

Alchemite™ Analytics

Gareth Conduit

Alchemite™ machine learning tool to



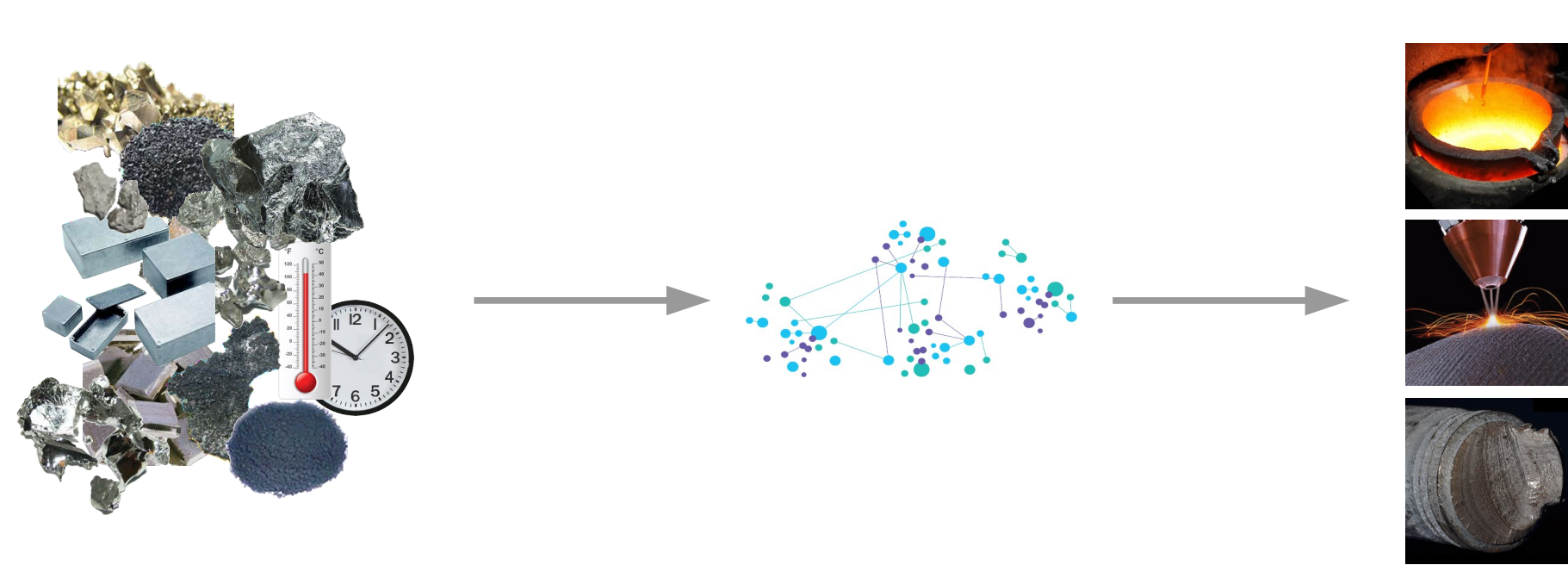
Reduce the need for experiments and **accelerate** discovery

Impute values from sparse data

Utilise **all available** information: computer simulations and real-life measurements

Broadly applicable with **proven** applications in drug design, industrial chemicals, and materials

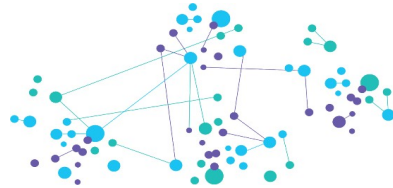
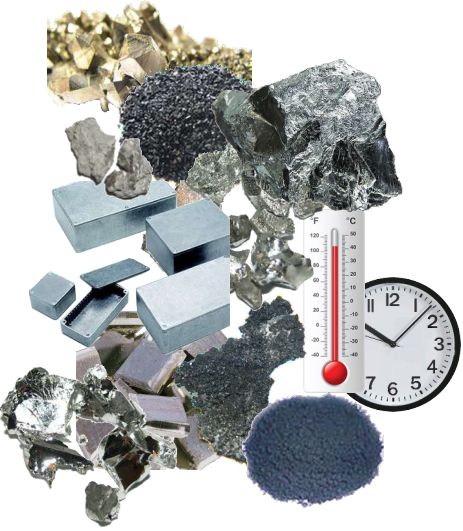
Machine learning to predict materials properties



