APPLICATION OF MACHINE LEARINING AND COMPUTER MODELING IN METALLURGY COMPHERENSIVE REVIEW

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Abstract

Machine learning (ML) and computational modeling have transformed metallurgy into a predictive and data-driven field with accelerated alloy design, optimized processing pathways, and improved microstructural properties. This review discusses the emerging trends in atomistic, mesoscale, and continuum modeling studies, such as Density Functional Theory, molecular dynamics, Monte Carlo simulations, phase-field modeling, crystal plasticity, and finite element analysis. More physics-based models are being complemented by ML models, such as classical statistical learning, deep neural networks, and physics-informed neural networks (PINNs). The combination of models has made it possible enabled significant advancements in designing inverse alloys, predicting microstructures, characterizing defects, and controlling processes in real time in casting, thermomechanical processing, heat treatment, and additive manufacturing. Based on a wide body of peer-reviewed literature, this review critically evaluates the strengths, limitations, and strategies for integrating ML into metallurgical systems. High-performance aluminum alloys, energy-relevant materials, and new ideas for digital twins have been emphasized. Major challenges, such as data quality, multiscale coupling, quantification of uncertainty, and interpretability of the model, are addressed, and future research directions based on autonomous and mechanism-aware metallurgical systems are described.

Keywords Machine learning, Computational metallurgy, Multiscale modeling, Alloy design, Digital twins.

1.Introduction

1.1Background and Motivation

The concomitant development of empirical practice, mechanistic knowledge, and computational modeling has long influenced metallurgy [1-3]. Initial developments were based on trial-and-error experiments, which were gradually replaced in the 20th century by theoretical models based on thermodynamics, kinetics, and solid-state physics [4]. This was followed by an increase in high-performance computing, which allowed simulations at various scales, including atomistic interactions, macroscopic deformation, and other schemes, such as Density Functional Theory (DFT) crystal plasticity, molecular dynamics (MD), Monte Carlo (MC), phase-field modeling, and finite element methods (FEM) [5-9]. These physics models have provided important insights into microstructure formation, phase stability, defect development, and thermomechanical response. However, they are often faced with obstacles owing to the increase in computational complexity, simplification of assumptions, and lack of an effective framework for the inverse design or optimization of processes in real-time [10-12].

The advent of data-driven science, the so-called Fourth Paradigm of research, has triggered a paradigm shift in the material properties. At the interface of machine learning (ML), statistics, and materials science, materials informatics is now accompanied by more traditional modeling by deriving actionable information from extensive experimental data, simulations, and industrial process information. This represents an opportunistic shift in the field of metallurgy. Contemporary alloy systems, including high-entropy alloys (HEAs), superalloys, and high-technology aluminum alloys, are multi-component systems with complex defect chemistries that do not fit current modeling paradigms. Simultaneously, the spread of digital manufacturing ecosystems, real-time sensing technologies, and mass repositories of simulations has resulted in a volume of metallurgical data that has never been observed before [13].

ML has been shown to rapidly forecast historical and synthetic mechanical properties, phase stability, defect distributions, and microstructural features based on computational models and both historical and synthetic data. Computer modeling provides mechanistic and scale-interpretive information. The integration of their capabilities, especially by means of hybrid methods such as physics-informed neural network (PINNs) surrogate models, digital twins, and adaptive learning systems, is a route to autonomous metallurgical design and control. Such combined systems have already demonstrated promising outcomes in tasks that involve predicting carbon levels in simple oxygen furnaces, forecasting tramp element build-up in scrap-based steelmaking, optimizing additive manufacturing (AM) parameters, porosity reduction, and continuous casting operations. Radical transformations also occur in industrial practices. Smart metallurgy: Owing to the convergence of cyber-physical systems, real-time monitoring, digital twins, and ML algorithms, smart metallurgy has been implemented to control furnaces, optimize rolling mills, detect process faults, and conduct predictive maintenance. These developments highlight the increasing need for scalable, interpretable, and physics-guided AI models that can be reliably used in data-constrained and high variability settings [14].

