UNIVERSITY OF CAMBRIDGE

Materials imputation with artificial intelligence

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Artificial intelligence

Composition

Artificial intelligence

Yield stress

UTS

Melting point

Oxidation resistance

Cost

Density

Fatigue life

Fracture toughness

Creep

Processibility

Artificial intelligence

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Yield stress
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Oxidation resistance
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Artificial intelligence

Composition

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Yield stress

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Oxidation resistance

Cost

Density

Fatigue life

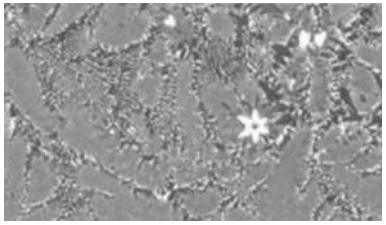
Fracture toughness

Creep

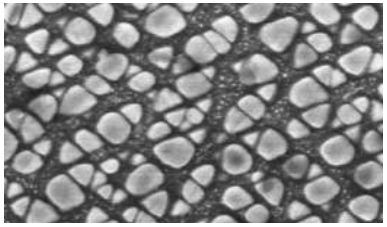
Processibility

Alloys discovered

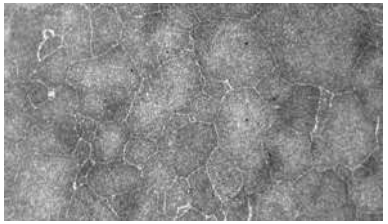
Cr-Cr_2Ta alloys
Intermetallics, 48, 62



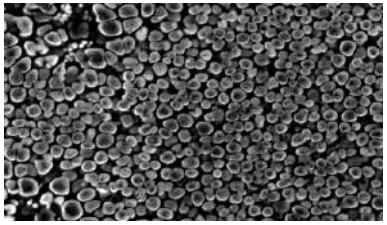
Combustor alloy
GB1408536



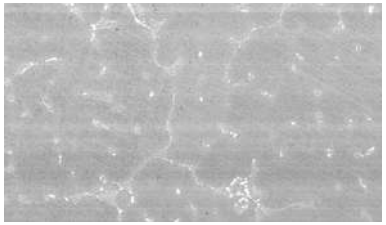
RR1000 grain growth
Acta Materialia, 61, 3378



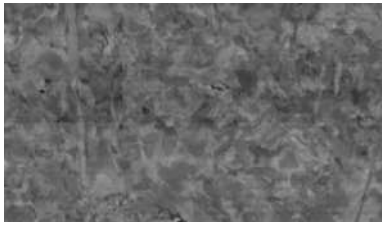
Ni disc alloy
EP14157622
US 2013/0052077 A2



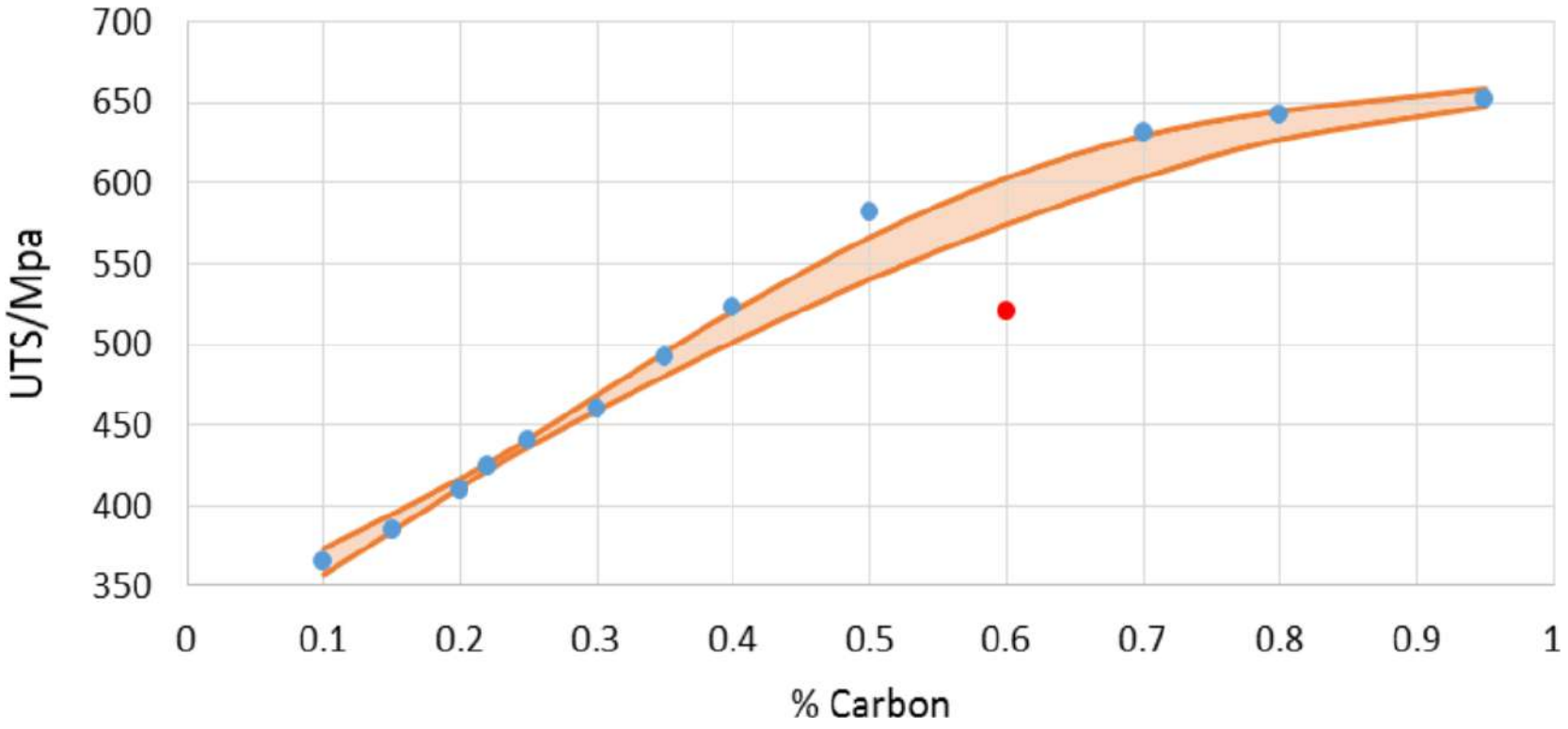
Mo-Hf forging alloy
EP14161255
US 2014/223465



Mo-Nb forging alloy
EP14161529
US 2014/224885



Detecting errors



Detecting errors

Alloy	Database YS / MPa	Predicted YS / MPa	#σ	Correct YS / MPa
Stainless steel, austenitic, AISI 301L, wrought	192.5	248.03	14.9	238
Stainless steel, austenitic, AISI 301, wrought, annealed	192.49	227.60	-14.2	221
Aluminum, commercial purity, 1080, wrought, H18	50.44	123.96	10.7	120
Aluminum, 5083, wrought, H112	116.79	190.55	-20.2	190

