UNIVERSITY OF CAMBRIDGE

# Materials discovery with artificial intelligence

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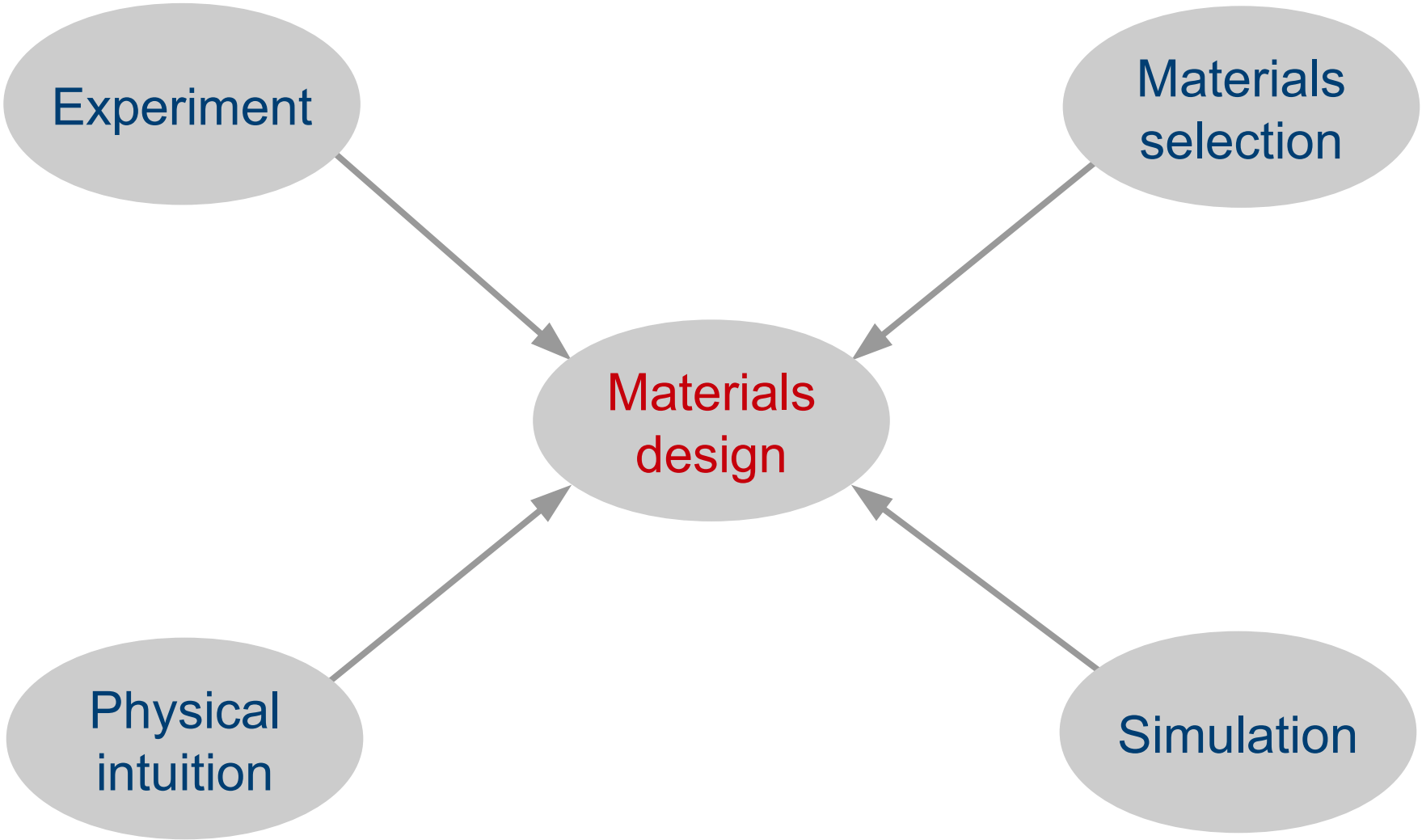
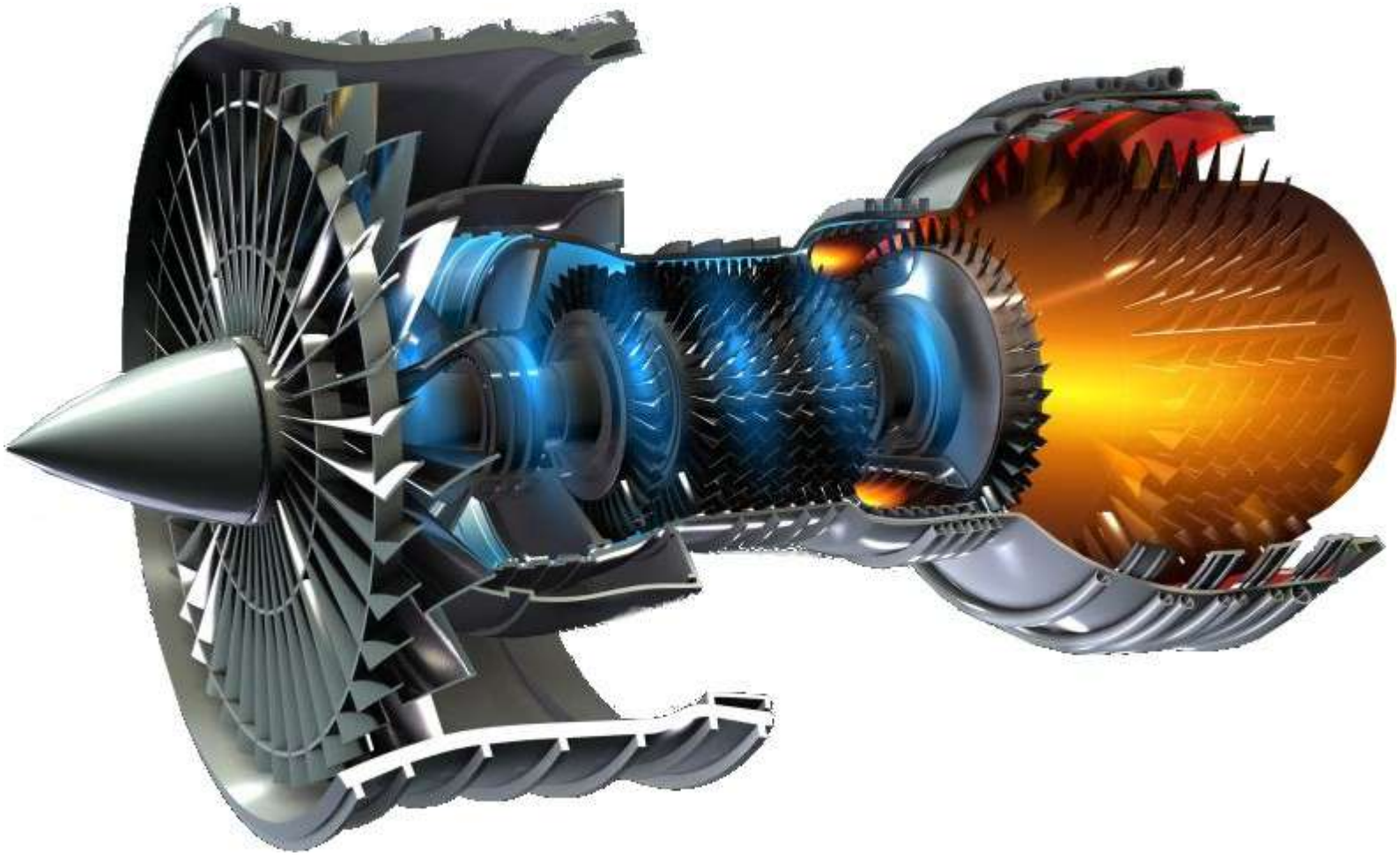
TCM Group, Department of Physics