1.2 History and Development of the Technology.

Computational metallurgy had its methodological origins in the early 1990s, with the introduction of parallel MD algorithms to simulate short-range interactions, early attempts to implement phase-field models to simulate microstructure evolution, and the development of the FEM to create and simulate thermomechanical processes. Towards the beginning of the 21st century, multi-scale modeling frameworks were commonly used to connect atomistic processes with continuum-scale behaviors. This changed in the mid-2010s, when materials informatics was formalized, and data-driven modeling was established as an inseparable part of metallurgy [15].

In the past decade, the 2020s, the use of MLs in metallurgy has increased. Examples of significant achievements include the classification of microstructures with conventional neural networks (CNNs) and an accuracy of over 95 percent, the design processes of alloys facilitated by machine learning, the predictive modeling of microstructural evolution in AM, and the optimization of high-energy processes in industry in real time. These innovations align with general industrial pressures related to energy efficiency, cost reduction, sustainability, and decarbonization. Recent research has shown that hybrid modeling can reduce alloy development times by as much as 70 percent, enhance process stability, and design next-generation materials for aerospace, automotive, and energy development [16].

1.3 Review Methodology

In this review, a structured, systematic survey and evaluation of the application of computer modeling-ML and ML integration in metallurgy was performed. Scopus, Web of Science, IEEE Xplore, and Science Direct were searched using keywords such as computational metallurgy, machine learning, materials informatics, physics-informed models, and digital twins in metallurgy to collect publications published between 2000 and 2025. The inclusion criteria were based on studies that used computational modeling, ML, or a mixed methodology to design alloys, predict microstructures, model processes, or optimize industries. The exclusion criteria eliminated

irrelevant, non-English, and strictly experimental studies without computational elements. They were identified using thematic clusters, research hotspots, and temporal trends as bibliometric tools, including VOS viewer.

More than 150 high-impact references, including foundational theories, methodological developments, and industrial case studies were included to provide a balanced analysis. The chosen literature is representative of the extent and scope of the technological integration channels of ferrous and non-ferrous systems, focusing on applications applicable to Industry 4.0, as well as predictive analytics and autonomous process control.

1.4 Scope and Structure of the Review.

This review provides a systematic overview of the use of computer modeling and machine learning in metallurgy, atomistic and mesoscale modeling, and more recent AI frameworks. The objectives are to:

- Overview of the history and theory of computational metallurgy on the scales.
- Summarized ML methods, such as supervised, unsupervised, and hybrid physics-informed methods, are applicable in metallurgy.
- Consider modeling-ML integration approaches with a particular focus on hybrid frameworks, including physics-informed neural networks (PINNs) and surrogate modeling.
- The major applications in alloy design, process control, additive manufacturing, and microstructural analysis are discussed.
- Determine issues related to data quality, interpretability, and multiscale coupling.
- Future research avenues in the fields of intelligent, autonomous, and sustainable metallurgical systems are suggested.

This review provides a critical analysis of the literature on the integration of computer modeling and machine learning in metallurgy. It discusses atomistic, mesoscale, and continuum modeling, underlying machine learning methodologies, and hybrid methods that use physical laws to supplement data-based inference. Its applications include alloy design, micro-structural prediction, process modeling, and optimization at the plant level, particularly in additive manufacturing and steel-making processes. Challenges, such as data scarcity, model interpretability, computational cost, and multi-scale integration, are discussed to explain the existing limitations of the area. The combination of length scales, computational approaches, and industrial fields will allow the continuation of physics-based and data-driven approaches to understand how these two avenues of knowledge can be collaboratively applied to achieve next-generation metallurgical sciences. It is designed for use by researchers, engineers, and industry practitioners who want to use intelligent modeling frameworks to develop materials faster and provide digitally enabled metal processing.

1.5 Evolution of Computer Modeling in Metallurgy

The principles of computational metallurgy are based on procedures that can be used to reproduce physical phenomena on different scales. At the atomic level, dislocation motion, diffusion, and phase transformations can be analyzed using molecular dynamics (MD) simulations pioneered by Plimpton. Later, phase-field modeling (PFM) was used to propose a mesoscale model of the micro-structural evolution of solidifying, precipitating, and recrystallizing materials [17].