Found and confirmed erroneous entries:
8 in yield stress, 4 in melting point, 7 in density

Materials databases

Training data

C	Mn	Ni	Cr	YS
✓	✓	✓	✓	✓
✓	✓	✓	✓	✓
✓	✓	✓	✓	✓
✓	✓	✓	✓	✓
✓	✓	✓	✓	✓

Materials databases

	C	Mn	Ni	Cr	YS
Training data	✓	✓	✓	✓	✓
	✓	✓	✓	✓	✓
	✓	✓	✓	✓	✓
	✓	✓	✓	✓	✓
	✓	✓	✓	✓	✓
Prediction	✓	✓	✓	✓	x
	✓	✓	✓	✓	x
	✓	✓	✓	✓	x

Materials databases

Training data

C	Mn	Ni	Cr	YS
✓	✓	✓	✓	✓
✓	✓	✓	✓	✓
✓	✓	✓	✓	✓
✓	✓	✓	✓	✓
✓	✓	✓	✓	✓

C	Mn	Ni	Cr	UTS
✓	✓	✓	✓	✓
✓	✓	✓	✓	✓
✓	✓	✓	✓	✓
✓	✓	✓	✓	✓
✓	✓	✓	✓	✓

Prediction

✓	✓	✓	✓	x
✓	✓	✓	✓	x
✓	✓	✓	✓	x

✓	✓	✓	✓	x
✓	✓	✓	✓	x
✓	✓	✓	✓	x

Materials databases

Training data

C	Mn	Ni	Cr	YS
✓	✓	✓	✓	✓
✓	✓	✓	✓	✓
✓	✓	x	x	✓
✓	✓	✓	✓	✓
✓	✓	✓	✓	✓

C	Mn	Ni	Cr	UTS
✓	✓	✓	✓	✓
✓	✓	✓	✓	✓
✓	✓	✓	✓	✓
✓	✓	✓	✓	x
✓	x	✓	x	✓

Prediction

✓	✓	✓	✓	x
✓	✓	✓	✓	✓
✓	✓	✓	✓	x

✓	✓	✓	✓	x
✓	✓	✓	✓	x
✓	✓	✓	✓	✓

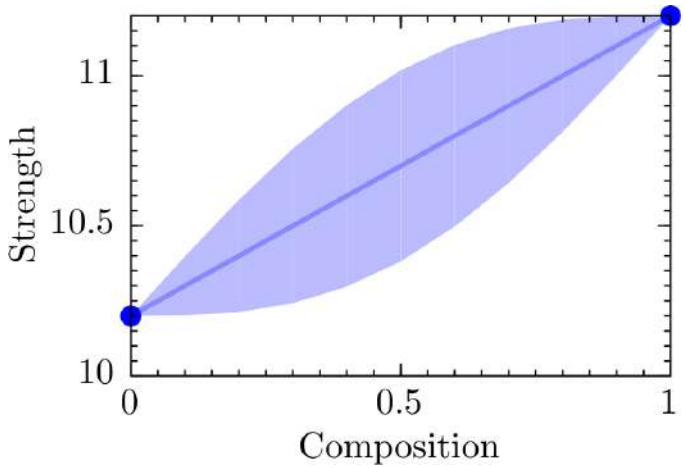
Fragmented database

	Composition	YS	UTS	Hardness
Training data	✓	✓	✓	✓
	✓	x	✓	x
	✓	x	✓	x
	✓	x	✓	✓
	✓	✓	x	x
Prediction	✓	x	x	x
	✓	✓	x	✓
	✓	x	✓	x

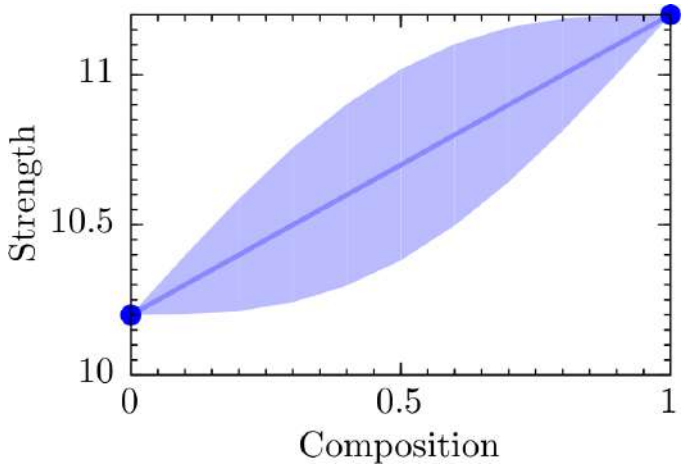
Fragmented database

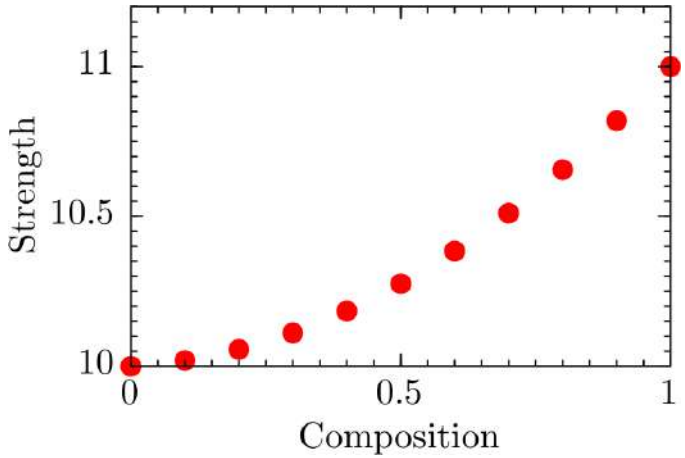
	Composition	YS	UTS	Hardness	Computed YS
Training data	✓	✓	✓	✓	✓
	✓	x	✓	x	✓
	✓	x	✓	x	✓
	✓	x	✓	✓	✓
	✓	✓	x	x	✓
Prediction	✓	x	x	x	✓
	✓	✓	x	✓	✓
	✓	x	✓	x	✓