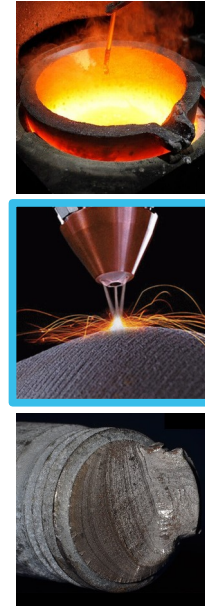
Not enough data to define a model



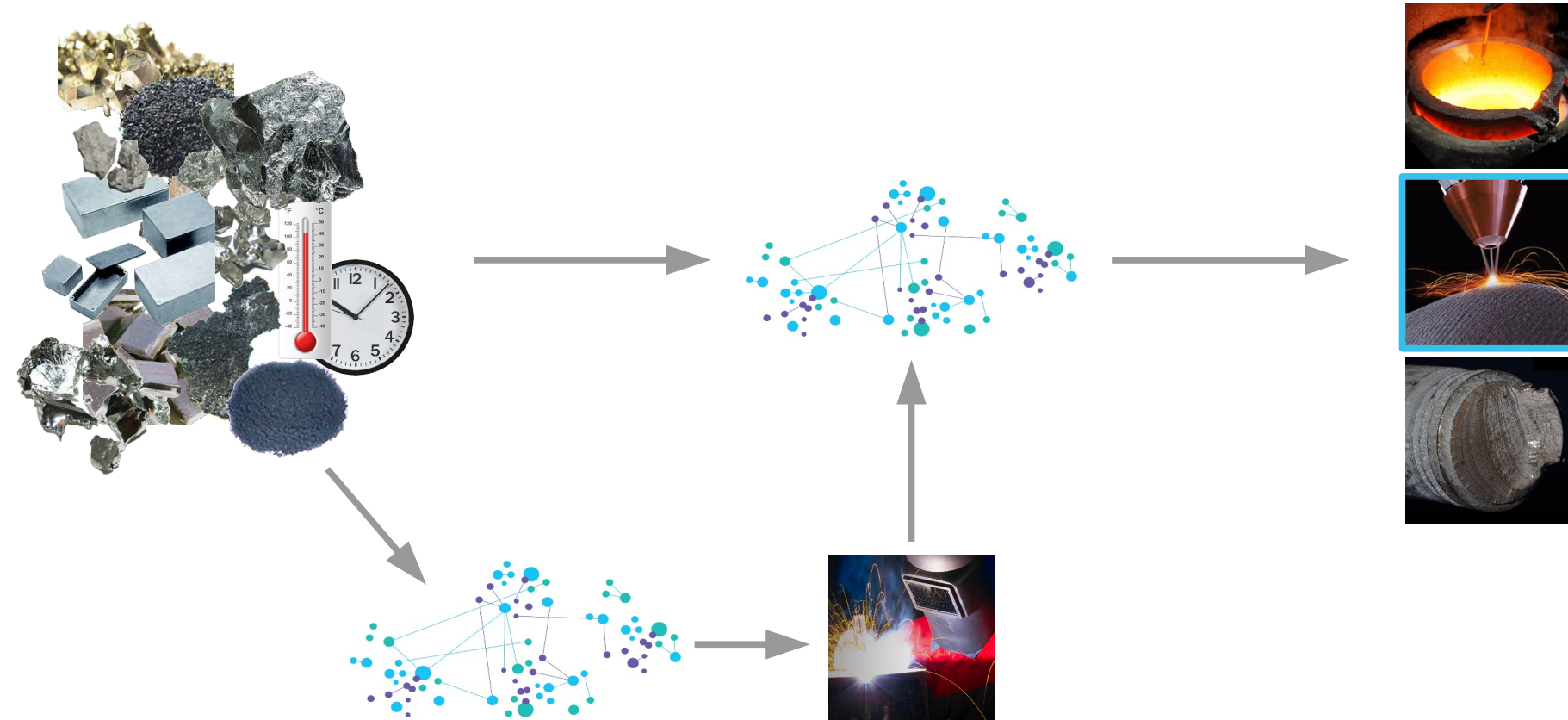
30 variables



10 database entries



Take advantage of data from analogous properties



Take advantage of data from analogous properties



Cr 19%



Co 4%



Mo 4.9%



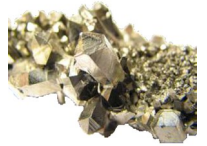
W 1.2%



Zr 0.05%



Nb 3%



Al 2.9%



C 0.04%



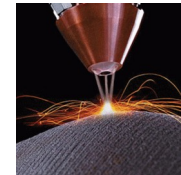