Finite element approaches, including the crystal plasticity finite element method (CPFEM) [18], enable explicit modeling of slip systems and texture changes, linking micro-structural deformation to macroscopic behavior in terms of stress-strain at the crystal plasticity and continuum scales. Finite element methods (FEM) have expanded the application of computational mechanics to the simulation of industrial processes such as casting, forging, and rolling.

Nonetheless, purely mechanistic models have constraints: they require precise constitutive parameters, are computationally expensive, and are not easily scalable to complex or multi-phase processes or stochastic

processes. This has encouraged the development of data-driven and hybrid modeling, in which ML serves as a surrogate, accelerator, or integrator of physics-based simulations [19].

1.6 Emergence of Machine Learning in Metallurgy

The addition of ML to the metallurgy industry is a major step towards deterministic simulation of probabilistic and adaptive systems. Neural networks have been applied to the design of superalloys and the prediction of their properties. As open material databases have increased in size (e.g., AFLOW, Materials Project, and NOMAD), algorithms such as random forests, support vector machines (SVMs), and deep neural networks (DNNs) have been used to project composition-micro-structure-property correlations [20]. Simultaneously, computer vision approaches using conventional neural networks (CNNs) have transformed the characterization of micro-structures. The microscopy images that CNNs can extract include features such as grain boundaries, inclusions, and precipitates, which saves time and improves the accuracy compared to manual analysis. Recently, hybrid and physics-informed methods have been developed to address the black box of ML. These include physics-informed neural networks (PINNs) that incorporate governing equations in loss functions and digital twins that combine real-time data with virtual process models [21].

1.7 Why Integrate Modeling and Machine Learning

Synergy between physics-based knowledge and data-driven learning was achieved by integrating computer modeling and ML.

- Faster simulation: ML surrogates are approximations of costly computational models (e.g., FEM and phase-field).
- Improving predictive accuracy: ML can rectify model biases through experimental learning.
- Data augmentation: The outputs of the simulated experiments can be used to augment small experiments to train the MLs models.
- Autonomous control: Frameworks of reinforcement learning (RL) and adaptive control involve models as computer-based simulations of process optimization.

This integration can be seen as a growing trend in more recent metallurgical applications: meta-PINN frameworks can be used to monitor induction furnaces, online neural predictive controlling annealing, and dynamic endpoint prediction in oxygen furnaces.[22] These in combination illustrate a shift towards self-learned metallurgical systems, which is one of the pillars of Industry 4.

2.Fundamentals of Metallurgical Processes and Modeling Approaches

2.1 Overview of Metallurgical Processes

The core issue in metallurgy is the possibility of converting raw materials and alloys into useful materials with certain mechanical, thermal, and chemical properties. It can be broadly categorized into extractive metallurgy, which examines the process of extracting metals from ores and scrap, and physical metallurgy, which examines the micro-structural processes that determine the behavior of materials [23]. The theme shared by both branches is the knowledge of phase transformations, solidification, diffusion, and thermo-mechanical processing, which determines the ultimate performance of the material [24].

Older metallurgical operations, including casting, forging, rolling, heat treatment, and sintering, are controlled by the complexity of interactions between thermodynamics and kinetics. Their tendency to form grains of different sizes, phase fractions, and defects, among others, are some of the outcomes that are traditionally challenging to predict without empirical evidence or semi-empirical models based on large-scale experiments. Although these models are quite accurate, they are difficult to extrapolate to complex nonequilibrium multi-component alloys. However, this has changed with the introduction of computational thermodynamics and

materials informatics. Multi-component systems have been predicted to have stable and metastable phase equilibria using a method termed Calculation of Phase Diagrams (CALPHAD), whereas simulations using phase field and molecular dynamics (MD) have been used to predict micro- and atomistic scales [25]. Nevertheless, despite these innovative tools, the growing complexity of contemporary alloys, including high-entropy alloys (HEAs) and Al-Mn-Zr-RE, imposes data-driven strategies capable of operating on large design spaces and non-linear relationships [26].