# Using data to design materials



# Schematic of a jet engine



# Artificial intelligence

Composition

Artificial intelligence

Yield stress

Hardness

Melting point

Oxidation resistance

Cost

Density

Fatigue life

Fracture toughness

Creep

Processibility

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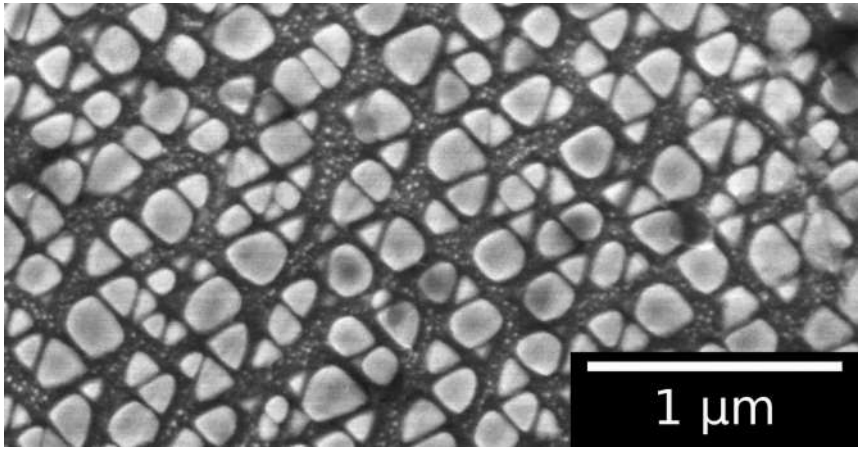
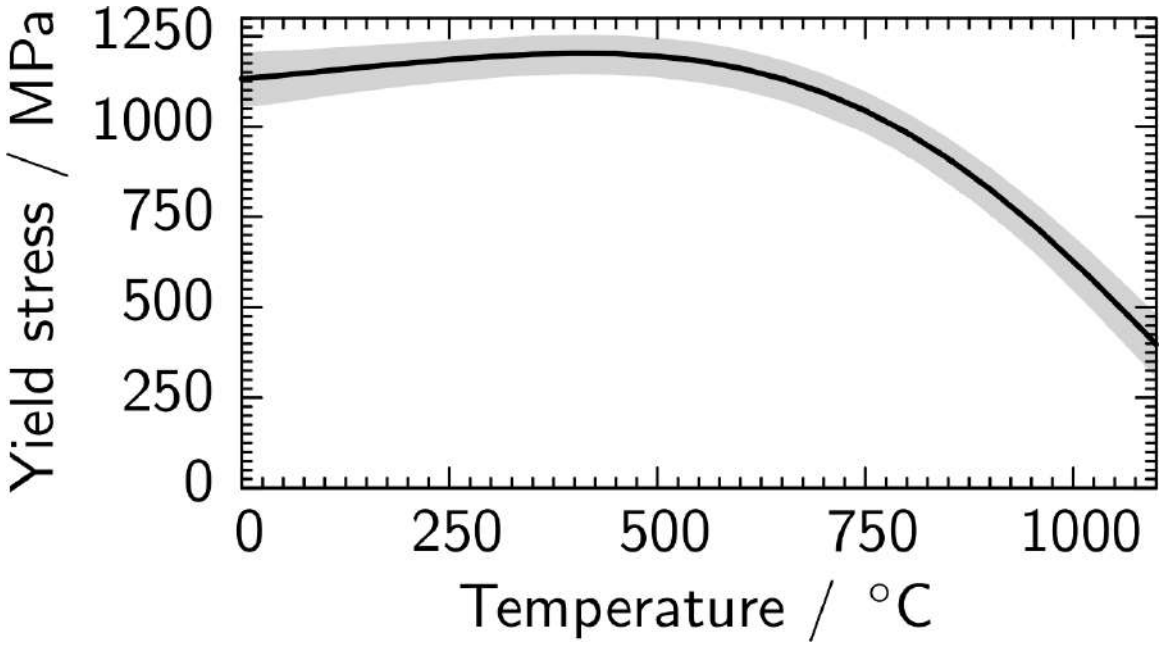
# Microstructure

