Tribo-informatics: An emerging new paradigm in the surface studies of materials based on the application of Artificial Intelligence and Machine Learning methods

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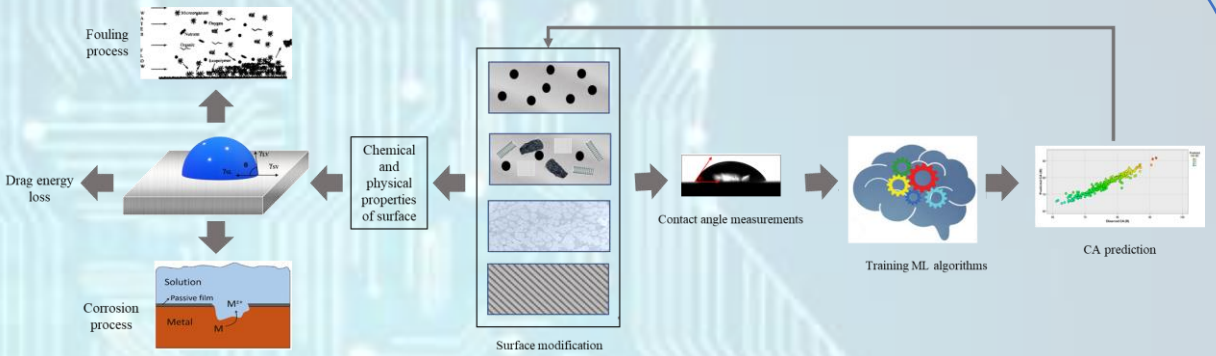
ABSTRACT

- Three major problems in water distribution system are corrosion, fouling, and energy loss due to drag. Literature shows that surface hydrophobicity impacts all these three phenomena. The contact angle of a water droplet on the surface is used to measure wettability.
- We engineered the surface of materials using different techniques such as alloying, compositing, microstructure modification, and altering roughness profile, and then we studied the changes in microstructural features such as second phase composition and distribution, grain size, and their effects on CA.
- After measuring CA for each condition, the results were used to train ML algorithms and the relationship between them and surface hydrophobicity were explored [1-3].

OBJECTIVES

- While many attempts have been made to formulate various laws or rules in the study of surface properties, such as wetting, this field often lacks derivation from physical or chemical first principles and, consequently, it remains data-driven inductive science.
- Due to the emergence and rapid development of new methods of "Big Data" analysis, it became possible to obtain and study new correlations in data-driven areas of science.
- This is required for optimized design of novel hydrophobic and superhydrophobic (the Lotus-effect) biomimetic materials with self-cleaning, anti-fouling, anti-corrosive, anti-bacterial, and anti-viral properties

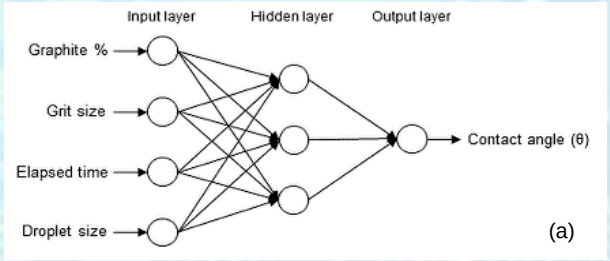
METHODOLOGY

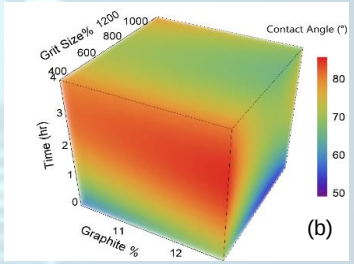


Research framework [3]

RESULTS

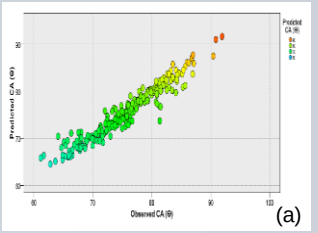
Ductile Iron





(a) According to the artificial neural network model, surface roughness was found to be the most important factor, (b) multivariate polynomial regression model of contact angle as a function of percent graphite in ductile iron, grit size and time. The optimal condition resulted in hydrophobicity improvement by 80% [1]

Aluminum Silicon Alloys



(a) Random Forest algorithms (r = 0.96), (b) Comparison of observed, theoretical, and ML predicted CA values. The prediction by the developed Random Forest algorithm outperformed the theoretical models [3]

CONCLUSIONS

- The results of the present study demonstrate that ML methods can be efficiently utilized to predict the water wettability of iron and aluminum based polyphase alloys and metal matrix composites
- This can lead to obtain new insights on the physical interactions relevant to the water CA.
- The finding can be used as a guide to design new high-performance materials with enhanced surface properties.
- This approach can become part of the emergent 'tribo-informatics' field, related to the application of machine learning methods to surface science and engineering.

REFERENCES

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[2]. Kordijazi, A., Behera, S. K., Suri, S., Wang, Z., Povolo, M., Salowitz, N., & Rohatgi, P. (2020). Data-driven modeling of wetting angle and corrosion resistance of hypereutectic cast Aluminum-Silicon alloys based on physical and chemical properties of surface. Surfaces and Interfaces, 20, 100549.
[3]. Kordijazi, A., Behera, S., Patel, D., Rohatgi, P., & Nosonovsky, M. (2021). Predictive Analysis of Wettability of Al–Si Based Multiphase Alloys and Aluminum Matrix Composites by Machine Learning and Physical Modeling. Langmuir, 37 (12), 3766–3777