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APPLICATION OF MACHINE LEARNING AND COMPUTER MODELING IN METALLURGY

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Introduction

The current state of metallurgy is changing towards anticipatory and information-focused engineering. Historically, the development of alloy and optimization of its processes were based on trial and error experimentation with the assistance of thermodynamics and kinetics. With the advent of high-performance computing, physics-based numerical techniques, including Density Functional Theory (DFT), molecular dynamics (MD), Monte Carlo (MC) simulations, phase-field modeling, crystal plasticity and finite element methods (FEM) could now be applied. The models enable to quantitatively describe phase stability, microstructure development, deformation processes, and defects.

Physics-based models however, are computationally costly and demand a lot of parameter tuning and are not conducive to inverse design and real-time industrial optimization. Concurrently, industrial metallurgy activities create large amounts of heterogeneous data in terms of sensors, simulations, and imaging devices. This has provided a powerful incentive to combine machine learning (ML) with computational modeling to enhance the speed and ease of materials design, microstructural prediction, and allow adaptive process control.

Main Part

In modern computational metallurgy, the following general categories of problems are tackled using mathematical and data-driven models:

1. Extrapolation of material properties and microstructures regarding composition and processing parameter.

Random forests, support vectors machines and deep neural networks are examples of machine learning algorithms that are used to forecast mechanical properties, phase stability, and microstructural features using experimental and simulated data. CNNs have broad application in the automated processing of microscopy images, which allows them to identify boundaries of grains, precipitates, and defects at a high level of accuracy.

2. Metallurgical processes modeling and optimization.

Hybrid methods that use simulations based on physics and surrogates based on ML are used to speed up phase-field and finite element simulation. Physics-informed neural networks (PINNs) are neural networks that include governing equations in the

learning models and enhance physical consistency and generalization. The applications in these processes are the optimization of processes in casting, heat treatment, rolling, and additive manufacturing, where ML can help to choose optimal process parameters in order to reduce defects and enhance performance.

Digital twins and control systems based on reinforcement learning can also be supported by the integration of modeling and ML. It is a system that uses real-time sensor-data with virtual process models in order to provide predictive maintenance, fault-detection, and autonomous control of industrial equipment. Irrespective of these developments, there are still issues pertaining to the quality of data, multiscale connectivity, measurement of uncertainties, and the explainability of complex learning models.

Conclusions

The comparison of existing strategies shows that the combination of machine learning and computational architectures can dramatically improve the predictive performance and effectiveness of metallurgical studies and factory application. Physics-guided ML Hybrid models, which provide faster alloy design, better microstructure forecasting, and real-time process optimization, are possible. Large-scale industrial applications to intelligent metallurgical systems demand further development of standardized data infrastructures, explainable ways of AI and multiscale coupling strategies.

References

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