The critical information on composition-processing-microstructure-property relationships that Eshetu et al. systematically investigate with systematic experimental research on the aluminum-based alloy systems are critical in machine learning applications. Detailed characterization of phase formation, grain refinement and mechanical properties in the study of ball-milled Al-Mn-Zr alloys with additions of Ce and Y showed strong relationships between alloy chemistry, milling conditions and microstructural stability [27]. The findings develop organized data sets that can be used in the supervised learning model to forecast hardness, microhardness and thermal stability in complex aluminum alloys.

The given modifications to microstructural refinement and mechanical performance brought by the introduction of rare-earth elements are especially pertinent to ML-based feature importance analysis, where the compositional descriptors (e.g., the content of Mn, Zr, Ce, Y) and processing variables (milling time, annealing conditions) are the important inputs. These experimentally verified relations are directly in line with regression-based ML models (e.g., random forests, gradient boosting) presented in contemporary metallurgical informatics.

Equally, studies into particle-reinforced aluminum during local laser melting observed how fast cycles of temperature reacted and reinforcing phases (SiC, TiC, TiB2) brought about microstructure and mechanical reaction [28]. These results can be closely related to data-driven optimization techniques in laser-based processing and additive manufacturing in which machine learning models are becoming more popular to correlate parameters of the laser between melt pool behavior and final product properties. The experimental results of the coupling of localized heat input with microstructural heterogeneity are similar to the input-output mappings that surrogate ML models are often trained on.

Phenomena involving diffusion control were studied within the Cu-Ni-Sn system where concentration gradient, phase evolution and diffusion kinetics were experimentally determined the studies of diffusion in the Cu-Ni-Sn system in 800-1100degC indicate interdiffusion coefficients in 10-12cm2/s, and the phase formations such as Ni3Sn4 and Cu6Sn5 depend on temperature and composition, provide benchmark data on the validity of MD simulations or ML models to predict the diffusion kinetics in ternary alloys [29]. The findings give mechanistic standards of validating physics-informed machine learning (PIML) and surrogate diffusion models, especially when the thermal stability of the long term is concerned, and phase transformation prediction.

Outside of structural metallurgy, porous silicon energy conversion work is evidence of the understanding of microstructural control, transport, and optimum performance using experimental evidence [30]. Even though the approach is used in electrochemical systems, the methodological similarities, namely, data organization, multivariate data analysis and property optimization, can be applied to the context of metallurgical informatics. Similarly, the research on chlorophyll-based photovoltaic materials included structure-property relations and materials performance modeling, which provided support to experience in data-driven materials analysis [31]. In the computational viewpoint, the methodological work of Novikov et al. offers a strict mathematical basis of

machine learning application to physical systems, such as metallurgy. His probabilistic modeling, scalable inference algorithms, and tensor-based learning models solve the key problems in metallurgical data science, including high dimensionality, quantification of uncertainty, and the integration of heterogeneous data.

The study by Alexander S. Novikov presents useful experimental data on lead-free solder alloys, especially Sn-Ag-Cu (SAC) alloys with Bi additions and is very relevant to the microstructure-property correlation in multi-component metallic systems. These papers highlight how alloying elements improve microstructures, inhibit intermetallic compounds (IMCs), and improve mechanical performance (i.e., creep resistance, hardness, and tensile strength), and provide extensive data into which to train ML models to predict hardness and tensile behavior based on composition and processing. Novikov et al. (2021) examined how Bi additions (0.5-3.5 wt.%) impact on Sn-1Ag-0.5Cu (SAC105) solder alloys. SEM and XRD were used to determine that Bi enhances eutectic refinement, decreases the size of b-Sn dendrites and inhibits Ag3Sn and Cu6Sn5 IMCs. Creep experiments demonstrated a lower steady state creep rate with the optimum Bi (2.5 wt.percent), and an activation energy of about 52 kJ/mol that dislocation climb through core diffusion is the predominant mechanism. Such microstructural transformations enhance mechanical stability at thermal stress, which offers data sets to the ML regression models to correlate the Bi content with creep resistance and hardness [32]. Novikov et al. (2025) considered Bi-Sn and Bi-Sn-Sb and Bi-Sn-Ag solder alloys to be used in electronics. The phase separation was observed in microstructural examination (SEM-BSE and EDS), Sb coarse Sn2Sb3 IMCs, and Ag finer needle-like Ag3Sn precipitates. Ag dispersion strengthened vickers microhardness, whereas Sb strengthened the structure. Such conclusions indicate the importance of these findings in precisely alloying tailors hardness and thermal stability, which is optimal in ML-based prediction of property improvements in low-melting solder systems [33].

