Learning to commercialize deep learning

Gareth Conduit

Neural network algorithm to

Merge simulations, physical laws, and experimental data

Reduce the need for expensive experimental development

Accelerate materials and drugs discovery

Generic with proven applications in materials discovery and drug design

2012: Working with Rolls Royce UTC

Design new materials that fulfil multiple target criteria in yield, hardness, melting, oxidation, cost, density, fatigue, toughness, creep, and processibility

2012: Working with Rolls Royce UTC

Design new materials that fulfil multiple target criteria in yield, hardness, melting, oxidation, cost, density, fatigue, toughness, creep, and processibility

Use a standard neural network to predict each property, combine results by multiplying likelihoods

$$L_{tot}=L_{yield}\,L_{hardness}\,L_{melting}\,L_{oxidation}\,L_{cost}\,L_{density}\,L_{fatigue}\,L_{toughness}\,L_{creep}\,L_{processibility}$$

2012: Alloy designed: composition

Cr:15.8

Co: 20.0

Mo: 0.5

W: 0.5

Ta: 4.9

Nb: 1.1

Al: 2.4

Ti: 3.0

Fe: 3.9

Mn: 0.2

Si: 0.2

C: 0.02

B: 0.06

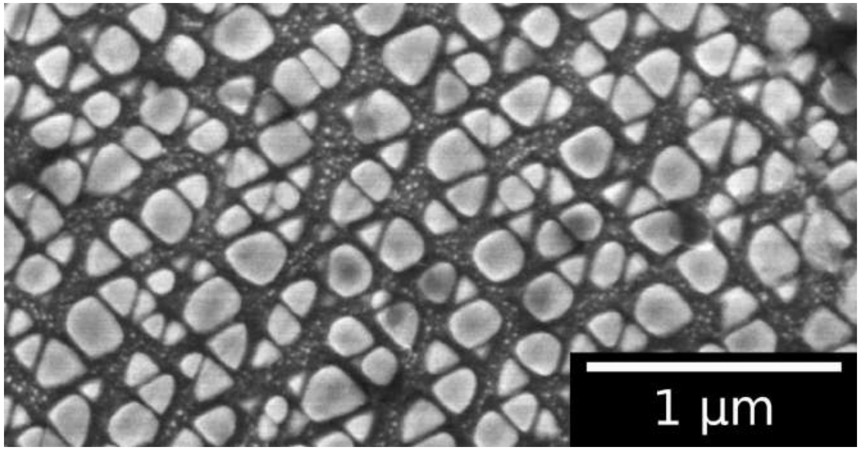
Zr: 0.18

Ni: 47.2

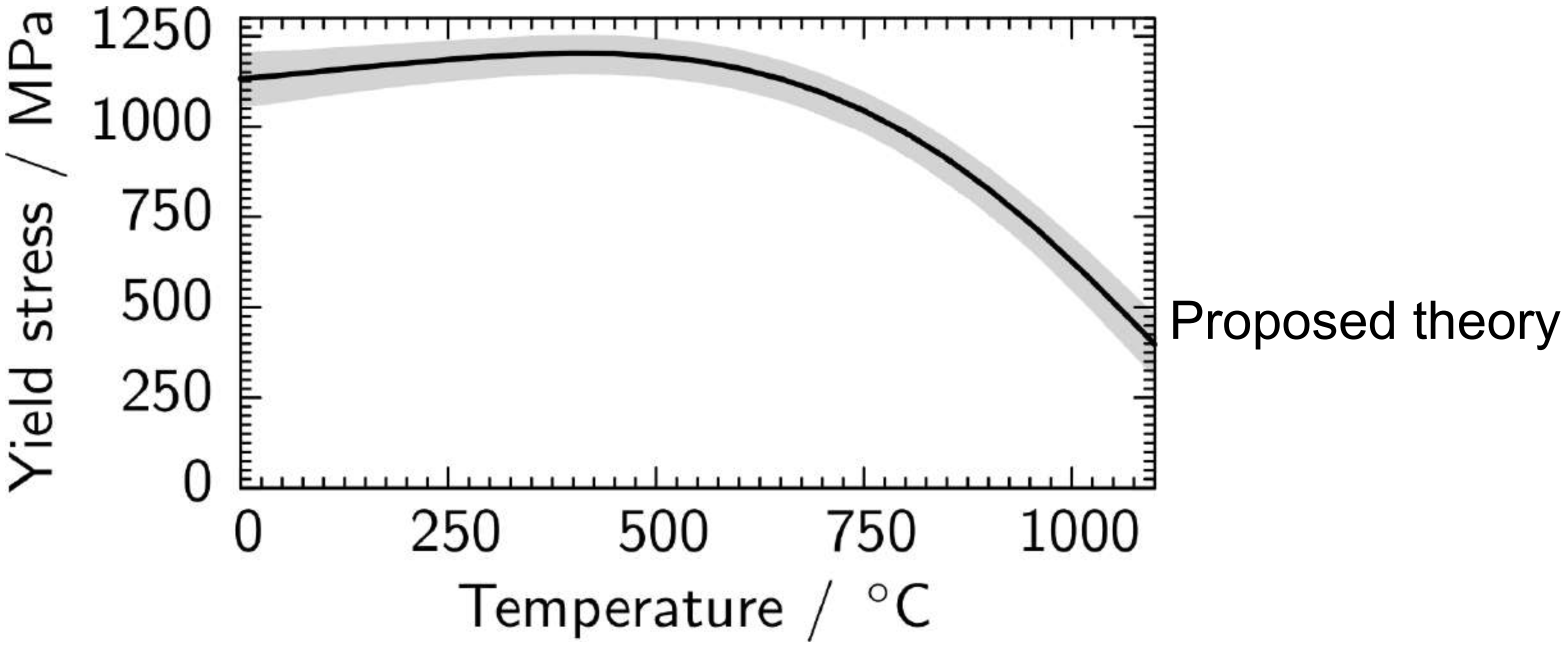
900ºC

30 hours

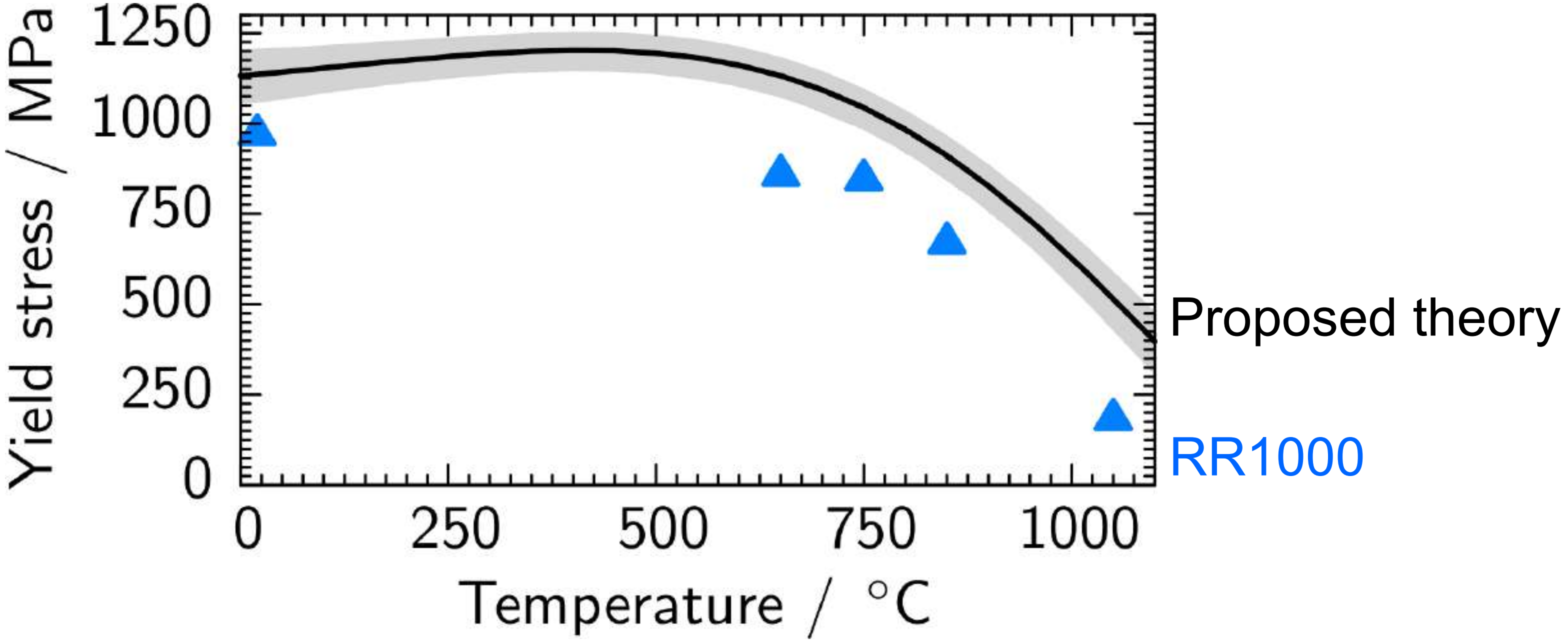
2012: Microstructure



2012: Predict the yield stress



2012: Test the yield stress



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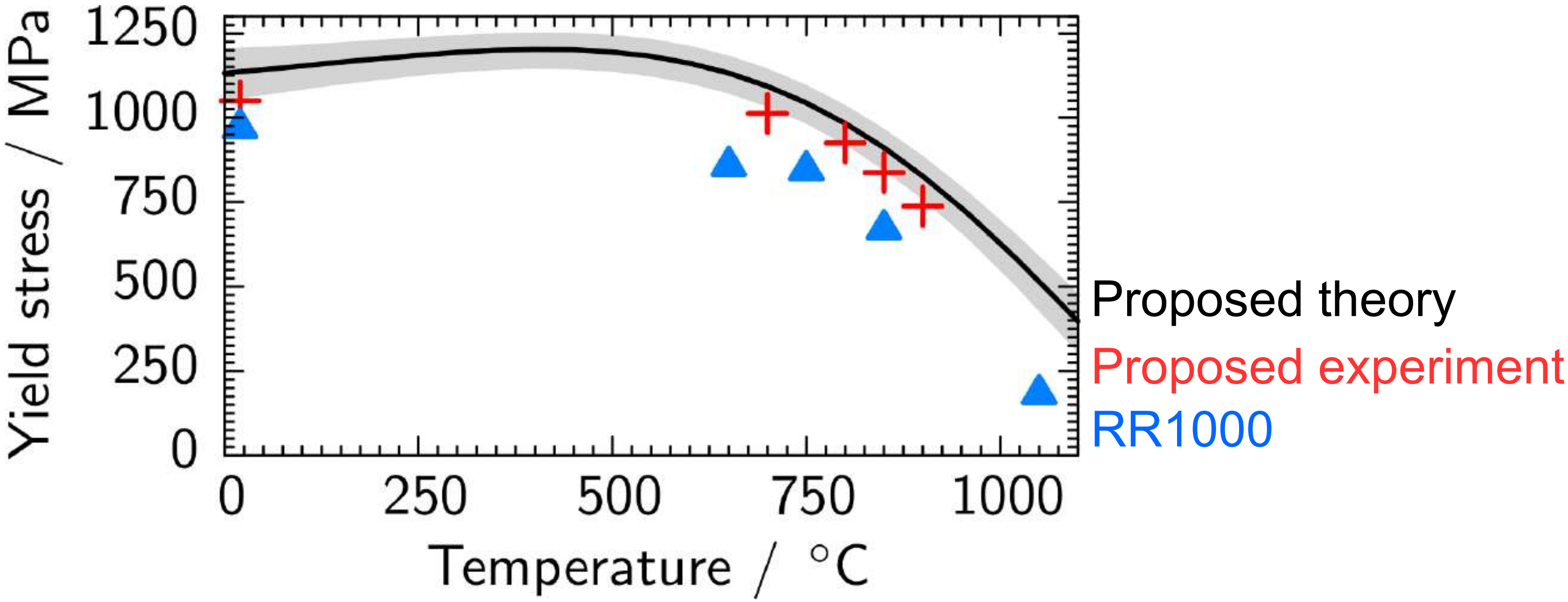
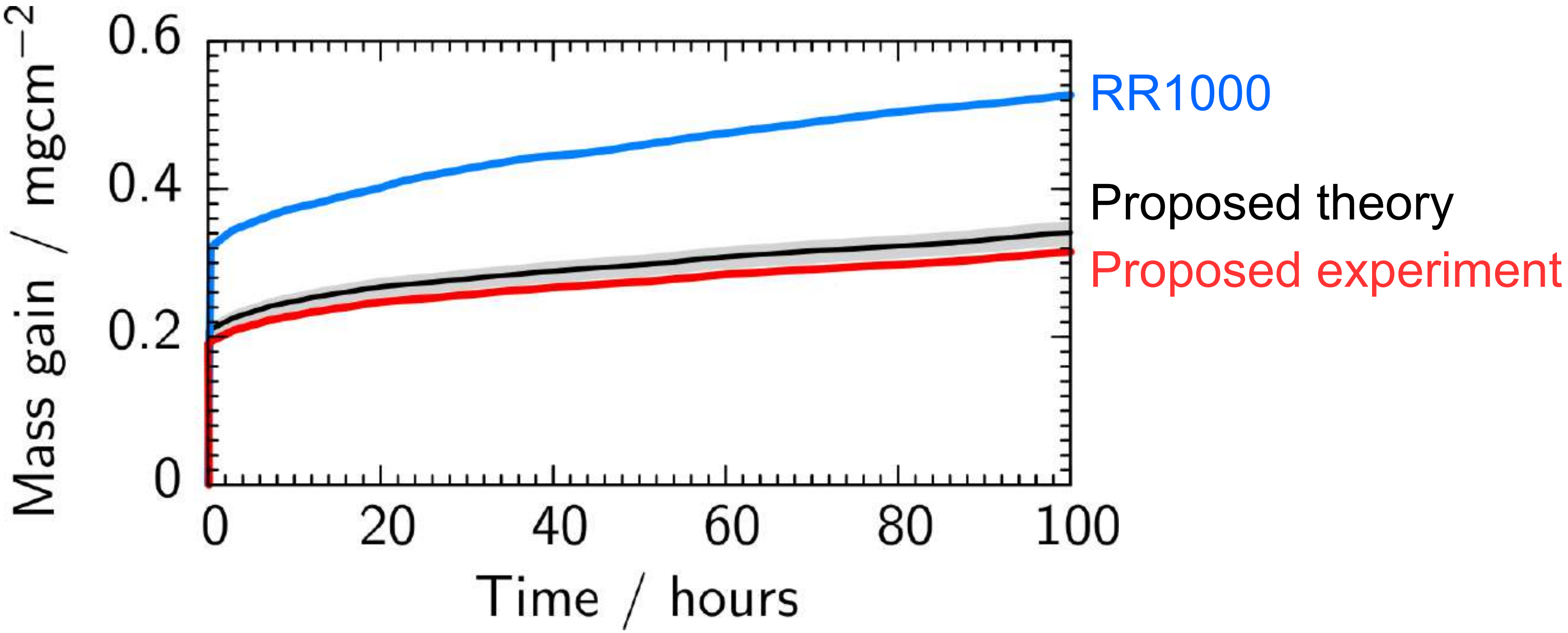
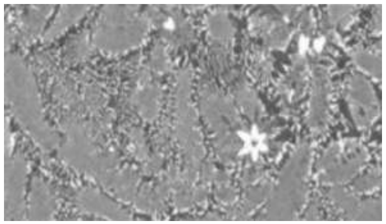