B 0.01%



Ni

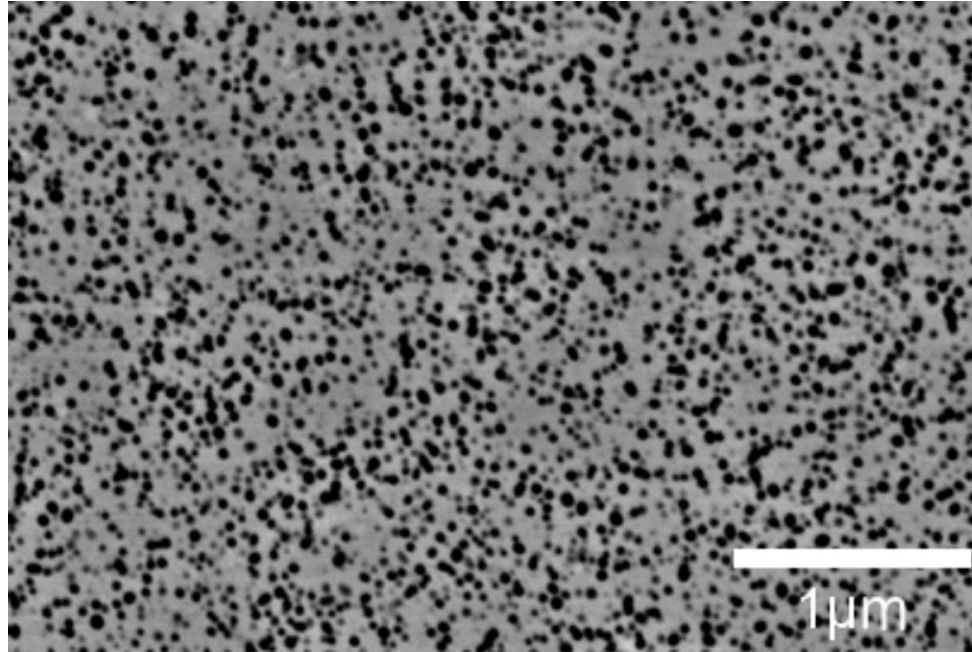


Expose 0.8



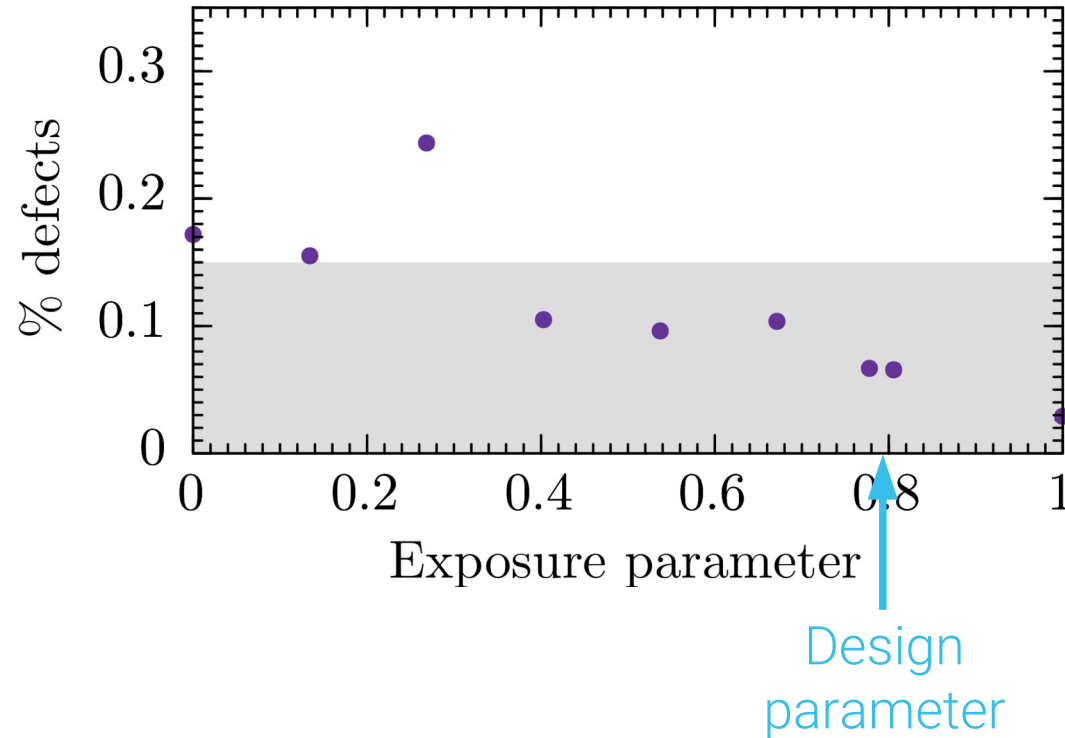
T_{HT} 1300°C





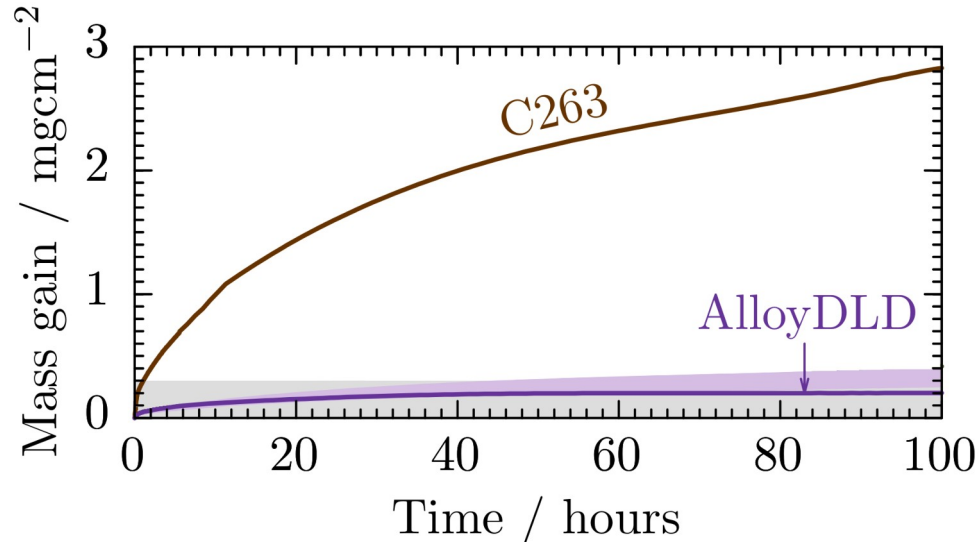
Probabilistic neural network identification of an alloy for direct laser deposition
Materials & Design 168, 107644 (2019)

Calculate probability distribution



Probabilistic neural network identification of an alloy for direct laser deposition
Materials & Design 168, 107644 (2019)

Oxidation resistance



Probabilistic neural network identification of an alloy for direct laser deposition
Materials & Design 168, 107644 (2019)

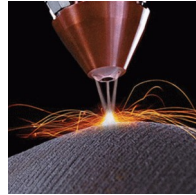
Other materials



Steel welding consumables



Titanium additive manufacturing



Battery cathodes



Lubricants



API for integration

intellegens

Search...