Merging experiment with simulation

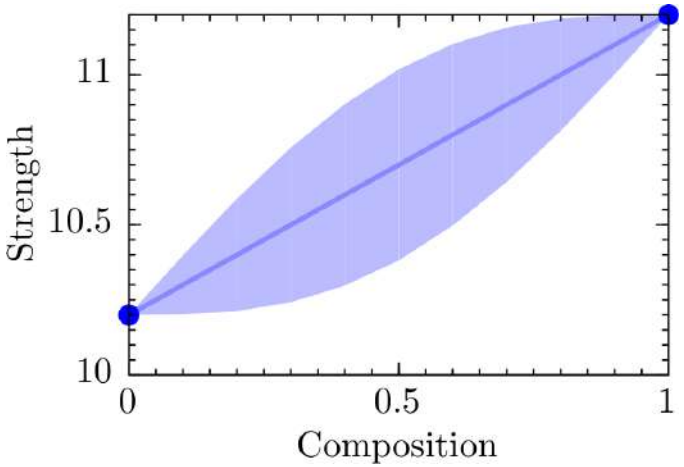


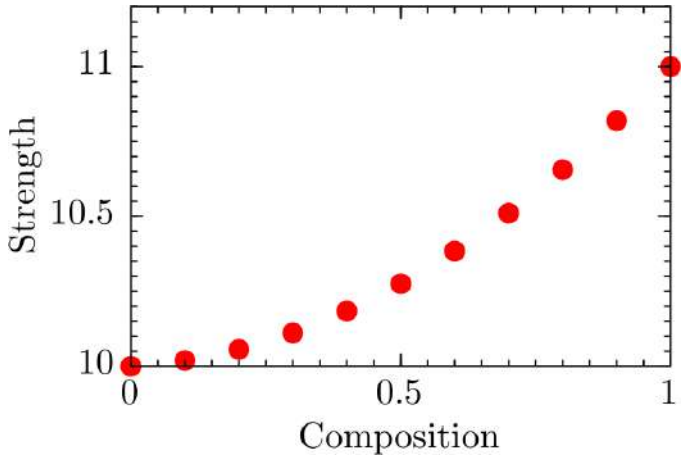
Merging experiment with simulation



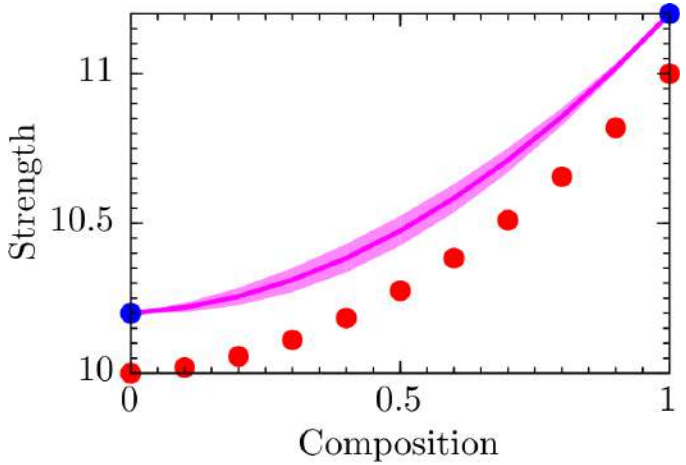


Merging experiment with simulation

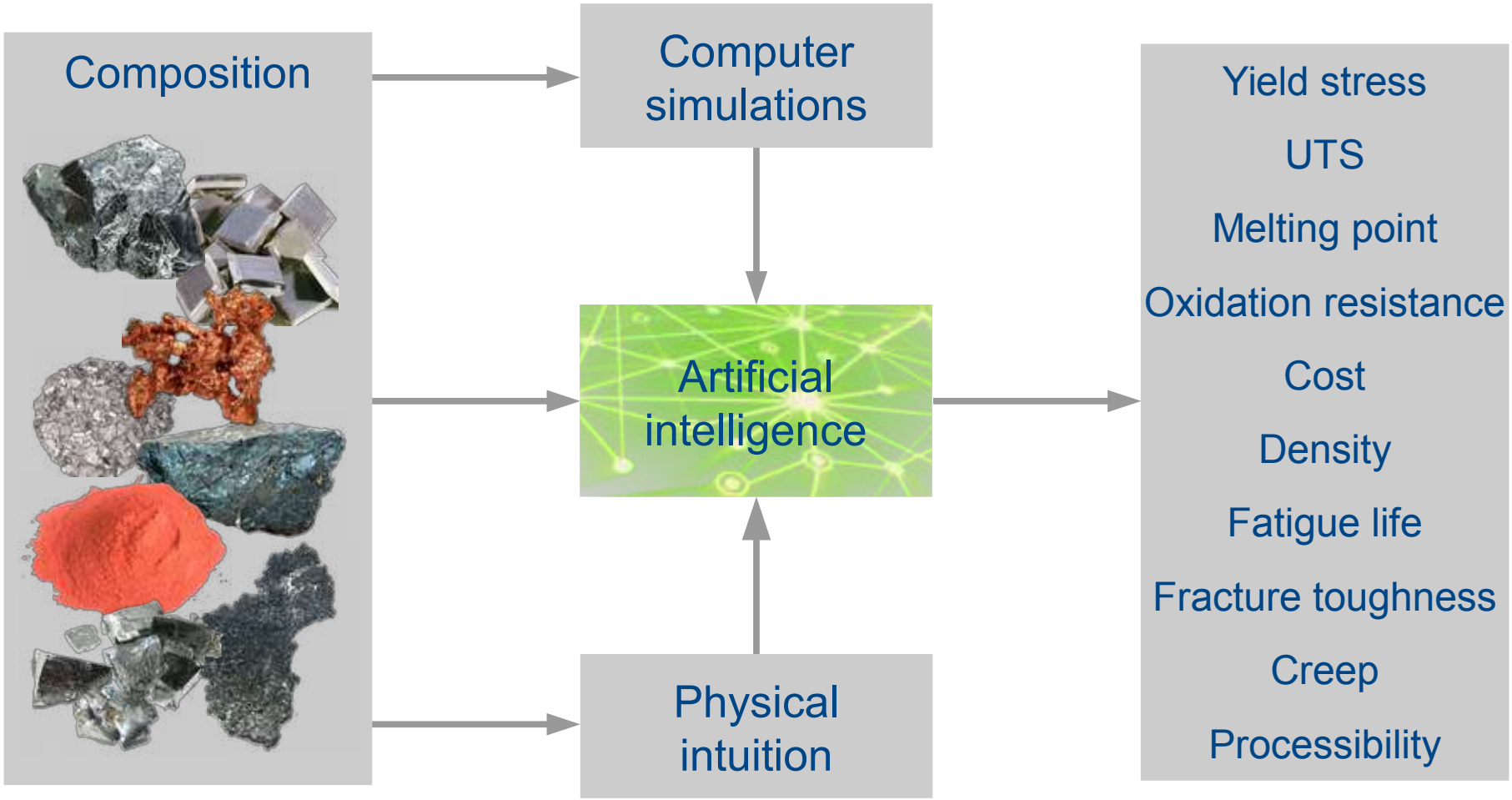