Novikov et al. (2016) examined the current developments in Sn-Ag-Cu lead-free solders containing alloy elements and nanoparticles. Among the issues highlighted in the work are the IMC growth, wettability, and mechanical reliability, and the work assesses improvement by making additions which refine microstructures and enhance tensile strength/elongation. This gives the hybrid ML-physics models the basis to optimize solder compositions in electronic packaging [34].

In metallurgical applications these frameworks can be directly applied in learning using mixed experimental-simulation data where uncertainty and missing information are necessitated. The focus on interpretable and statistically based ML models can be aligned with the necessity to apply physics-guided learning methods, such as surrogate modeling and physics-informed neural networks (PINNs). Underpins of Novikov in hybrid computational-ML methodologies, which underpin integration of governing equations, constraints and prior knowledge in the data-driven models are essential in promoting industrial acceptance of AI in metallurgy [35].

The field of materials informatics is a paradigm shift in metallurgy, in which big data techniques are used to identify patterns and predict the behaviors of materials that could not have been observed before via empirical processes. The informatics of materials, as described in the fourth paradigm of materials science, involves the use of data-driven methods to supplement theory, experimentation, and computation. This paradigm combines large datasets of simulations, experiments, and real-world processes to accelerate the design and optimization of alloys. For example, high-throughput library production allows for rapid screening of thousands of material compositions and correlates with the underlying physics. This is especially applicable in metallurgy to solve problems such as phase stability in high-entropy alloys (HEAs), where big data analytics minimizes the trial-and-error of the conventional development of alloys. Foundation models in material discovery emphasize the role of large-scale datasets made available by computational simulations in predicting inorganic material properties, which are not usually available in experimental datasets. This is similar to the review on ML in metal additive manufacturing (AM), where big data obtained by process-monitoring sensors are used to optimize parameters to reduce defects such as porosity. With big data, machine-readable representations of metallurgical

data can be obtained by integrating big data with informatics tools, including databases such as the Materials Project, and these representations can be used in machine learning to predict mechanical or thermodynamic behavior [36].

This is particularly the case for the management of heterogeneous data sources in metallurgy, such as micro-structural images, spectral data in converters, and process records in furnaces [37-39], this provides a broad overview of ML in materials informatics with a focus on the opportunities of levels of hierarchical learning between the atomic and macroscopic images. This has resulted in innovations such as big data to predict tramp elements in basic oxygen furnaces (BOF), where ML models can be used to predict impurities based on scrap mix compositions. Nevertheless, issues such as lack of data and poor quality of data still exist and thus can bias the models. Recent bibliometric reviews indicate that there is an increase in the volume of publications, but the quality of data is still scarce. AI optimization in production chains and ore extraction applies big data to reduce the consumption of energy and the amount of waste, in line with the principles of circular economy [40]. Figure 1 illustrates the metallurgy, mechanistic models, and machine learning in metal printing. The development timelines can be depicted in visual form to demonstrate how the initial computational models emerged in the 1990s and evolved into information-intensive ML in the 2020s.

