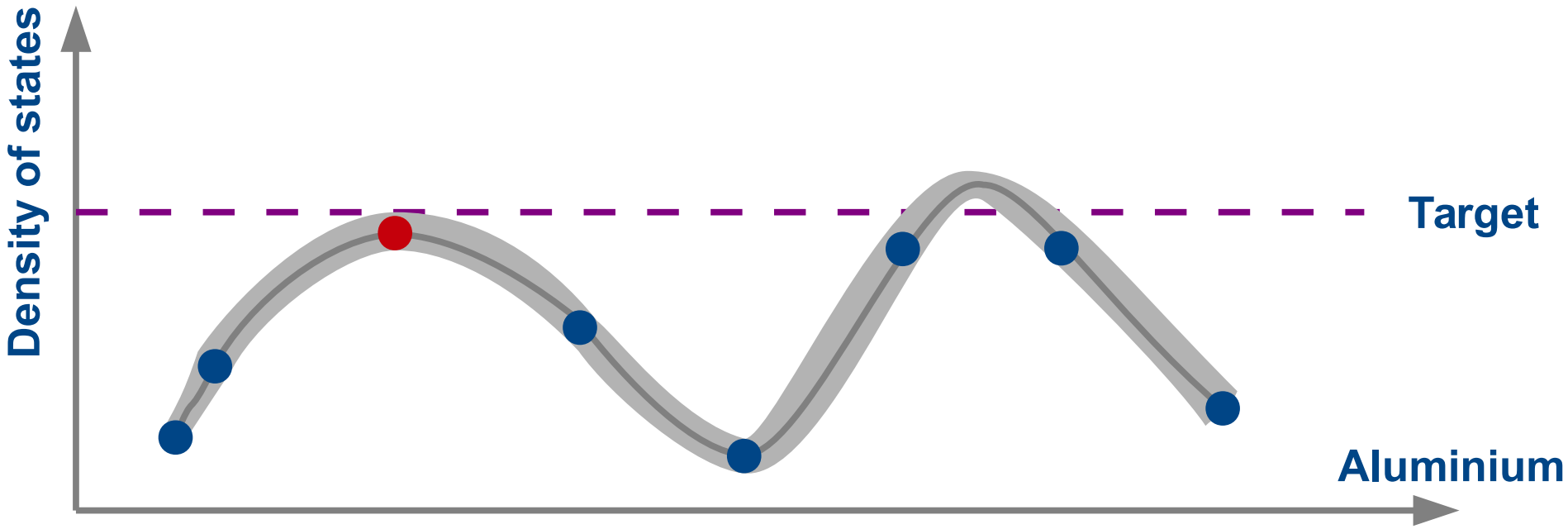
Generate neural network models

Search for optimal solution

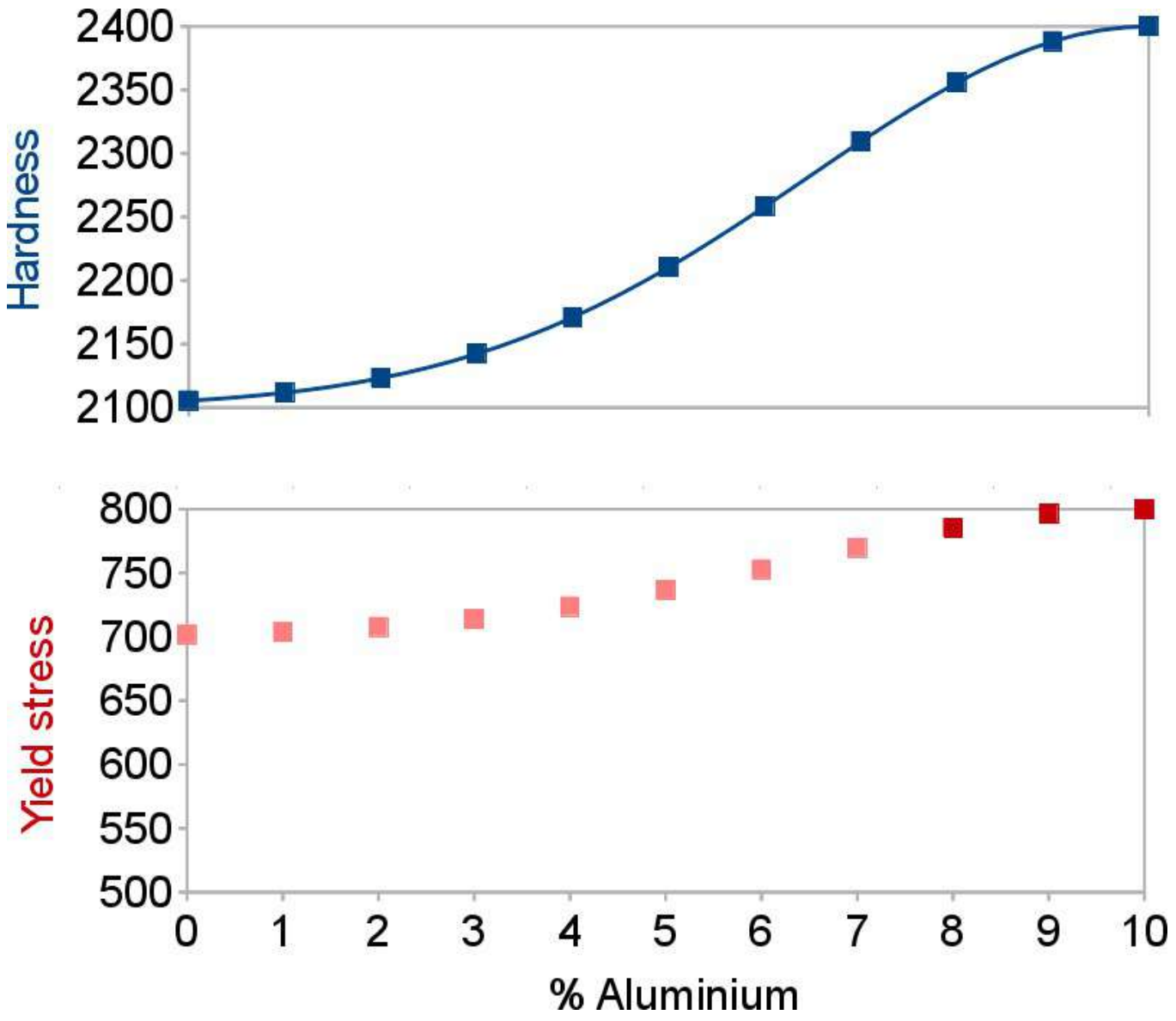