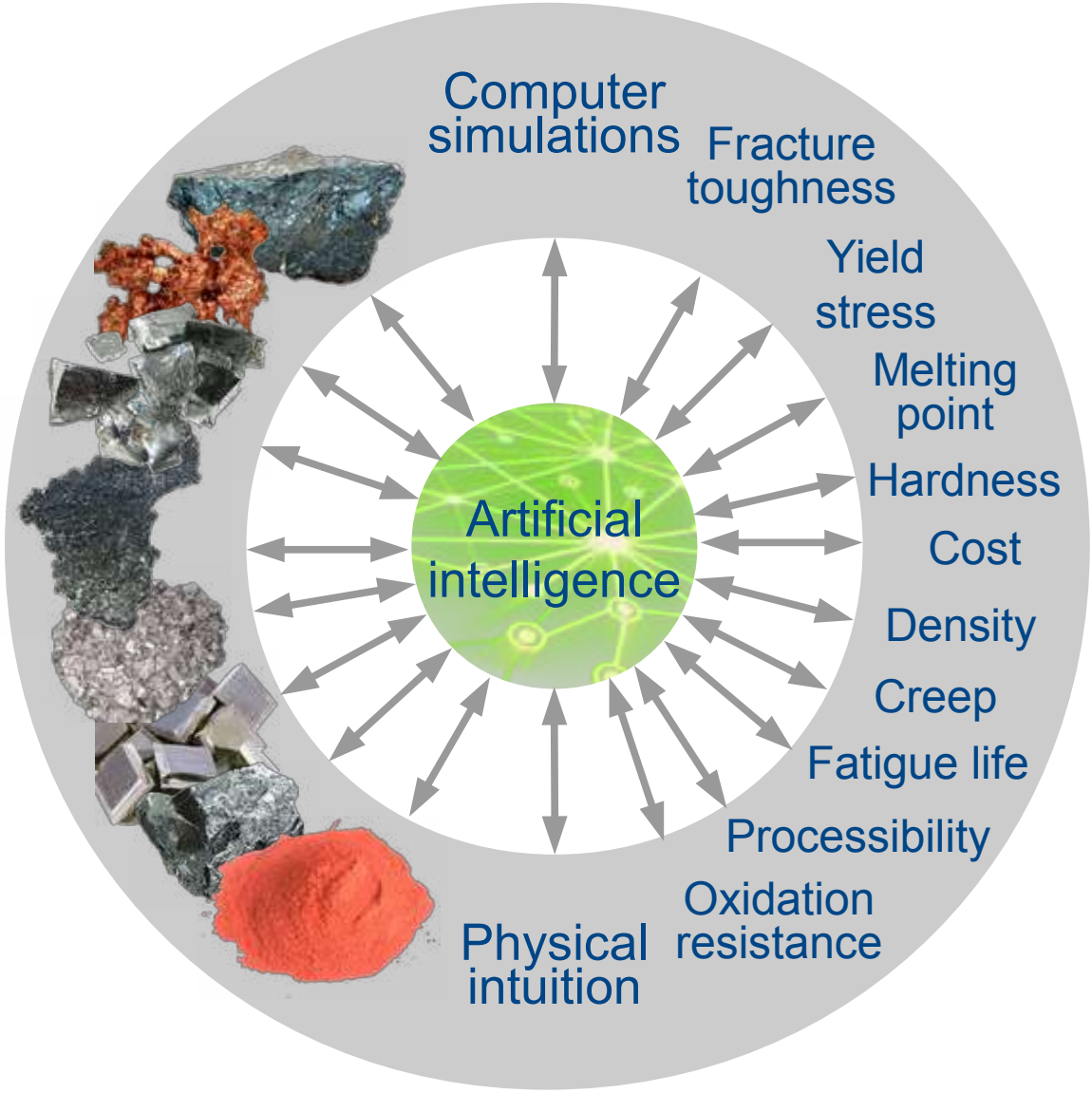
Combine



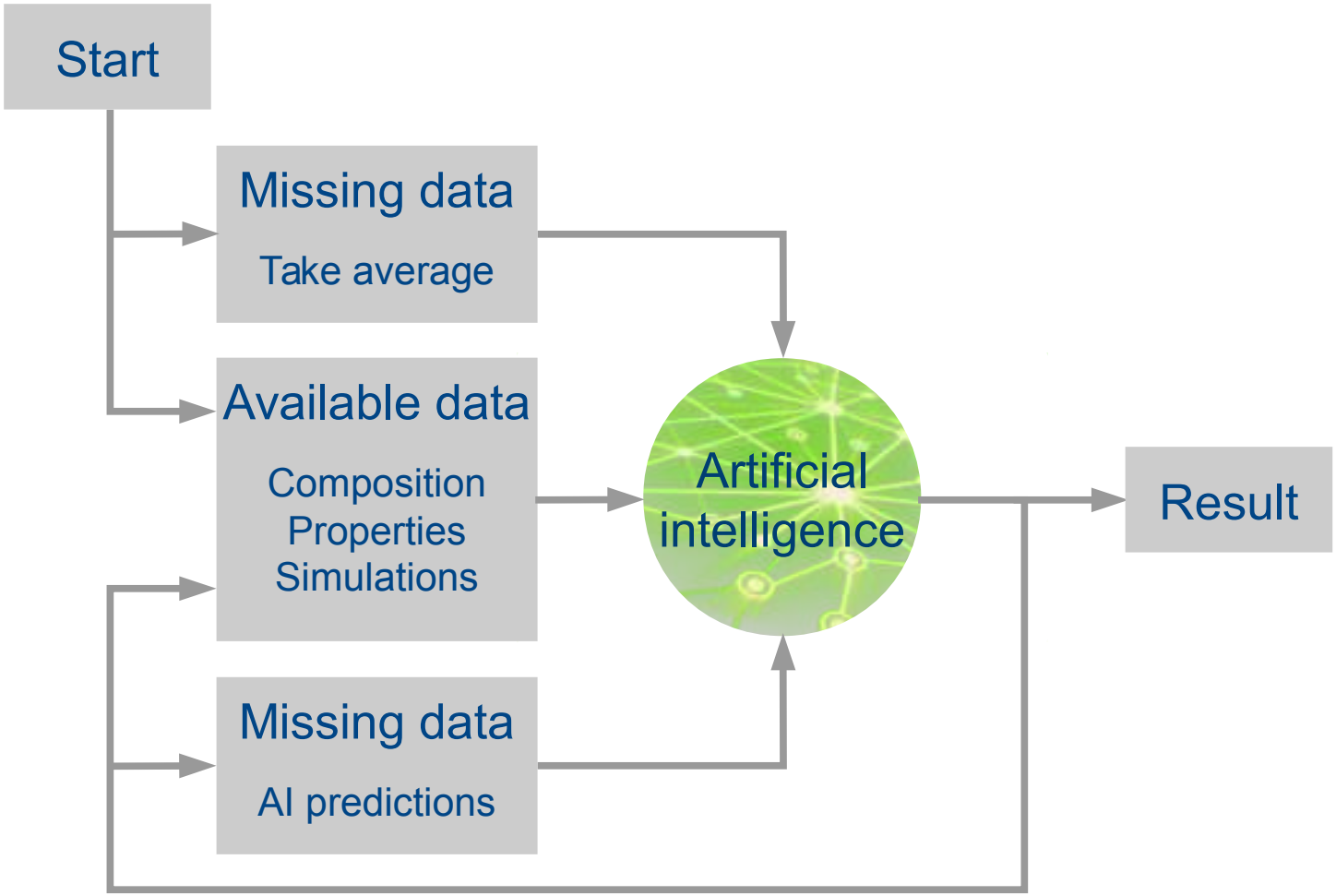
Standard artificial intelligence



Enhanced artificial intelligence



Recursive artificial intelligence



Choice of basis set

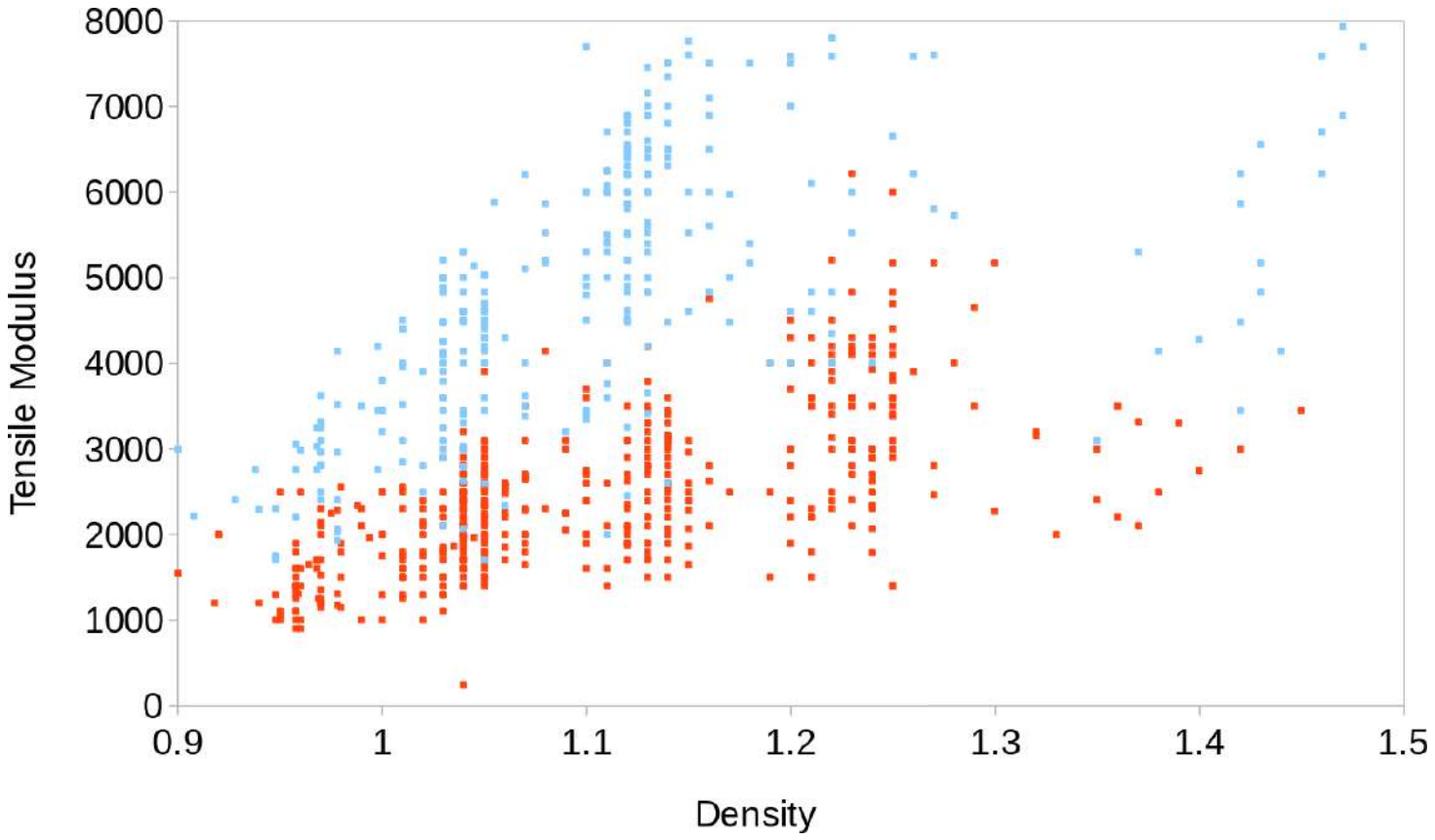
Alloys

Composition