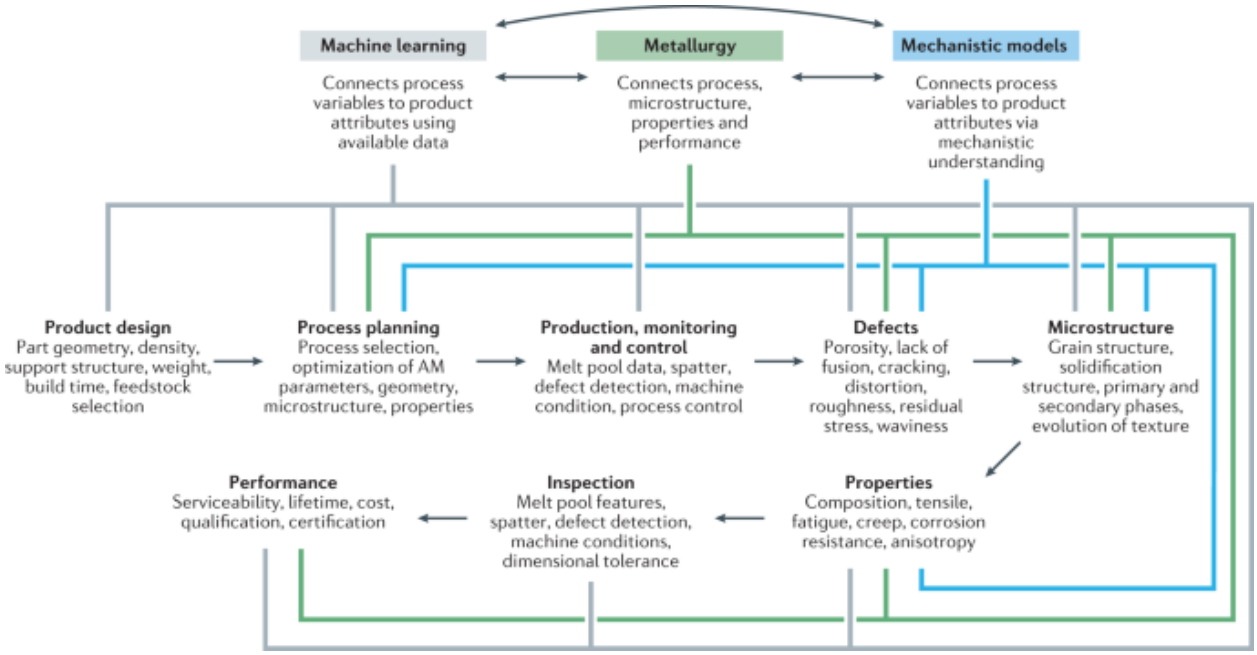

Figure 1 – Metallurgy, mechanistic models and machine learning in metal printing [136]

This foundational overview sets the stage for understanding how big data not only inform but also transform metallurgical research, with evidence suggesting a 50% reduction in the development time for new alloys through informatics-driven approaches [41–45]. Further depth reveals counterarguments: while big data promises efficiency, over-reliance on correlations without physical insights can lead to nongeneralizable models. The transition from data correlation to mechanistic understanding is essential for robust metallurgical applications. Materials informatics and big data form the bedrock of modern metallurgy, enabling predictive capabilities that align with industrial needs for sustainability and innovation [46–50].

2.2 Computational Modeling in Metallurgy

Computational modeling serves as the backbone of predictive metallurgy, bridging experimental insights and theoretical understanding. These methods can be categorized into three primary levels: atomistic, mesoscale, and macroscale modeling, each with distinct strengths and limitations.

2.2.1 Atomistic and Mesoscale Modeling

Atomistic modeling provides insights into the fundamental behaviors of materials at the atomic level by simulating interactions using techniques such as MD and density functional theory (DFT). Fast parallel algorithms for short-range MD have been foundational, enabling efficient simulations of large systems to study phase stability and defect dynamics in metals [51-53]. Recent advances include the 2024 atomistic simulation of primary micro-structure formation during molten metal solidification [54]. investigated the microscopic mechanisms responsible for dendrite growth and grain boundaries and revealed how undercooling influences the nucleation rates. These models are crucial for predicting alloy properties, advancing in situ atomic-scale methods to understand energy materials under operating conditions, and linking local structural changes to macroscopic performance. Figure 2 elaborates on the Modeling and simulation of micro-structures in metallic systems.