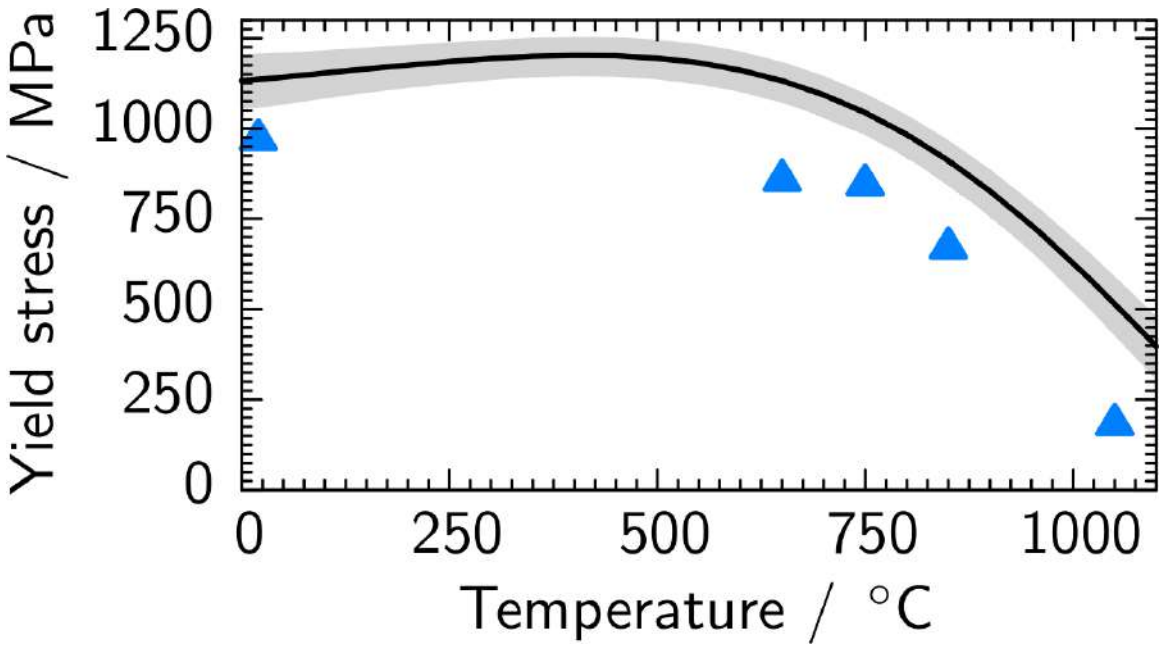


# Testing the yield stress




Proposed theory

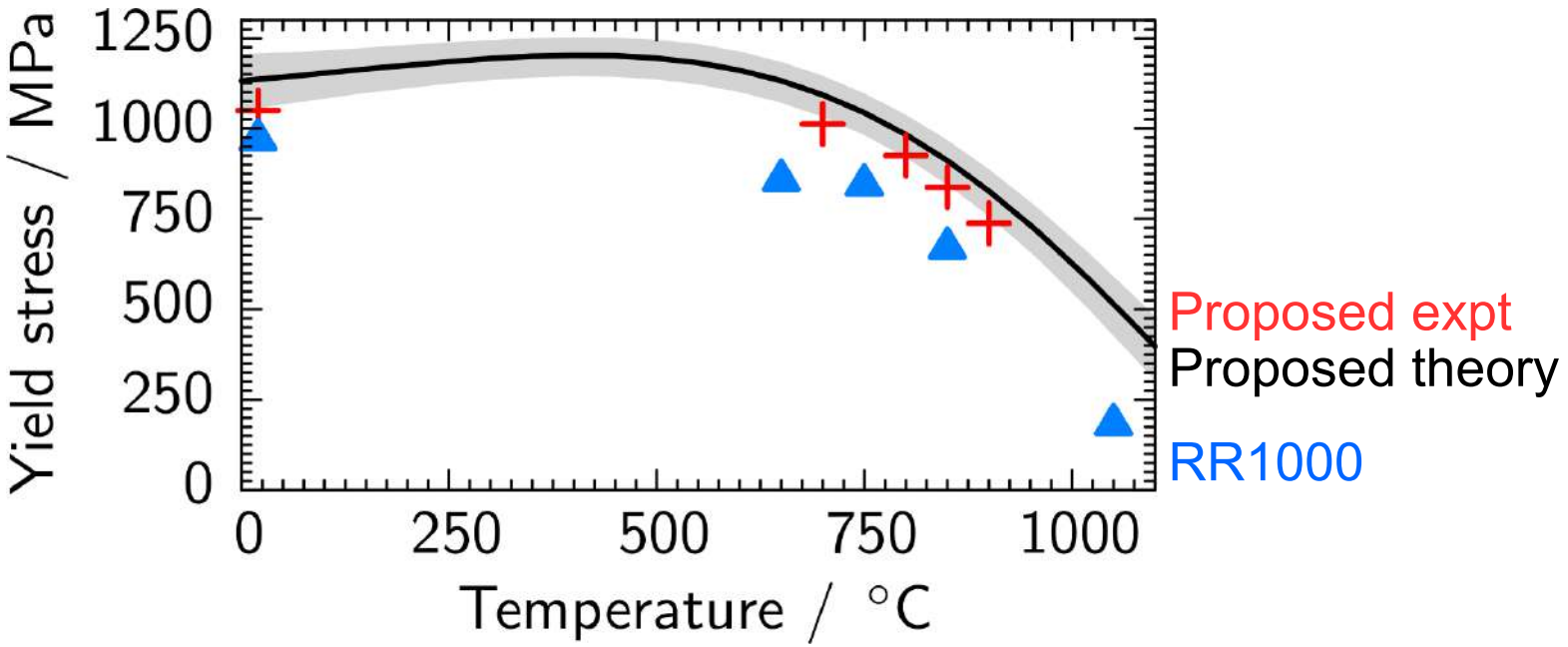
# Testing the yield stress



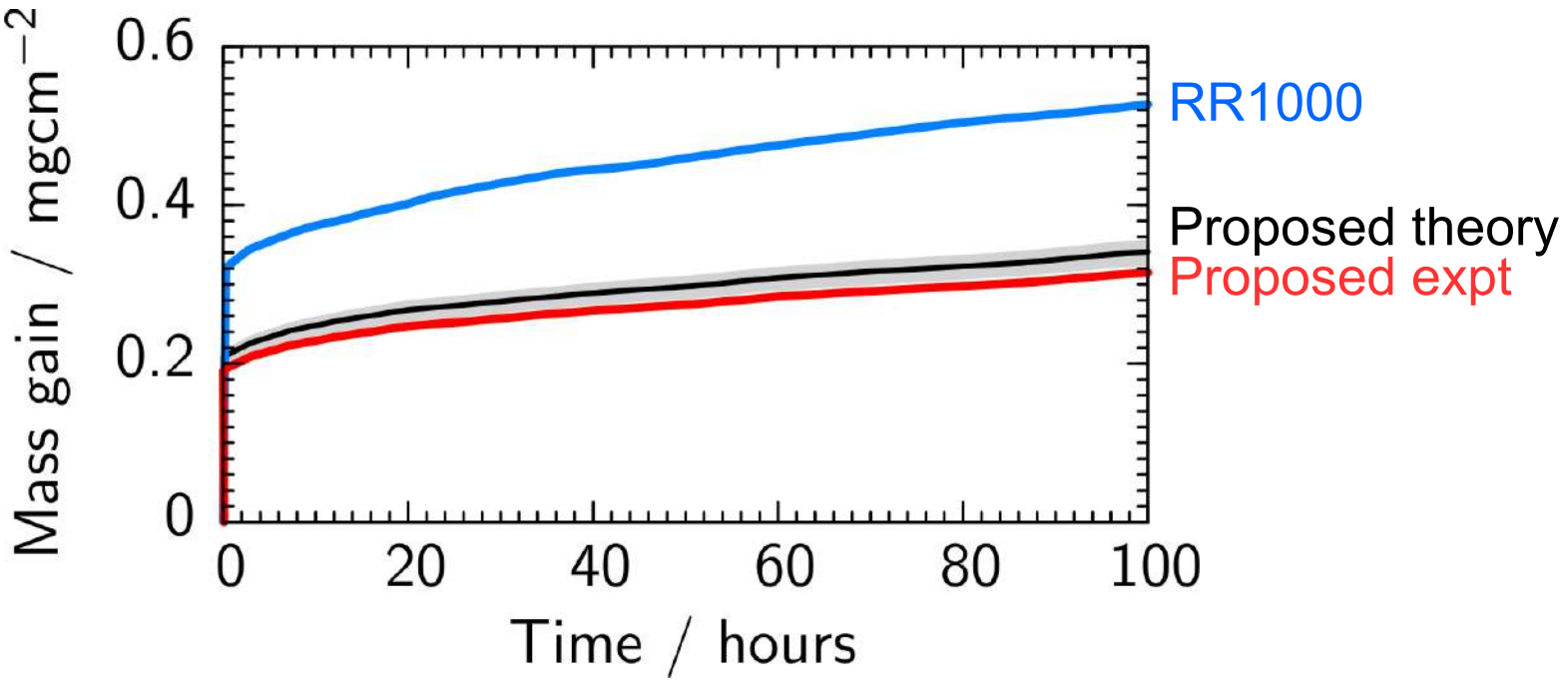

Proposed theory

RR1000

# Testing the yield stress

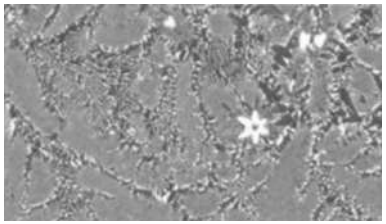


# Testing the oxidation resistance

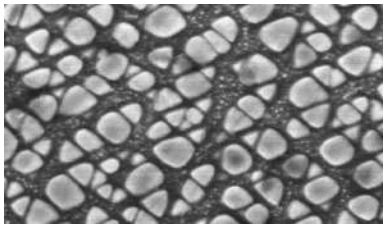


# Alloys discovered

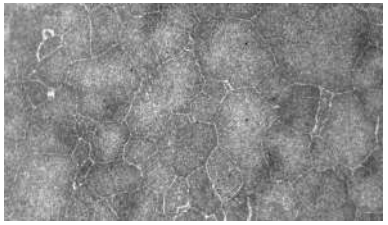