Heat treatment

Polymers

Filler type and volume
Properties

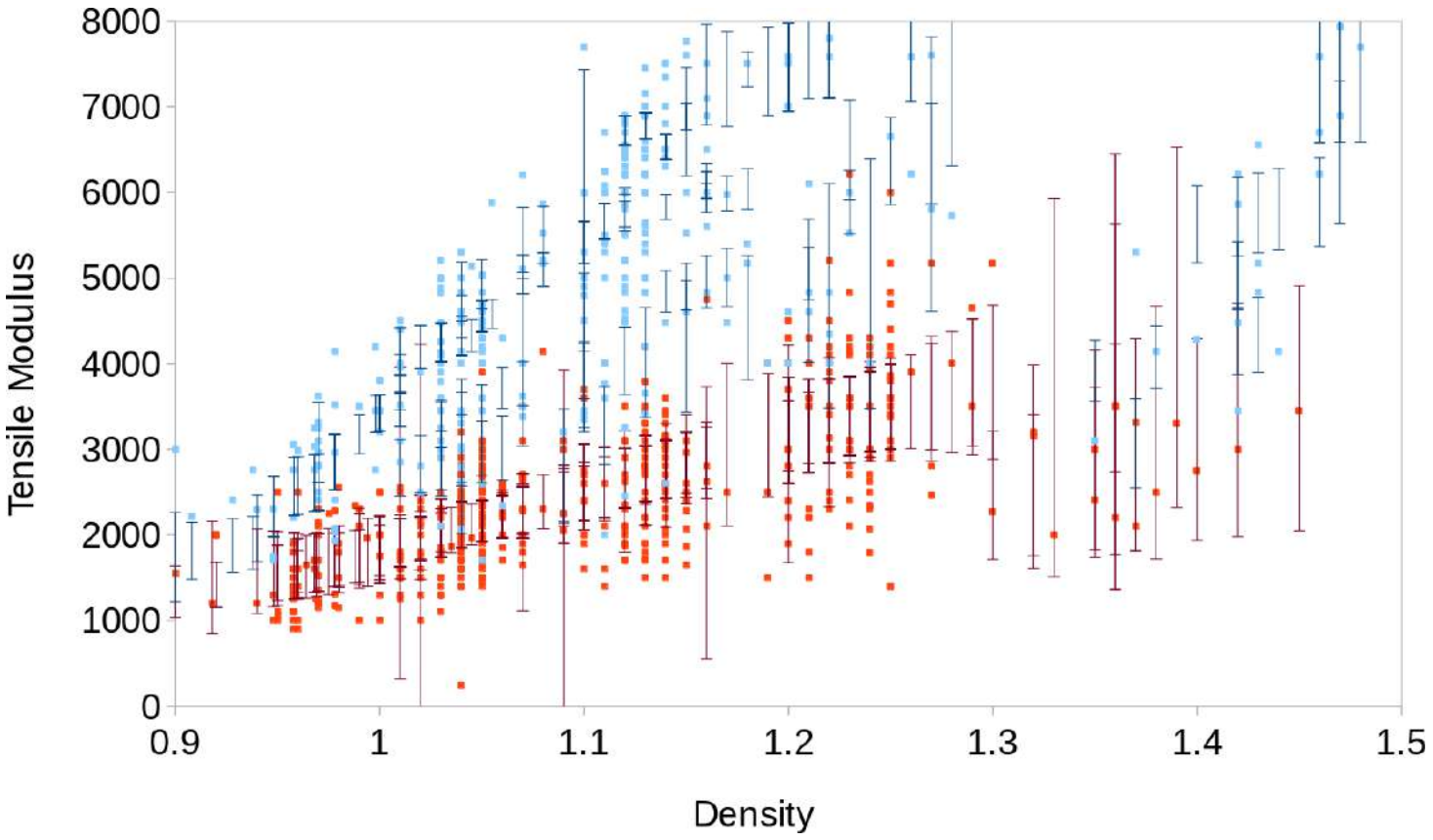
Polymers: all data present



Glass filler

Mineral filler

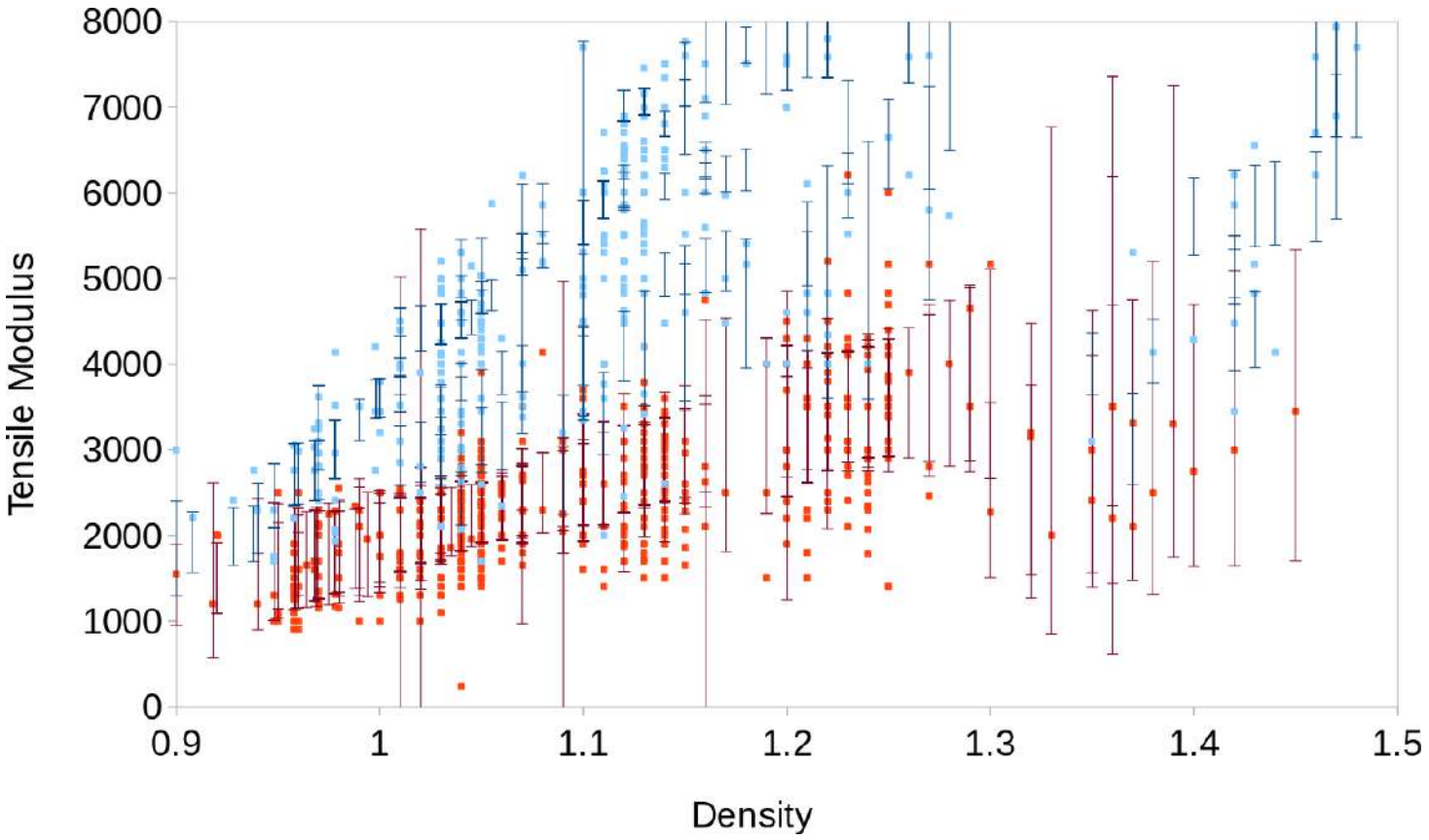
Polymers: all data present



Glass filler

Mineral filler

