Intellegens

Deep learning in materials design and drug discovery

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Neural network algorithm to

Merge all possible sources of information

Reduce the need for expensive experimental development

Accelerate materials and drugs discovery

Generic with **proven** applications in materials discovery and drug design

Neural network: a black box

Neural network: train on complete data

Materials design

Materials design

Neural network: train on complete data

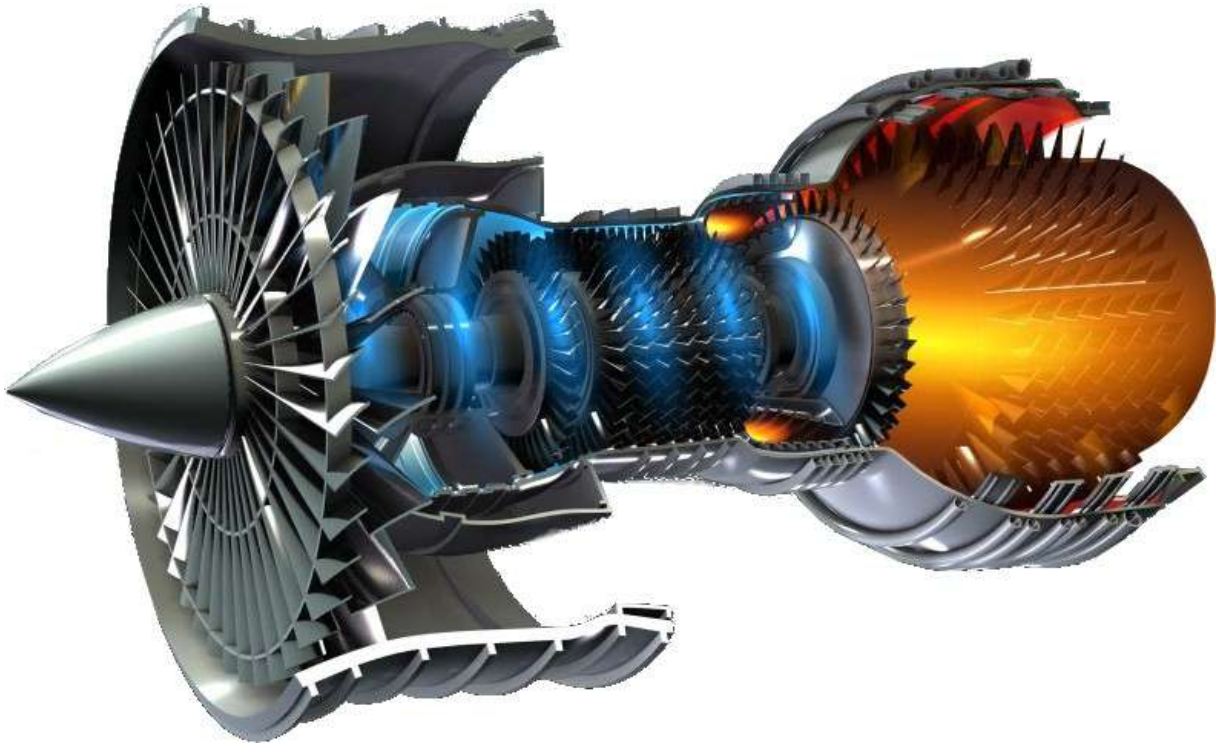
Neural network trains on fragmented data