**Cr-$Cr_2Ta$ alloys**
Intermetallics, 48, 62



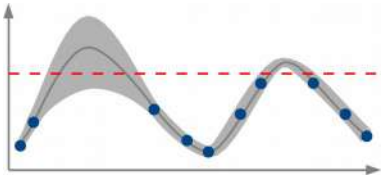
**Combustor alloy**
GB1408536



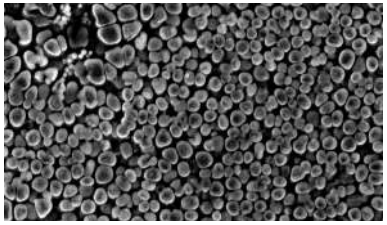
**RR1000 grain growth**
Acta Materialia, 61, 3378



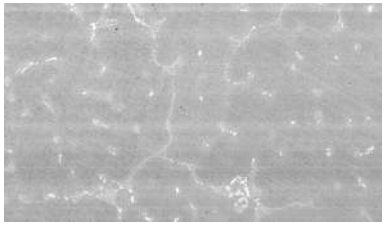
**Discovery algorithm**
EP14153898
US 2014/177578



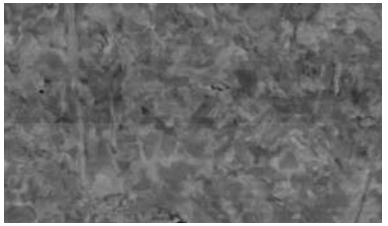
**Ni disc alloy**
EP14157622
US 2013/0052077 A2