Recursive learning DFT

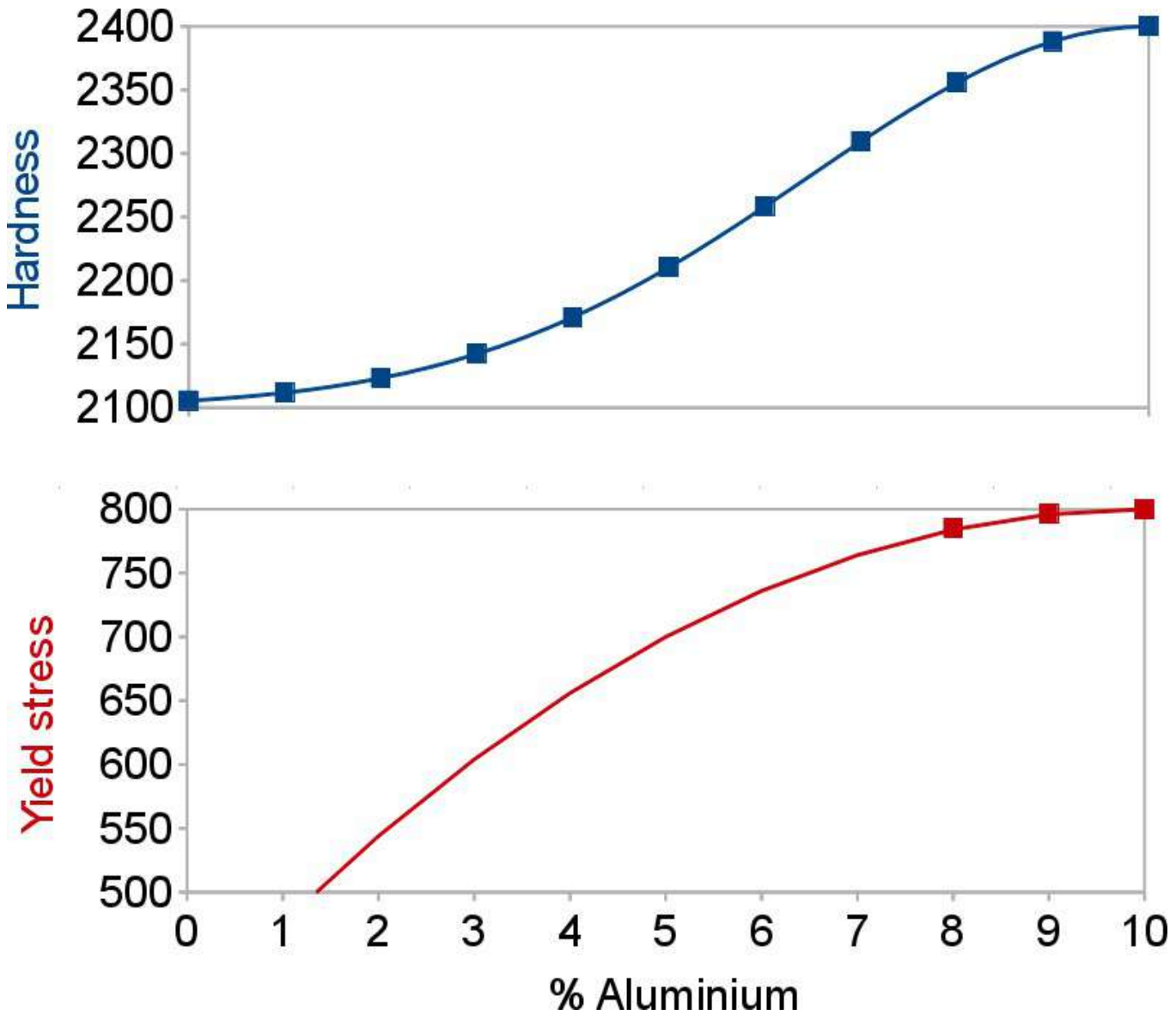




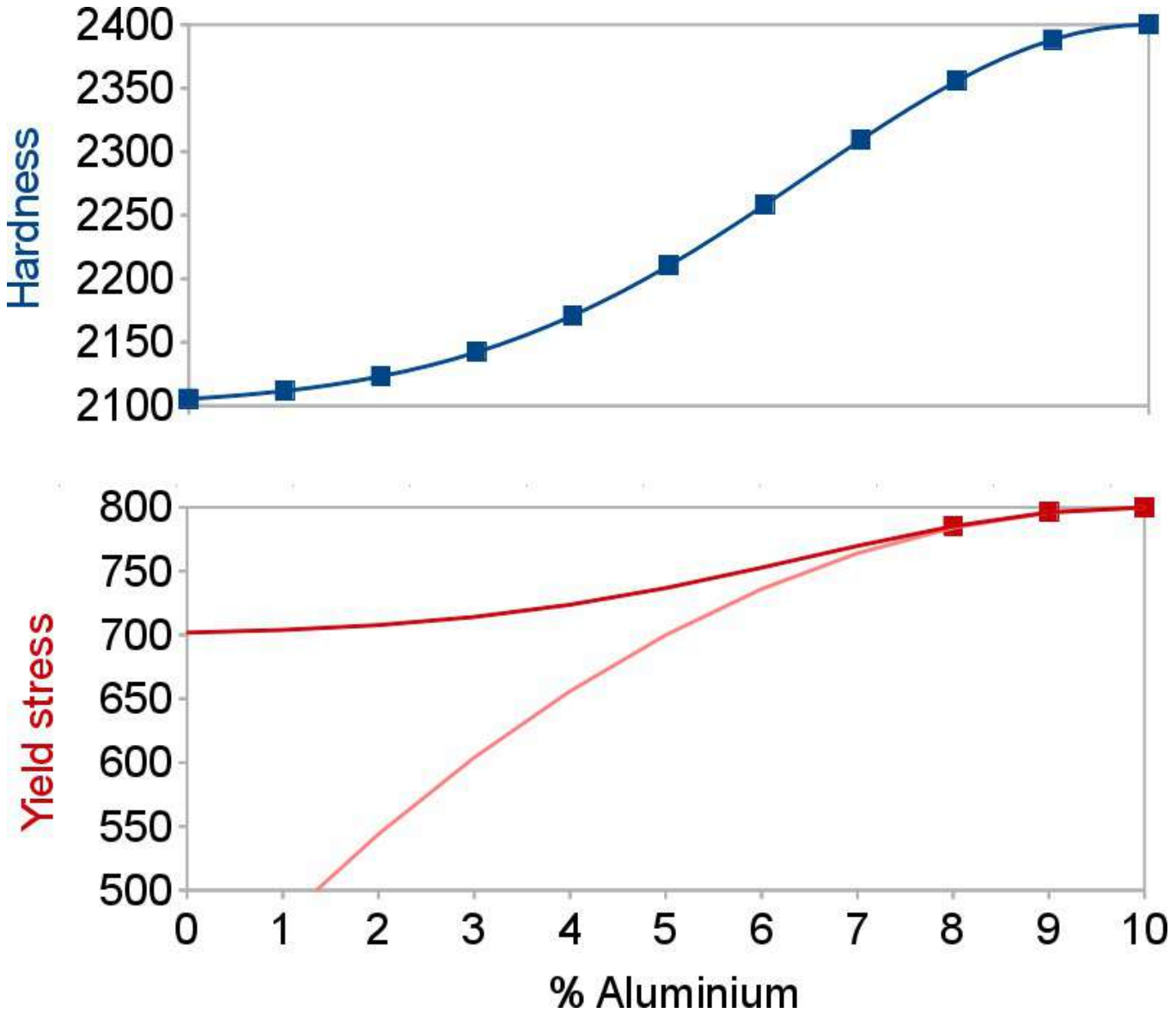
Correlations between properties