2012: Test the oxidation resistance

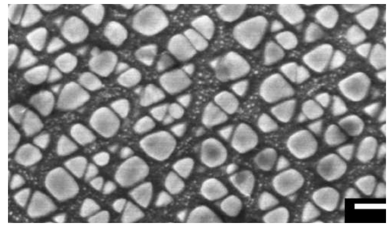


2012: Alloys designed

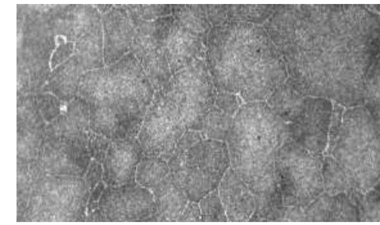
Cr-Cr_2Ta alloys
Intermetallics, 48, 62



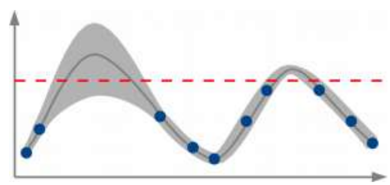
Combustor alloy
GB1408536



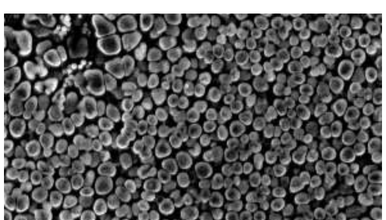
RR1000 grain growth
Acta Materialia, 61, 3378