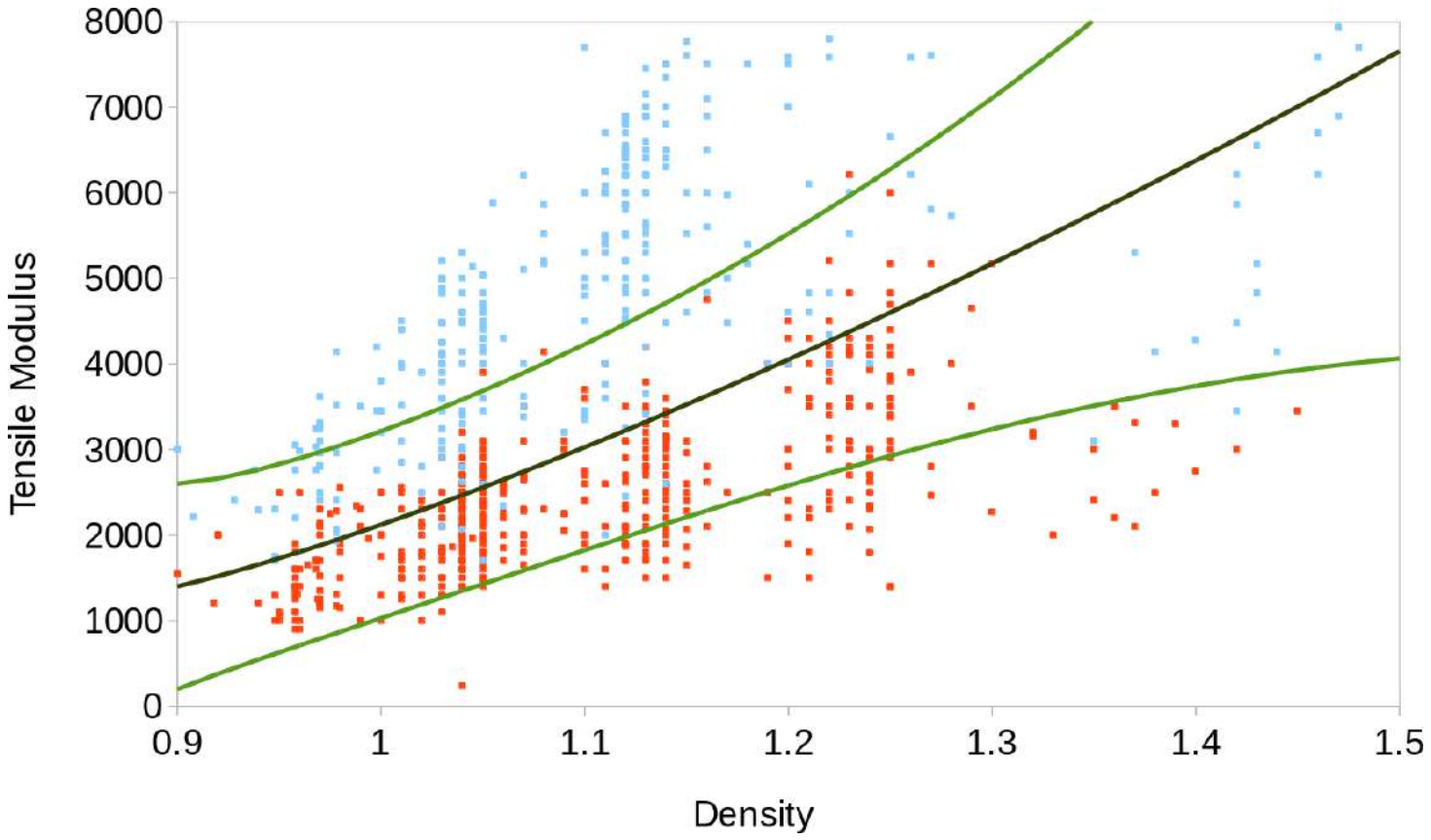
Polymers: 50% training data missing



Glass filler

Mineral filler

Polymers: entry missing filling information

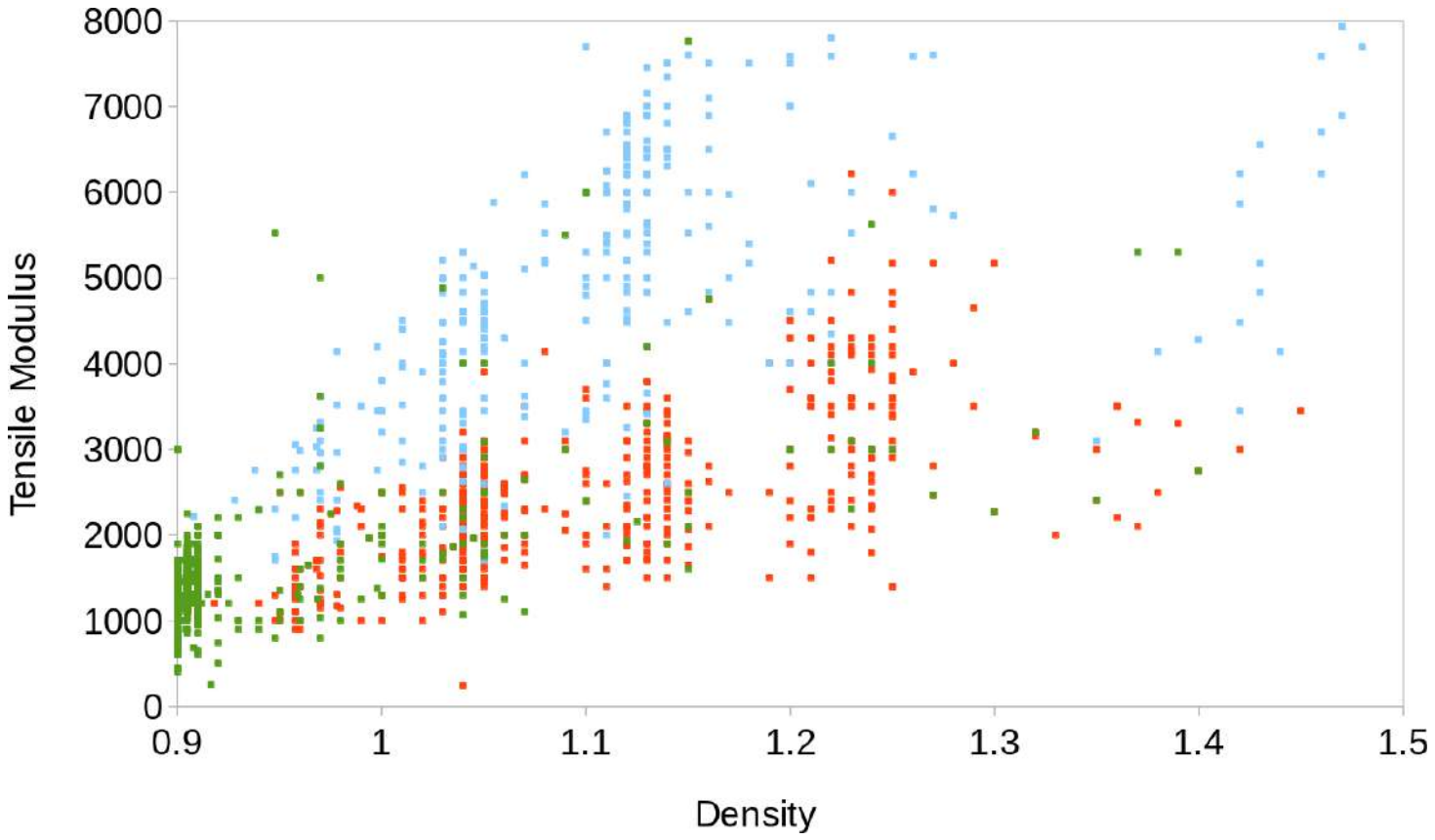


Glass filler

Unknown

Mineral filler

Polymers: tensile modulus vs density

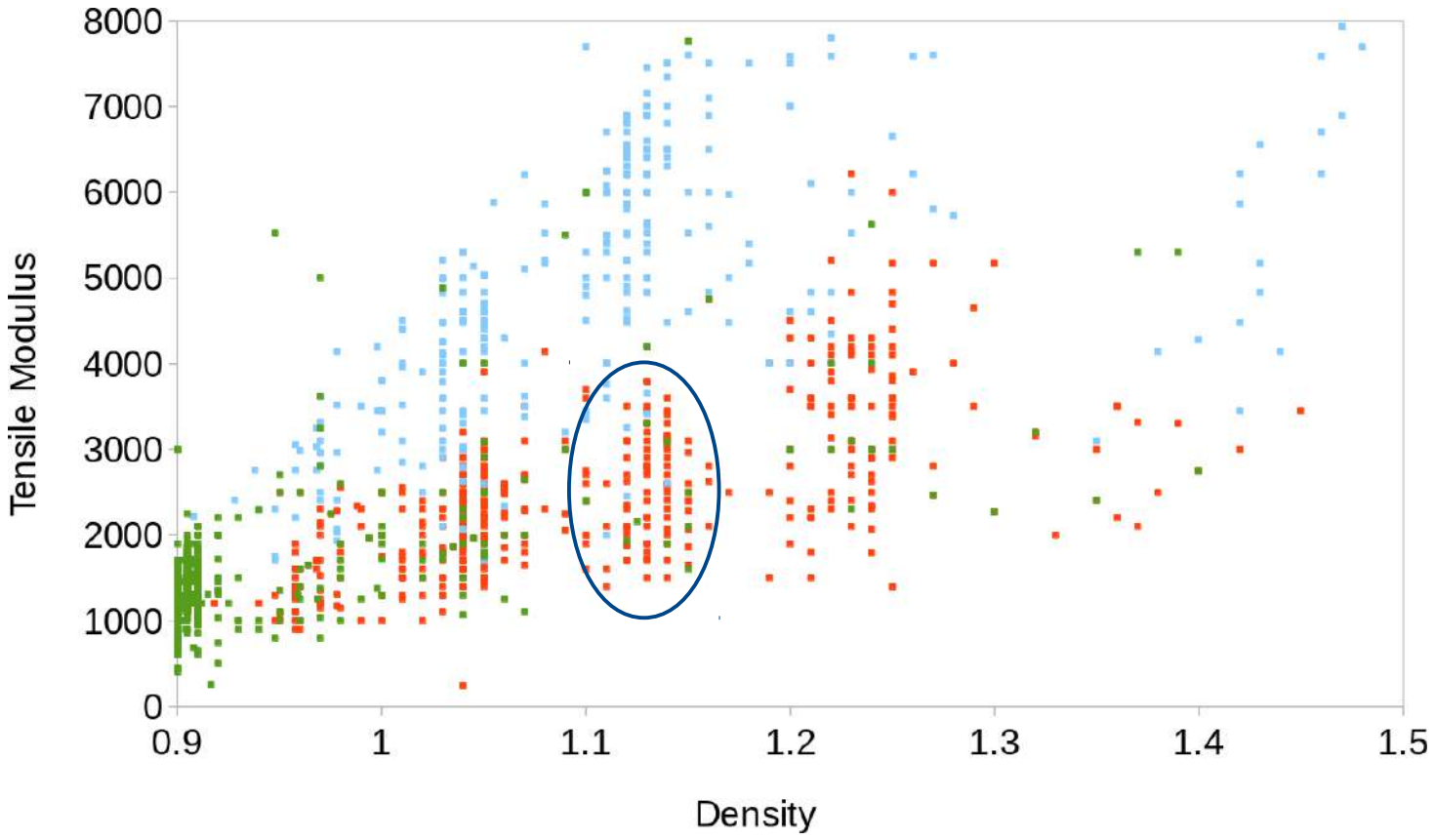