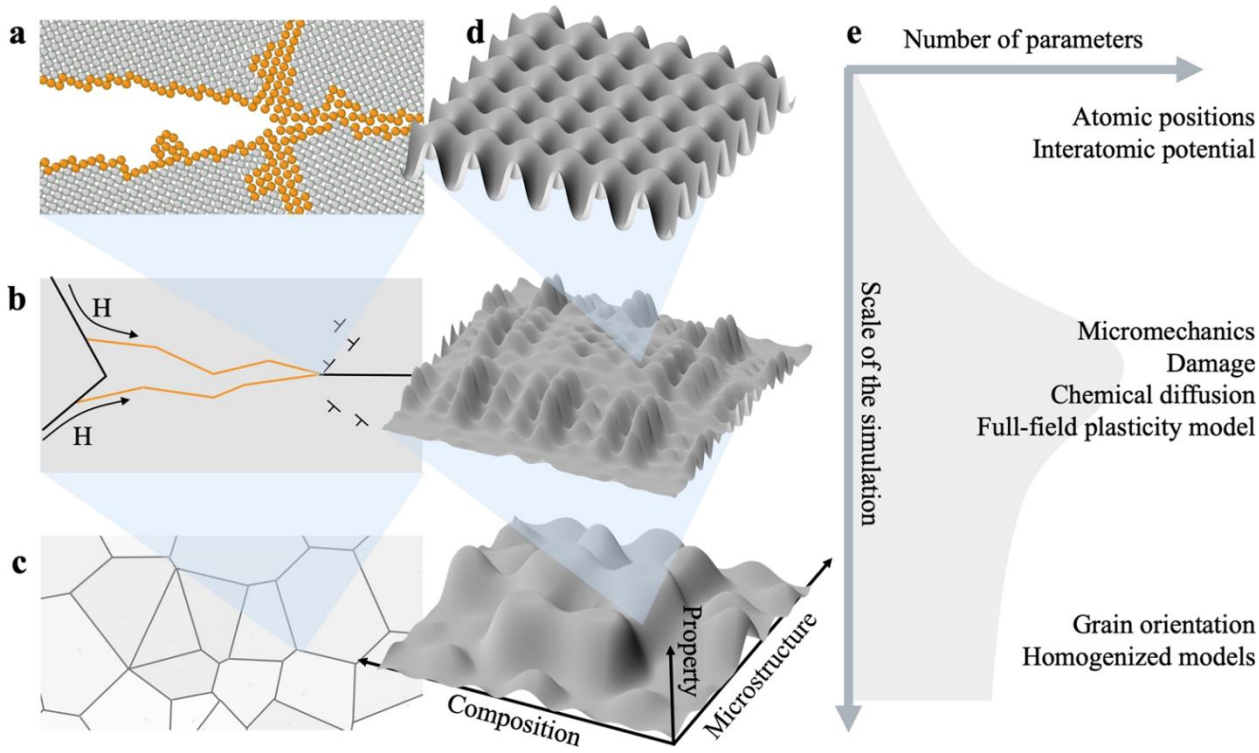

Figure 2 – Modeling and simulation of micro-structure in metallic systems based on multi-physics approaches [137].

Transitioning to the mesoscale, phase-field models simulate micro-structural evolution by treating interfaces as diffuse regions governed by partial differential equations. on phase-field models for micro-structure evolution outline their application in solidification, grain growth, and precipitation in alloys. Crystal plasticity finite element modeling (CPFEM) incorporates constitutive laws, kinematics, and homogenization to simulate deformation in polycrystalline metals, providing a bridge between micro- and macro-scales. Atomistic and mesoscale modeling of micro-structure development during sintering highlights the interfacial dynamics in nanostructured materials, using SEAKMC (Self-Evolving Atomistic kinetic Monte Carlo) to extend simulation timescales. the Modeling and simulation of micro-structures in metallic systems based on multi-physics

approaches, which address challenges such as bridging atomistic and continuum simulations, with advancements in Multiphysics modeling applying atomistic Monte Carlo to predict defect structures in multi-scale contexts [55].