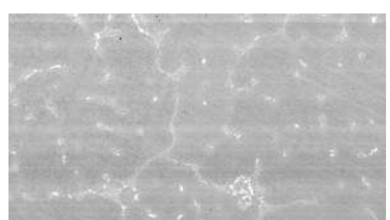
Discovery algorithm
EP14153898
US 2014/177578



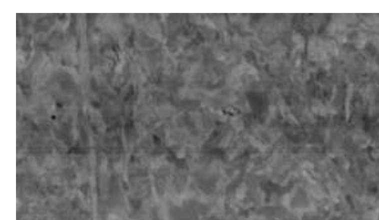
Ni disc alloy
EP14157622
US 2013/0052077 A2



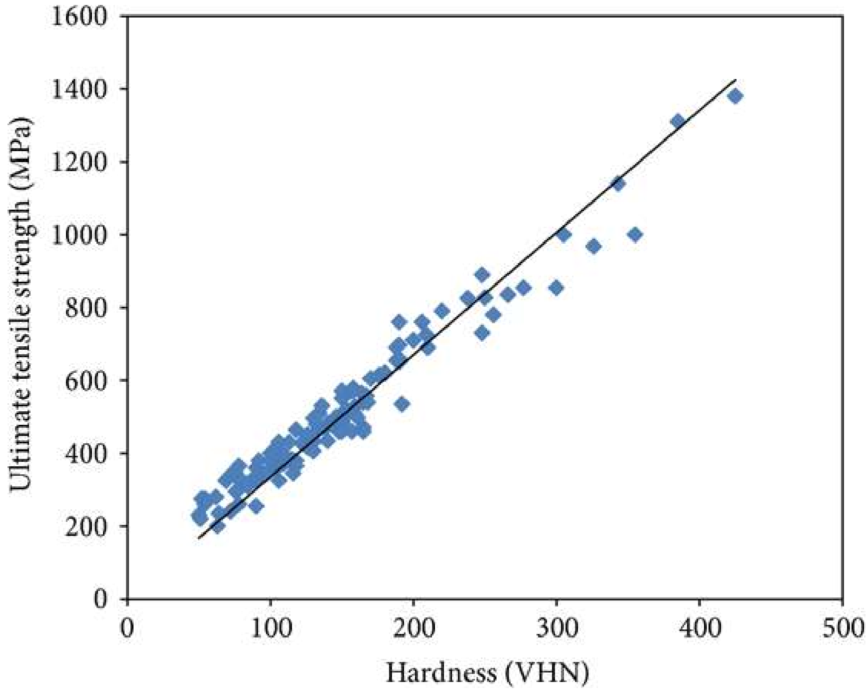
Mo-Hf forging alloy
EP14161255
US 2014/223465



Mo-Nb forging alloy
EP14161529
US 2014/224885

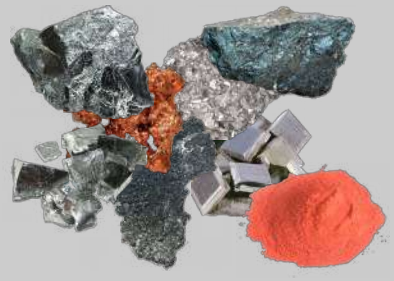


2013: Property-property correlations



2013: Alloy for 3D printing: property-property correlations

Composition



Properties

Weldability

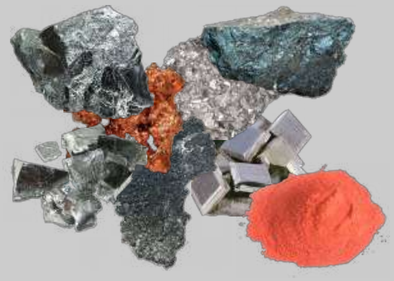
Processibility

Cost

2013: Alloy for 3D printing: property-property correlations

Extrapolate ten results for processibility with weldability

Composition



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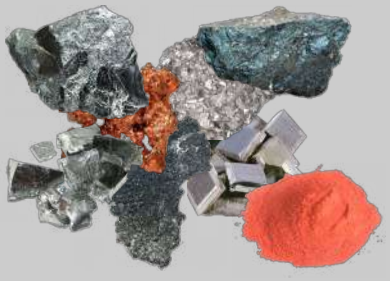