**Mo-Hf forging alloy**
EP14161255
US 2014/223465



**Mo-Nb forging alloy**
EP14161529
US 2014/224885



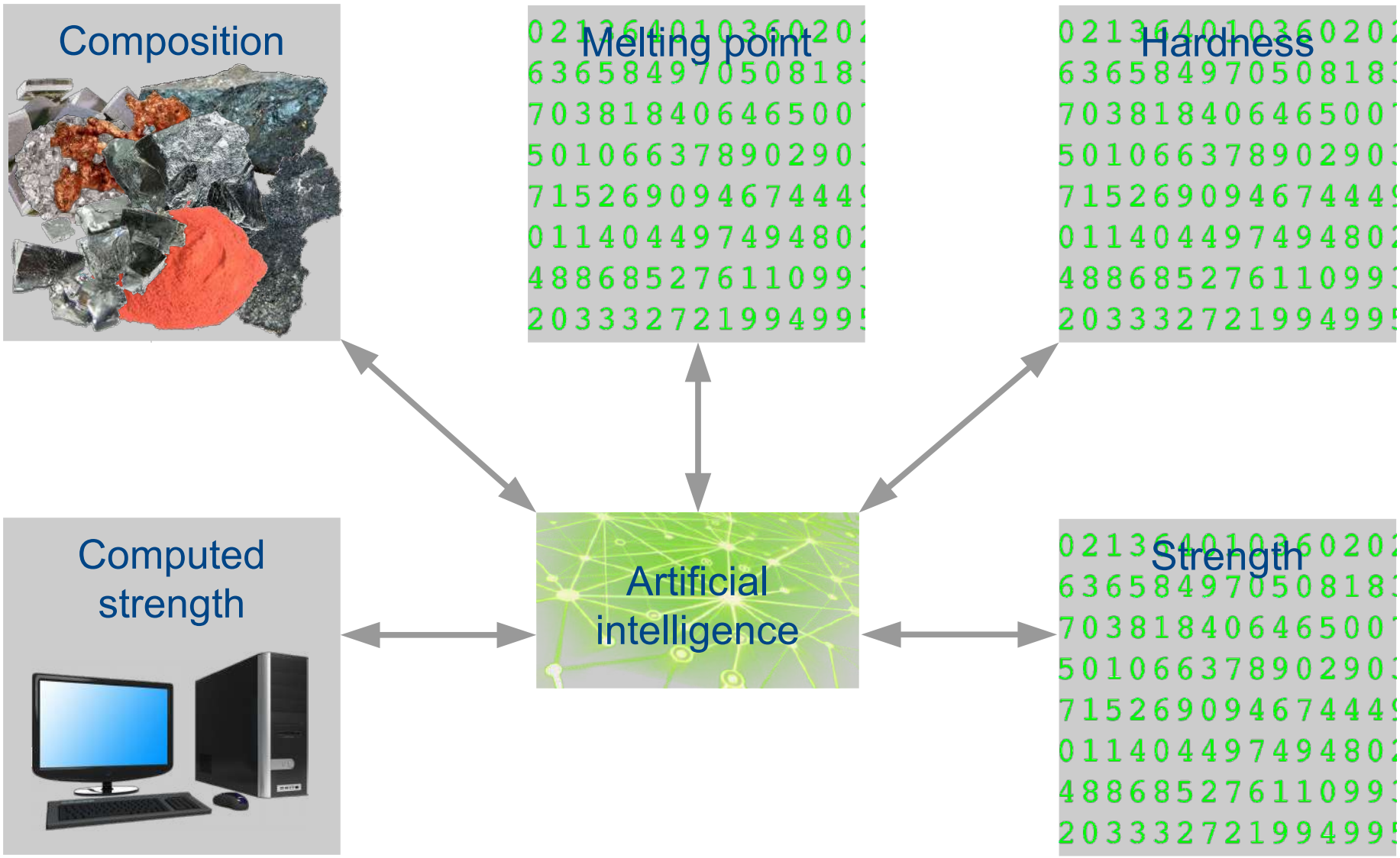
# Materials databases

| Nickel | Aluminum | Tungsten | Titanium | Strength |
|---|---|---|---|---|
| ✓ | ✓ | ✓ | ✓ | ✗ |
| ✓ | ✓ | ✓ | ✓ | ✗ |
| ✓ | ✓ | ✓ | ✓ | ✗ |
| ✓ | ✓ | ✓ | ✓ | ✗ |
| ✓ | ✓ | ✓ | ✓ | ✗ |
| ✓ | ✓ | ✓ | ✓ | ✗ |
| ✓ | ✓ | ✓ | ✓ | ✗ |

# Fragmented databases

| Composition | Computed strength | Melting point | Hardness | Strength |
|---|---|---|---|---|
| ✓ | ✓ | ✓ | ✓ | ✓ |
| ✓ | ✓ | ✗ | ✓ | ✓ |
| ✓ | ✓ | ✗ | ✗ | ✓ |
| ✓ | ✓ | ✓ | ✓ | ✗ |
| ✓ | ✓ | ✓ | ✗ | ✗ |
| ✓ | ✓ | ✗ | ✓ | ✗ |
| ✓ | ✓ | ✗ | ✗ | ✗ |