- PUT Train a model
- POST Load model into memory
- PUT Unload model from memory
- PUT Impute missing data
- PUT Validate given data
- PUT Predict given and missing data
- PUT Find the outlying values in a dataset
- PUT Suggest which missing values to provide from the training dataset to improve future predictions.
- GET Get all optimize jobs for given model ID
- POST Optimize for specified

Suggest which missing values to provide from the training dataset to improve future predictions.

Get a specified number of suggestions for additional measurements which are currently omitted from the data used to train the model. These measurements, if provided, would best improve subsequent predictions for a given list of 'targetColumns'.

AUTHORIZATIONS: `oauth (alchemiteapi.models.suggest)`

PATH PARAMETERS

→ `id` required string <uuid>
 Example: 00112233-4455-6677-8899-aabbccddeeff
 Unique identifier for the model.

REQUEST BODY SCHEMA: `application/json`

→ `numberOfSuggestions` integer
 Default: 10
 Request the top numberOfSuggestions values that will most improve predictions for the requested targetColumns.

→ `targetColumns` Array of strings
 A list of column headers which all appear in the training data. Suggested measurements will be targeted to best improve predictions for these columns. If not given then targetColumns will be treated as being all columns.

Within the browser

intellegens Alchemite™ Analytics Create model

M0 Cheddar/Akawi ha...
432 rows 9 cols

Analytics All properties

ACTUAL VS PREDICTED PROPERTY VS PROPERTY IMPORTANCE

HARDNESS R²: 0.8206

3D Scatter Plot: Predicted vs Actual vs Spill (ml (dry))

Powered by Alchemite API v0.17.4

Battery management software



Juxtapose physics-based modelling with machine learning

In-service data from a particular battery and others deployed to make bespoke predictions of remaining useful life

Model that spans time-scales to permit simultaneous state-of-health and state-of-charge predictions

Data from testing in first few cycles to predict long-term battery performance



Predicting the state of charge and health of batteries using data-driven machine learning

Man-Fai Ng¹, Jin Zhao², Qingyu Yan², Gareth J. Conduit³ and Zhi Wei Seh⁴

Machine learning is a specific application of artificial intelligence that allows computers to learn and improve from data and experience via sets of algorithms, without the need for reprogramming. In the field of energy storage, machine learning has recently emerged as a promising modelling approach to determine the state of charge, state of health and remaining useful life of batteries. First, we review the two most studied types of battery models in the literature for battery state prediction: the equivalent circuit and physics-based models. Based on the current limitations of these models, we showcase the promise of various machine learning techniques for fast and accurate battery state prediction. Finally, we highlight the major challenges involved, especially in accurate modelling over length and time, performing in situ calculations and high-throughput data generation. Overall, this work provides insights into real-time, explainable machine learning for battery production, management and optimization in the future.

With rising concerns about global warming, electrification of transport has recently emerged as an important vision in many countries. The successful development of electric vehicles (EVs) depends highly on the cycling performance, cost and safety of the batteries. Rechargeable lithium-ion (Li-ion) batteries are currently the best choice for EVs due to their reasonable

where C_{cur} is the capacity of the battery in its current state, C_{full} is the capacity of the battery in its fully charged state, C_{nom} is the nominal capacity of the brand-new battery².

In essence, SOC denotes the capacity of the battery in its current state compared to the capacity in its fully charged state (equivalent of a fuel gauge), while SOH describes the capacity of the battery

Predicting the State of Charge and Health of Batteries using Data-Driven Machine Learning
Nature Machine Intelligence 2, 161 (2020)