Glass filler

Unknown

Mineral filler

Polymers: tensile modulus vs density



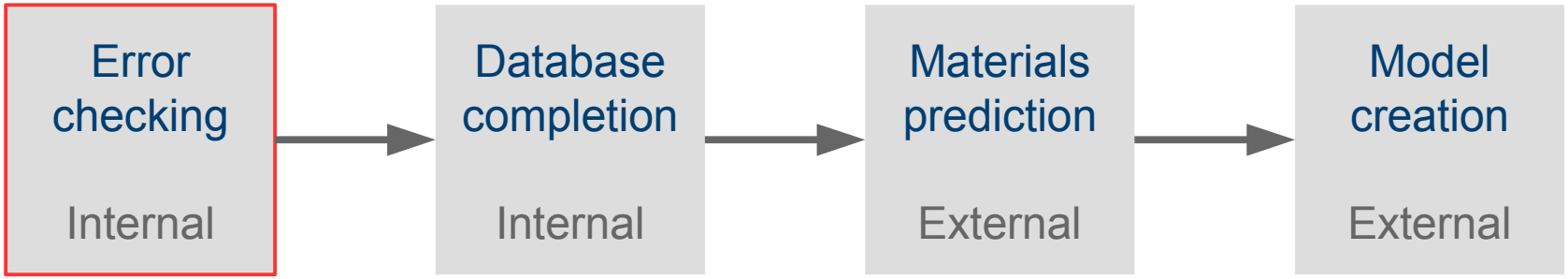
Glass filler

Unknown

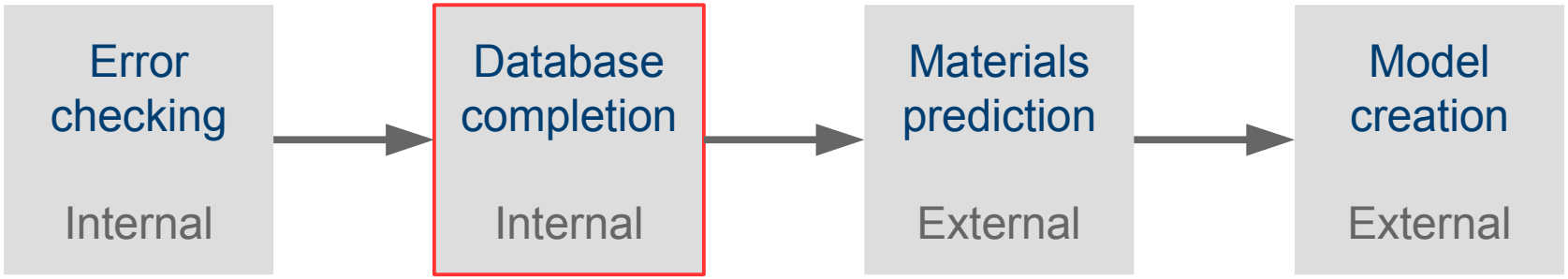
Mineral filler

Confirmed 9 errors, predicted and verified 8 missing values