Neural network predicts on fragmented data

Materials: experimental interlude

Materials: experimental interlude

Schematic of an engine



Proposed alloy

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

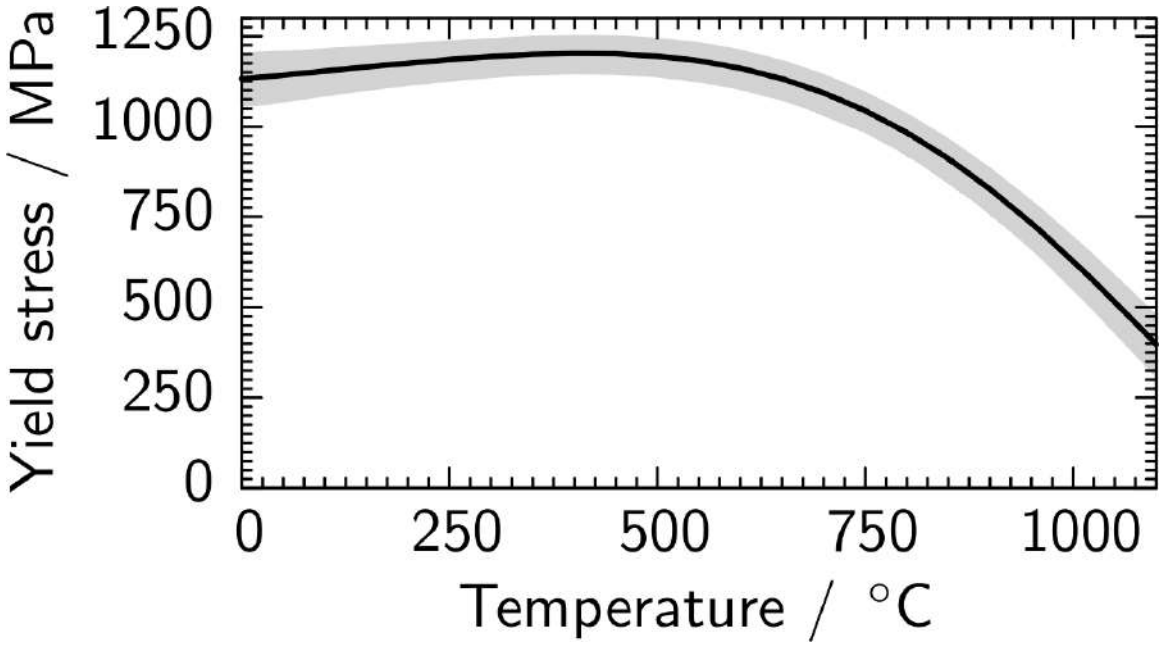
Zr: 0.18

Ni: 47.2

900ºC

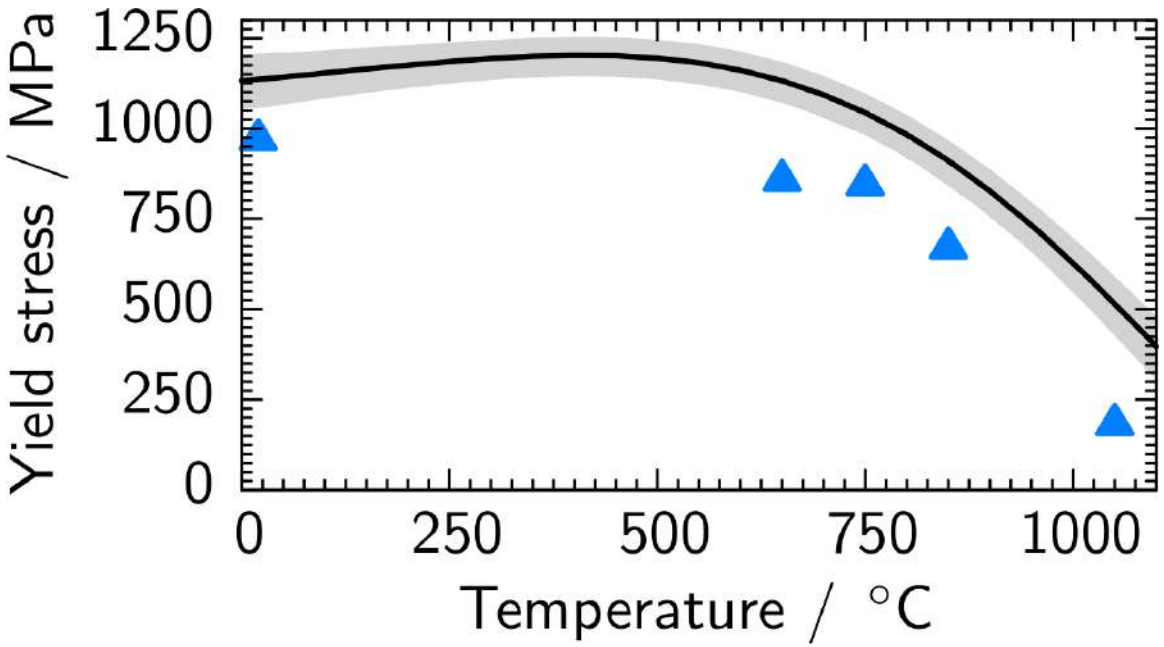
30 hours

Predict the yield stress



Proposed theory

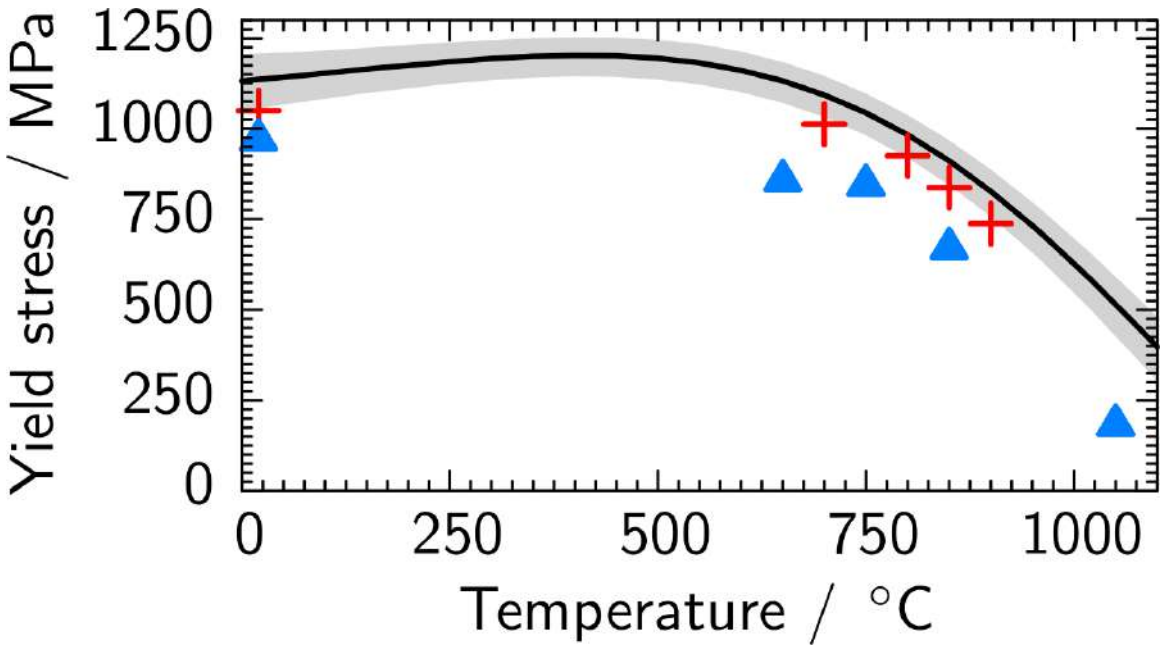
Test the yield stress



Proposed theory

RR1000

Test the yield stress



Proposed theory