# Merging simulation and experiment



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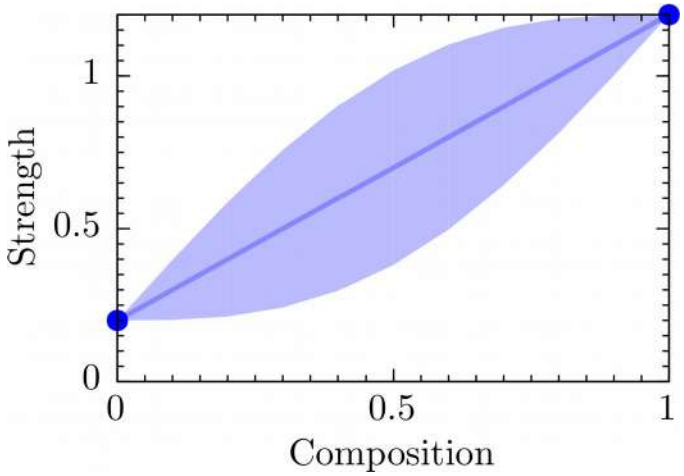

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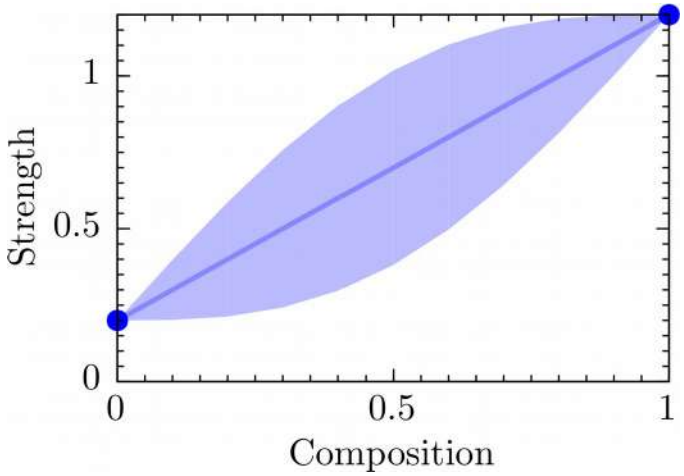


