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)
Four new tools

Experimental databases

Physically based

Computational

Materials characterization
Four new tools

- Experimental databases
- Neural network fitting
- Physically based
- Recursive learning
- Property correlations
- Computational
- Materials optimization
Neural network fitting & optimization

Yield stress vs. Aluminum

Target
Neural network fitting & optimization

Yield stress

Target

Aluminum
Probability of alloy satisfying all properties

- Yield stress
- Cycle fatigue
- Cost
- Weldability

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

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

Physically based → Recursive learning → Property correlations

Computational
Correlations between properties

Aluminum

Hardness

Graph showing correlation between Aluminum and Hardness.
Correlations between properties
Correlations between properties

Aluminum

Hardness

Yield stress

Aluminum

Hardness

Aluminum
Correlations between properties

Aluminum

Hardness

Titanium

Hardness

Aluminum

Hardness
Correlations between properties

- Relationships between material properties & computer simulations
- Search for LEDs with Samsung Electronics

- Relationships between material families
- Alloy for direct laser deposition with Rolls-Royce
Four new tools

- Experimental databases
- Neural network fitting
- Physically based
- Recursive learning
- Computational
- Property correlations

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
Recursive learning

- Calculate material property
- Generate neural network models
- Search for optimal solution

Precipitate

Target

Aluminum
Mo-base alloy

Proposed
MHC
TZC
TZM
ZHM

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