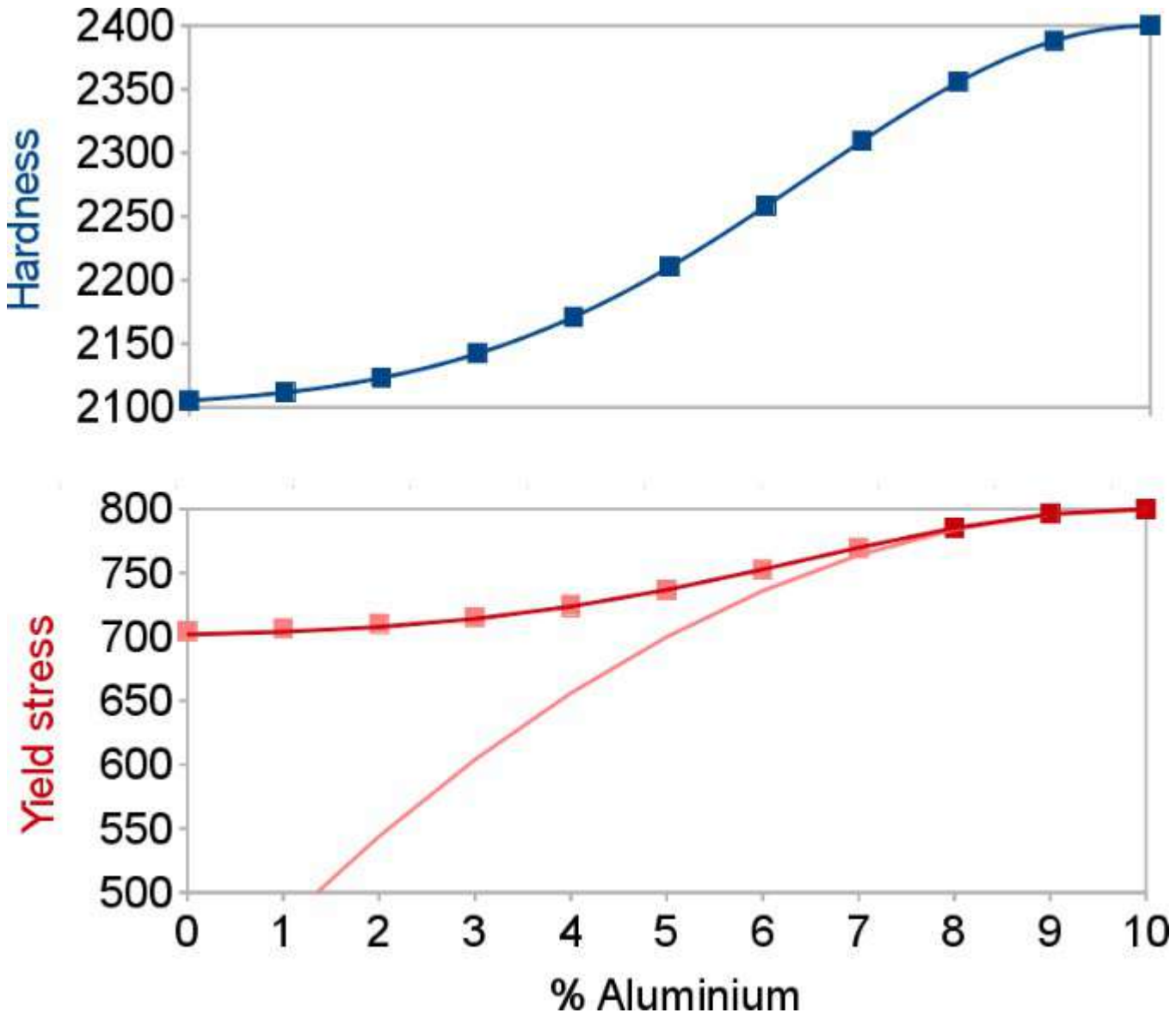
Correlations between properties



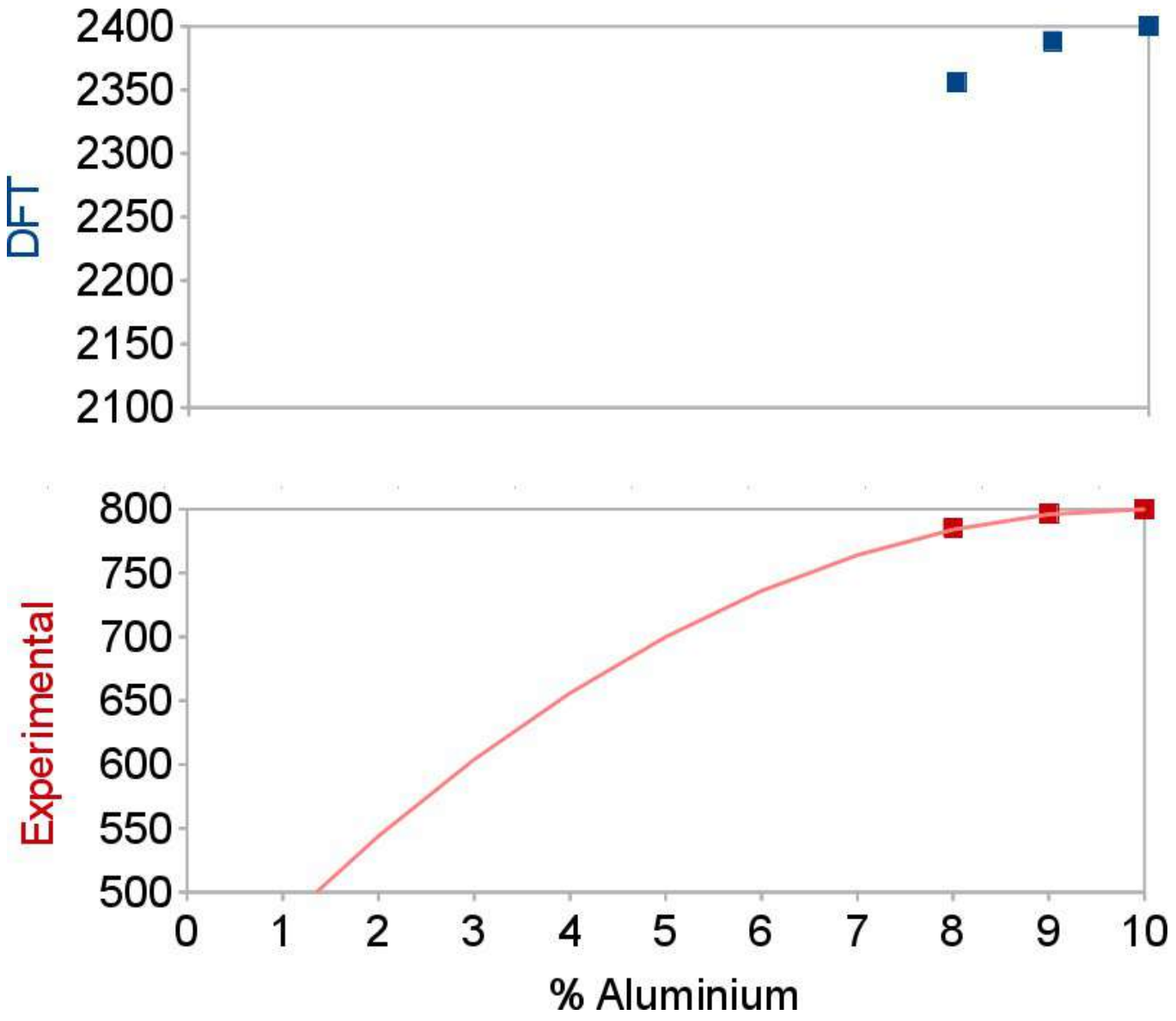
Correlations between properties



