Analysis of alloy steel composition-property relationship using machine learning: beyond human physical intuition

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This is the abstract, write it at last.

I. MOTIVATION

why are you doing this? flowchart

II. DATA ACQUISITION

how and where did you get it. how did you deal with blocking problems.

portable code

III. FEATURIZATION

What is the format of raw data, how did you collect them to one dataframe, how to convert them to float64, why pick these elements and properties (number count).

IV. DATA ANALYSIS WITH HUMAN INTELLIGENCE

Carbon: increase tensile strength and hardness; decrease ductility, toughness.

Sulfur: improve machinability; decrease weldability; impact toughness and ductility.

Silicon: increase tensile/yield strength, hardness, forgeability and magnetic permeability; deoxidier and degasifier.

Phosphorous: increase strength and hardness; improve machinability and corrosion resistance.

Manganese: increase tensile strength, hardness and reduce brittleness; deoxider and degasifier.

Chromium: increase tensile strength, hardness and corrosion resistance.

Nickel: increase strength, hardness, toughness and resistance to corrosion.

Molybdenum: increase toughness, strength, hardness, machinability, resistance to corrosion.

Copper: increase corrosion resistance.

Density Hardness, Vickers: Thermal conductivity: Specific heat capacity: CTE, linear: Electrical resistivity: Elongation at break: Bulk modulus: Modulus of elasticity: Shear modulus: Poissons ratio: Tensile strength, yield: Tensile strength, break:

Iron: decrease thermal conductivity, decrease specific heat capacity, slightly increase modulus of elasticity, slightly decrease CTE

Carbon: decrease thermal conductivity, slightly increase specific heat capacity, increase electrical resistivity, decrease shear modulus

Sulfur: increase specific heat capacity, slightly increase electrical resistivity

Silicon: decrease density, slightly increase specific heat capacity and CTE, slightly increase electrical resistivity

Phosphorous: decrease thermal conductivity, slightly increase specific heat capacity, increase electrical resistivity, slightly increase modulus of elasticity

Manganese: slightly increase specific heat capacity, slightly increase electrical resistivity, slightly decrease shear modulus

Chromium: decrease density, increase thermal conductivity, slightly increase CTE, slightly decrease modulus of elasticity

Nickel: increase thermal conductivity, slightly increase specific heat capacity and CTE, slightly decrease modulus of elasticity, slightly increase tensile strength

Molybdenum: increase specific heat capacity, increase electrical resistivity

Copper: increase specific heat capacity, increase electrical resistivity

Discuss influence of element to properties, discuss their correlation, whether it is expected/intuitive, find some weakly correlated target props

V. DATA ANALYSIS WITH ARTIFICIAL INTELLIGENCE

CTE linear is dropped for more instances to learn.

A. NEED NEW NAME

benchmark (x-axis: algo, y-axis: log(r2+1), dataset: predict x from the rest dataset) table of hyper-parameters

B. predicting composition-property relationship

plot (single algo, x-axis: element, y-axis: log(r2+1)) Overfitting, plot learning curve

VI. CONCLUSIONS