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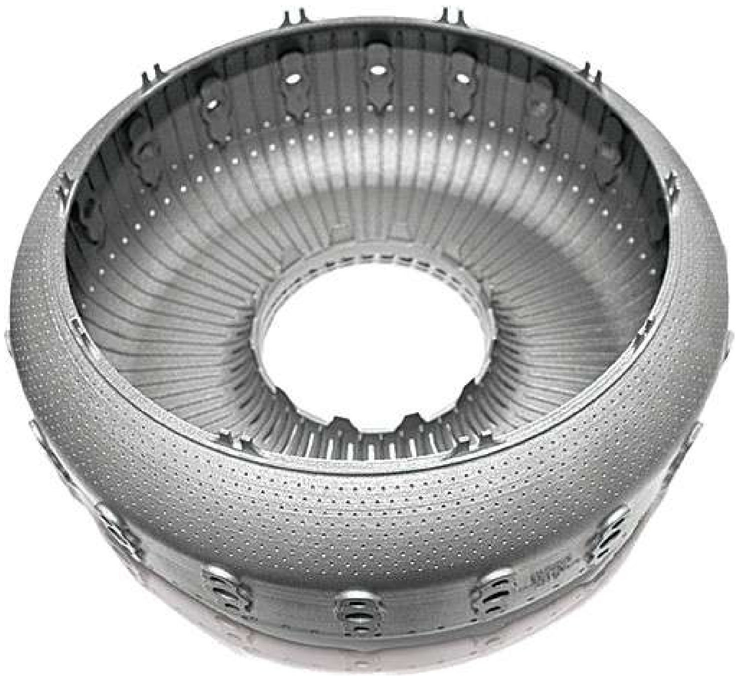


2014: Further materials design

Battery design
with DFT and
experimental data

2014: Further materials design

Battery design with DFT and experimental data

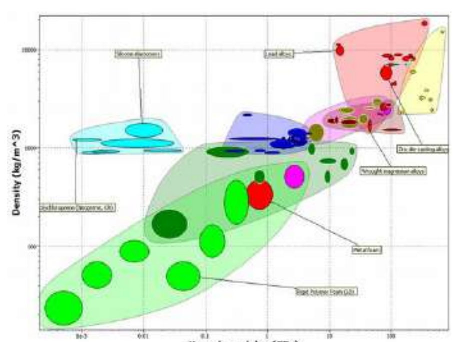
Designing lubricants with DFT and experimental data

2014: Further materials design

Battery design with DFT and experimental data

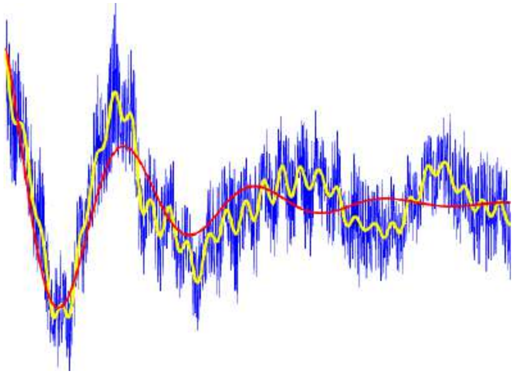
Designing lubricants with DFT and experimental data

Identified and corrected errors in materials database



2015: Further capabilities

Extract information
out of noise



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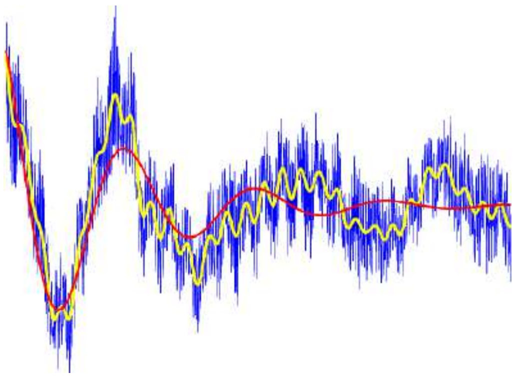