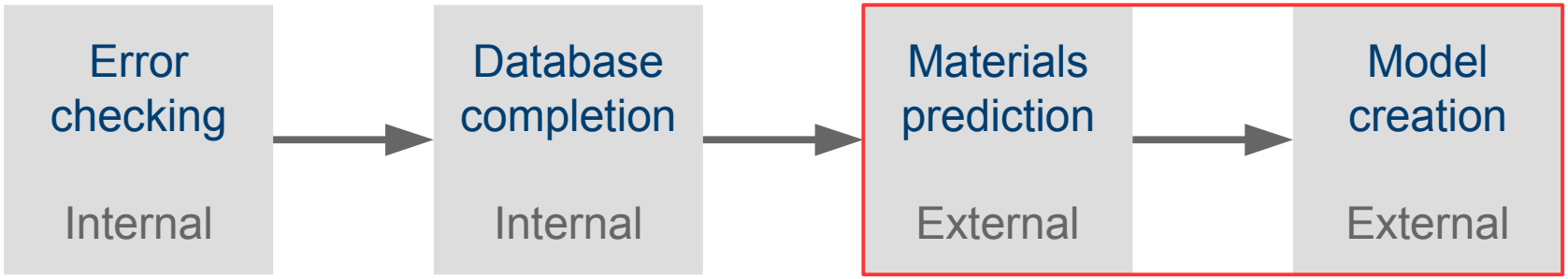
Route to exploitation



Route to exploitation



Route to exploitation



Summary

Artificial intelligence tool that can handle fragmented data

Discover four new alloys that are experimentally verified

Materials database verification and analysis