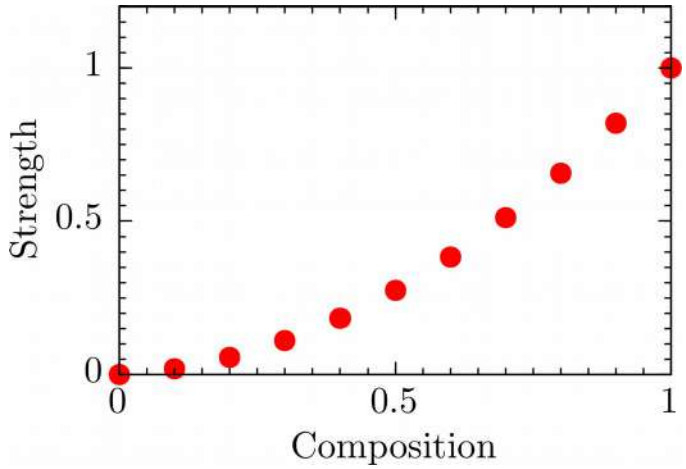

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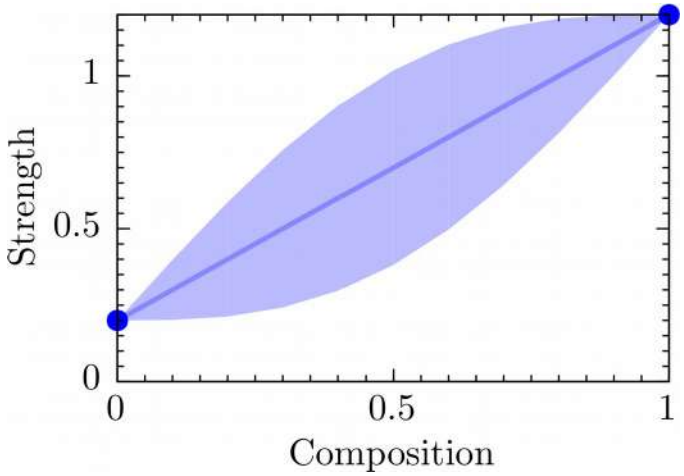
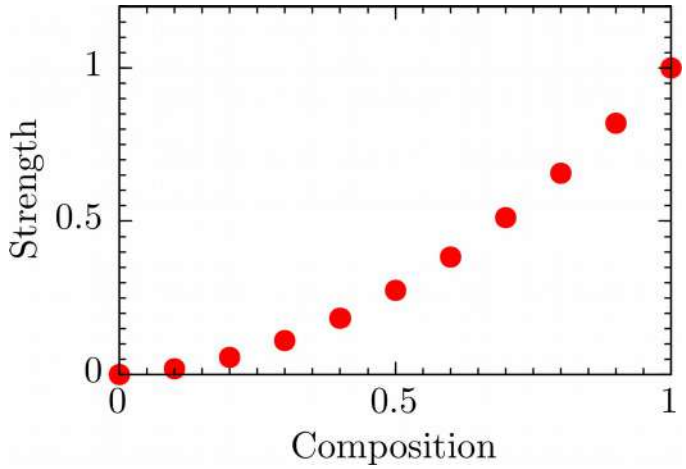
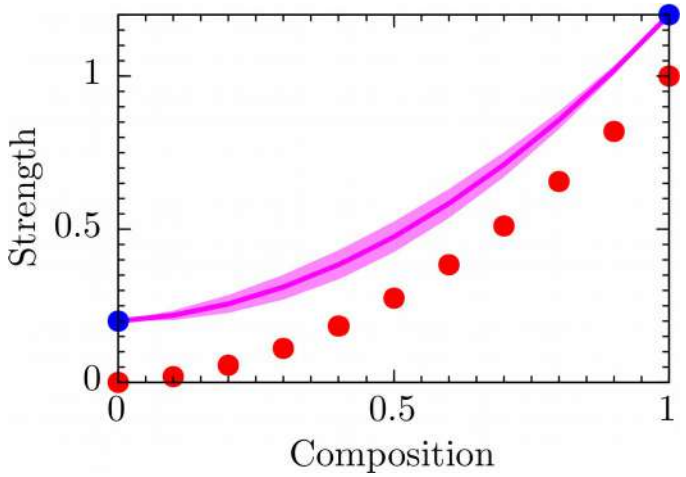


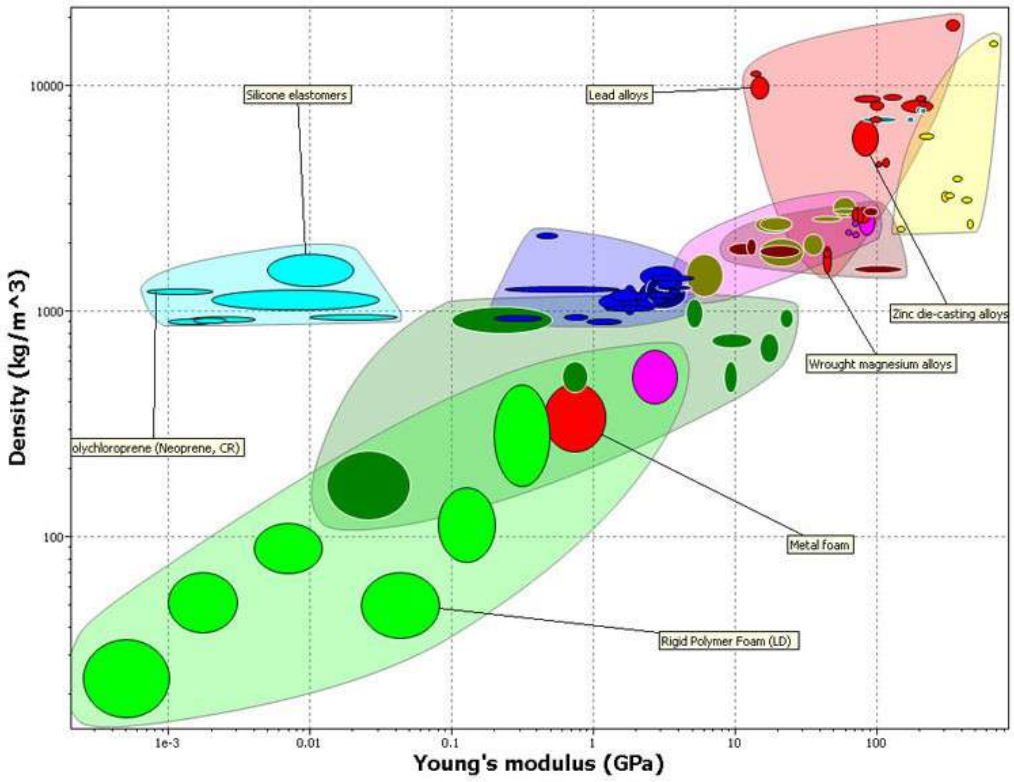

Combine



# Designing a lithium cathode


Experiment ⟷ Computational

# Database verification




Database contains >$10^7$ separate entries

# Summary

Analyze databases with artificial intelligence to discover four new alloys

Merge fragmented computational and experimental databases

Materials database verification and completion