Merge two datasets together

2015: Further capabilities

Extract information
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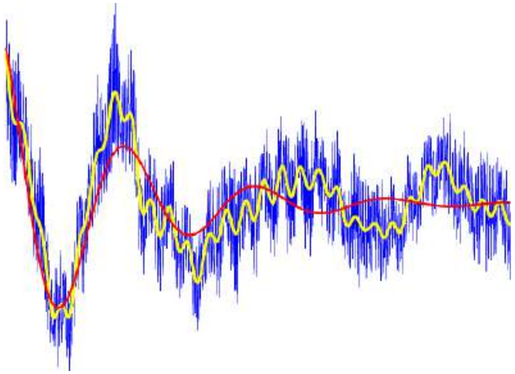
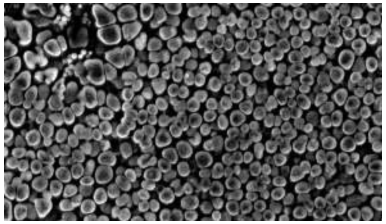


Merge two
datasets together

Train on
encrypted data

2016: Understanding of business models

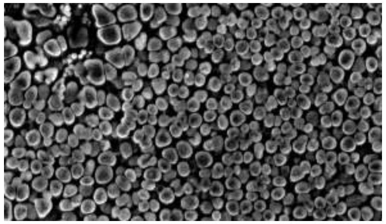


Proposal
5%

Initial testing
10%

Certification
100%

2016: Understanding of business models



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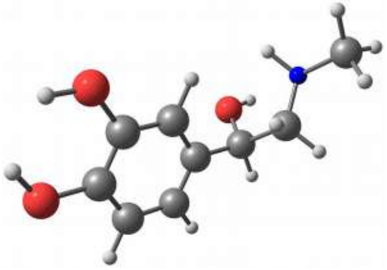


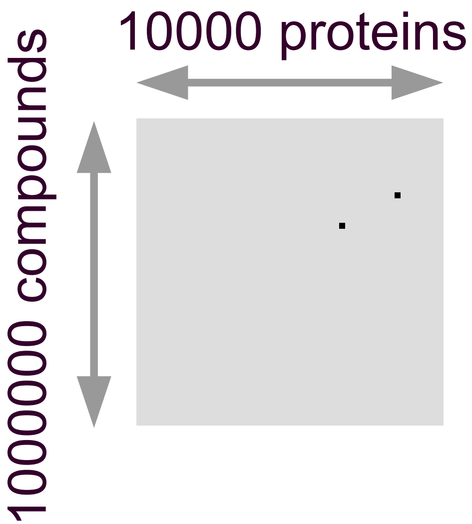
Proposal
30%

Initial testing
70%

Certification
100%

2016: Drug discovery

Protein activity dataset from 0.1% complete



e-therapeutics

2016: Drug discovery

Enhance protein activity dataset from 0.1% to 20% complete

2017: Startup Intellegens

Dr Gareth Conduit

Ben Pellegrini

2017: Startup Intellegens

Dr Gareth Conduit

Ben Pellegrini

Graham Snudden

Dr Elaine Loukes

2017: Startup Intellegens

Dr Gareth Conduit

Ben Pellegrini

Graham Snudden

Dr Elaine Loukes

Dr Thomas Whitehead

Gerald Fux

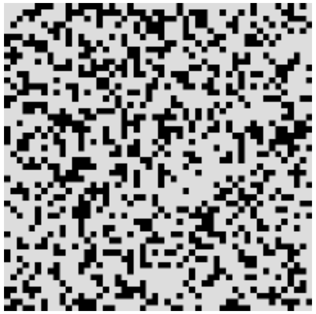
2017: Startup: initial contracts

Drug discovery

e-therapeutics

2017: Startup: initial contracts

Drug discovery



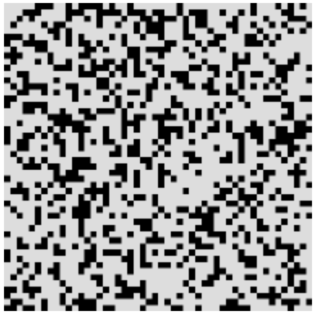
e-therapeutics

Materials design

BenevolentAI

2017: Startup: initial contracts

Drug discovery



e-therapeutics

Materials design

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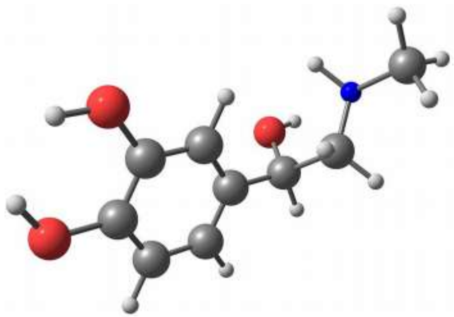
Drug discovery