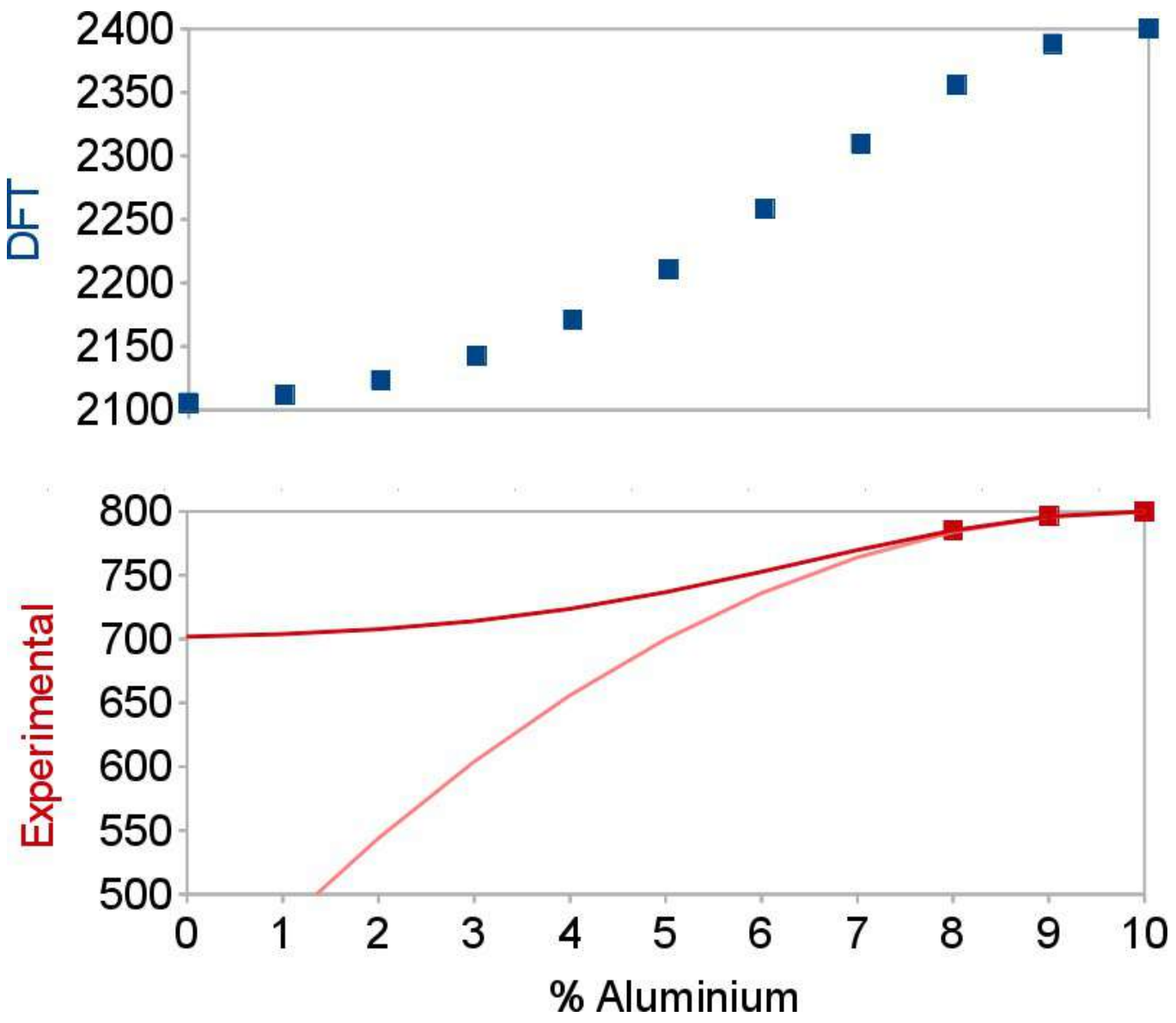
Correlations between properties



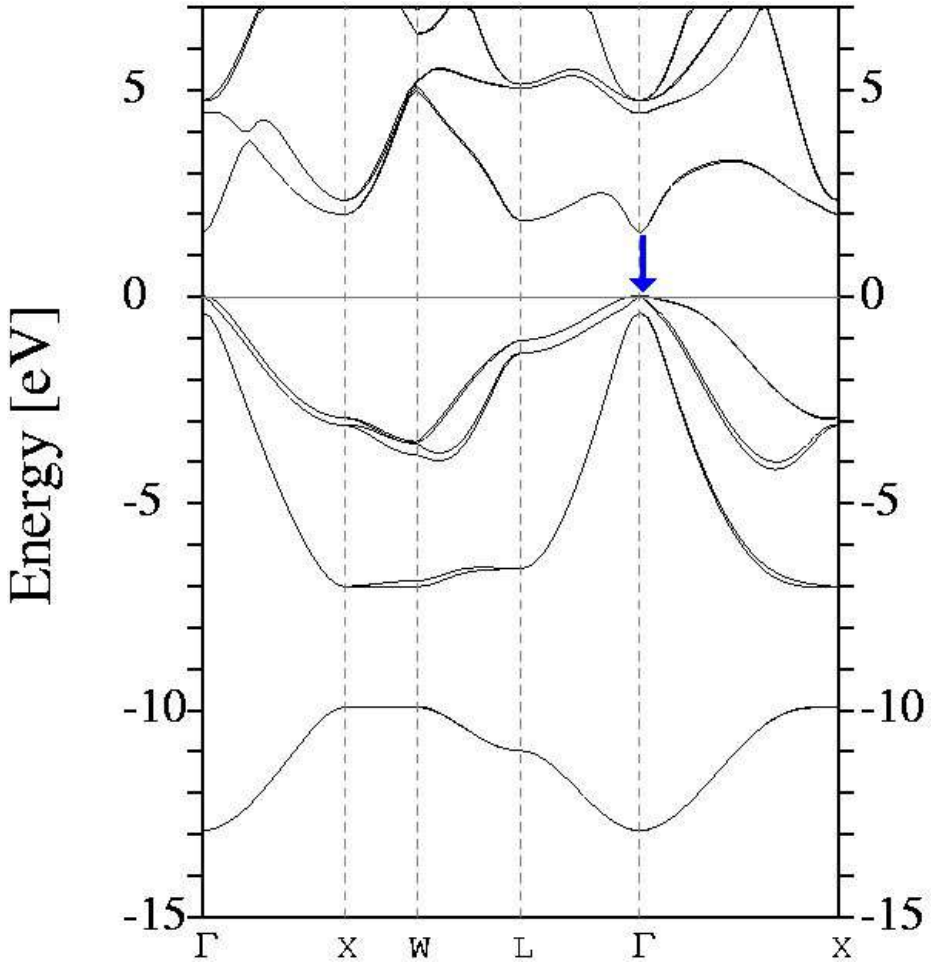
Correlations between properties



Correlations between properties



Semiconductors



Working with Samsung to propose and experimentally verify new LED materials

Use DFT combined with experimental data to search for:

Reduced cost

Improved efficiency

Four new tools

Neural network fitting & optimization	Mo and Ni alloys
Phonons in DFT	Alloy phase predictions
Recursive learning DFT	LED semiconductors
Correlations between properties	LED semiconductors

Precipitate formation