Concurrent materials design

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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

Experimental databases

Computational

Materials characterization
Two new tools

Experimental databases → Neural network fitting → Computational

Materials optimization
Neural network fitting & optimization

Hardness

Aluminum

Target
Probability

Hardness

Cycle fatigue

Weldability

Cost

Probability of alloy satisfying all properties

EP14153898.3; US 2014/177578; GB1302743.8
Ni-base superalloy
Two new tools

Experimental databases → Neural network fitting

Computational → Materials optimization
Three new tools

- Experimental databases
- Neural network fitting
- Property correlations
- Materials optimization

Computational
Correlations between properties

Aluminum

Hardness
Correlations between properties

Aluminum

Hardness
Correlations between properties

Aluminum

Hardness

Yield stress

Aluminum

Hardness

Aluminum
Correlations between properties

Aluminum

Hardness

Titanium

Hardness

Aluminum
Exploiting correlations: 3D printing

7 points for 3D printability + Weldability
Heat capacity
Conductivity
Precipitates → Accurate predictions for 3D printability
Exploiting correlations: LEDs

1. Band gap from experiment
2. DFT predictions of band gap
3. Accurate band gaps at all compositions
Three new tools

Experimental databases

Neural network fitting

Property correlations

Computational

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

1. Calculate material property
2. Generate neural network models
3. Search for optimal solution

Precipitate

Target

Aluminum
Recursive learning

1. Calculate material property
2. Generate neural network models
3. Search for optimal solution

Large uncertainty

Precipitate
Mo-base alloy

Proposed
MHC
TZC
TZM
ZHM

UTS / MPa

Temperature / °C

Patents GB1307533.8 (2013), GB1307535.3 (2013)
Mo-base alloy

The graph illustrates the relationship between UTS (MPa) and cost per cycle ($), with different compositions of Mo and Hf. The properties targets are satisfied within the shaded region.

- **UTS (MPa)**: The Y-axis represents the ultimate tensile strength in MPa.
- **Cost per cycle ($)**: The X-axis represents the cost per cycle in dollars.
- **Composition**: The color coding indicates the weight percentage of Mo and Hf, with Mo rich and Hf rich compositions.

Target areas are marked with dashed lines and specific points are highlighted with a cross.