Proposed experiment

RR1000

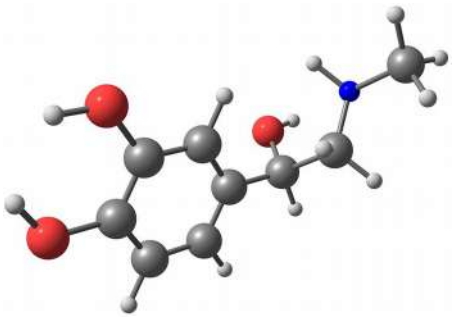
More materials designed

ROLLS ROYCE

Materials Solutions

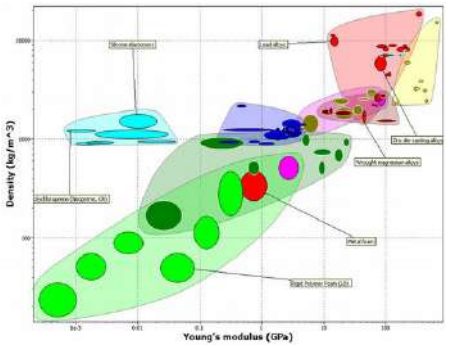
bp

SAMSUNG



e-therapeutics

optibrium



GRANTA

MATERIAL INSPIRATION

Summary: future prospects

Apply deep learning to high-value fragmented data

Merge all sources of information into a holistic design tool

Experimentally proven materials and drugs design

Steels demonstrator: https://app.intellegens.ai/steel_search