optibrium

2018: Startup: plan to productize

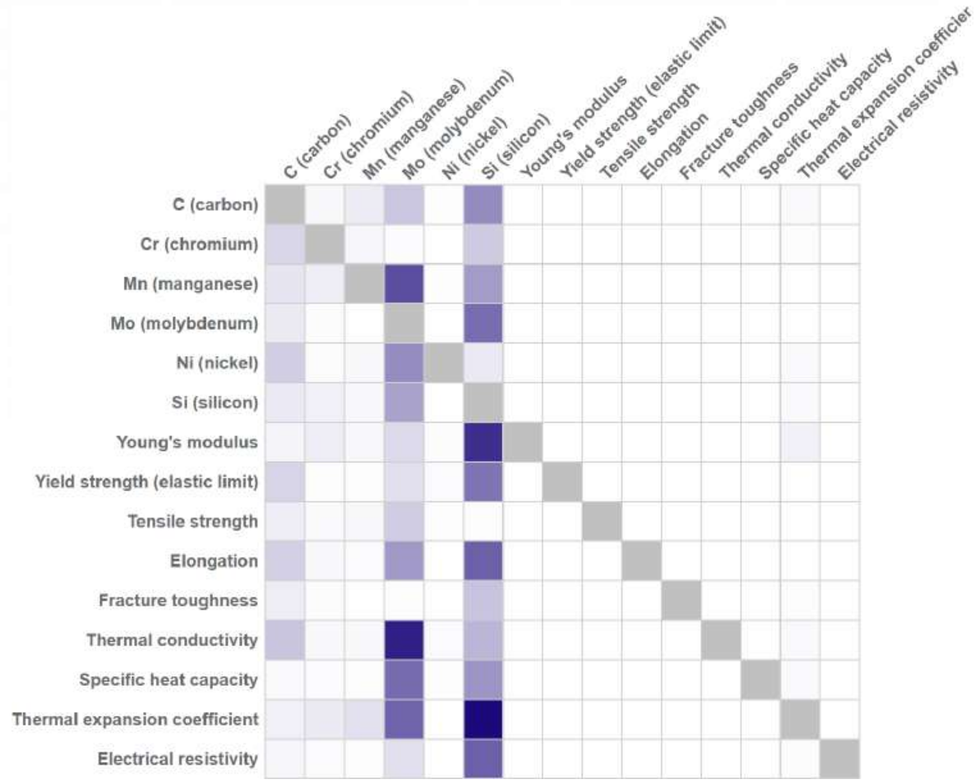
Input composition

Iron	52.93	remain %
Carbon	0.2	0 to 0.43 %
Manganese	1	0 to 3.0 %
Silicon	2	0 to 4.75 %
Chromium	9	0 to 17.5 %
Nickel	10	0 to 21.0 %
Molybdenum	4.5	0 to 9.67 %
Vanadium	2.1	0 to 4.32 %
Nitrogen	0.07	0 to 0.15 %
Niobium	1.2	0 to 2.5 %
Cobalt	10	0 to 20.1 %
Tungsten	4	0 to 9.18 %
Aluminium	1	0 to 1.8 %
Titanium	2	0 to 2.5 %
Heat treatment	1000	800-1150 C

PREDICT

Output properties - predicted

Yield stress	1320	± 322	MPa
Ultimate tensile strength	1951	± 209	MPa
Elongation	9	± 3	%



2018: Exploring other verticals

Autonomous vehicles

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Autonomous vehicles

Ordnance Survey

Healthcare

CARE fertility

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Autonomous vehicles

Ordnance Survey

Healthcare

CARE fertility

Infrastructure

SKANSKA

Conclusions

Develop technology motivated by problems

2012
Multiple targets
Superalloys

2013
Inter-property
3D printing

2014
DFT-experiment
Batteries

2015
Merge datasets
Commercial data

2016
Business model
Drug discovery

2017
Angel investor
Drug discovery

2018
Productization
New verticals

?

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Flexibility to adapt to market need

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Develop technology **motivated** by **problems**

- 2012 Multiple targets Superalloys
- 2013 Inter-property 3D printing
- 2014 DFT-experiment Batteries
- 2015 Merge datasets Commercial data
- 2016 Business model Drug discovery
- 2017 Angel investor Drug discovery
- 2018 Productization New verticals
- ?

Flexibility to **adapt** to market need

Willingness to take **risks** to enable greater returns