In-depth analysis revealed that atomistic models excel in high-fidelity predictions of thermodynamic properties but are computationally intensive, limiting system sizes to nanometers. Mesoscale approaches mitigate this by coarse graining, allowing simulations of micrometer-scale micro-structures. For instance, in aluminum alloys, mesoscale models predict hot tearing during solidification, incorporating continuum mechanics for defect formation.it emphasize cross-scale modeling, where atomistic data informs mesoscale parameters for grain growth simulations. Challenges include parameter calibration and validation against experiments, with hybrid methods emerging to enhance the accuracy [56,57].

2.2.2 Atomistic Modeling

Atomistic simulations, such as molecular dynamics (MD) and density functional theory (DFT), provide a basic picture of the interaction between atoms and the processes of diffusion. MD simulations can capture the short-term behavior of defect migration, dislocation movement, and solidification fronts, whereas DFT provides highly accurate information on the electronic structure, cohesive energy, and thermodynamic stability [58].

As an illustration, DFT has been effectively used to explore solute-vacancy interactions in aluminum alloys and the stabilization of L12-Al3Zr phases with the aid of rare-earth additions. These atomistic understandings inform alloy design procedures, particularly in complicated alloys such as Al-Mn-Zr-Ce and Al-Mn-Zr-Y alloys, where micro-structural stability plays a vital role in high-temperature performance. Nevertheless, MD and DFT have limited use in small systems and short time intervals because of their high computational cost. This drawback encourages the use of machine learning-based interatomic potentials (MLIPs), including Gaussian Approximation Potentials (GAP) and Neural Network Potentials (NNP), which approximate potential energy surfaces with near-DFT accuracy at a fraction of the cost [59,60].

2.2.3 Mesoscale Modeling

Phase-field modeling (PFM), cellular automata (CA), and kinetic Monte Carlo (kMC) are mesoscale techniques that simulate microstructural evolution in processes such as solidification, precipitation, and recrystallization. These models are based on thermodynamic and kinetic inputs of atomistic simulations or experimental measurements to explain grain growth, coarsening of phases, and development of defects [61].

Specifically, phase-field models have become extremely useful in connecting thermodynamic driving forces with the morphology of the micro-structure, enabling the prediction of dendritic solidification in Al-Si or prediction of coarsening of Al3Zr dispersoids in Al-Mn-Zr alloys. However, such models are usually complex for solving coupled non-linear partial differential equations that require substantial computational power and accurate parameterization. Recently, data-driven phase-field models that use neural networks to solve phase-field equations much faster (and even entirely replace them with surrogate ML models) have been proposed [62–65]. These hybrid models demonstrate how AI can be used to complement traditional models in the metallurgy industry.

2.2.4 Macroscale Modeling

The macroscale model uses continuum modeling to model large-scale metallurgy and concentrates on thermal, mechanical, and fluid dynamics. The stress, strain, and heat transfer analyses in processes such as forging and rolling are based on the finite element method (FEM). used FEM to simulate the compaction and sintering processes and predict density distributions and residual stresses. in macroscale FEM simulations of additive manufacturing (AM) categorizes models of thermal and mechanical behavior and focuses on their application in post-processing simulations to mitigate distortions [66].

Process-specific modeling deals with phenomena that are complex in steel-making and casting. As an illustration, the AM macroscale thermal simulation strategy based on track-scale resolution combines typical temperature fields to effectively compute part-scale temperatures. Simulation analysis was used to optimize the gold recovery of the small-scale mining in hydrometallurgy through leaching and adsorption kinetics. The current developments in 2025 involve multi-physics simulations treating models according to length and physics scale, ranging between melt pool dynamics and part-scale residual stresses in metal AM. These models combine thermomechanical features, such as the connection between macro- and microscale equipment to the AM of maraging steel and forecasting the micro-structure in terms of process parameters [67].

Limitations such as the assumption of homogeneous ma trials are discussed further, as they do not consider microstructural heterogeneities. Case-study-based validation, including the reuse of old data to optimize the plant, has practical value and lowers the cost of operation. Future outlooks include connecting it to AI to achieve real-time process control [68].

Macroscale modeling incorporates phenomena that occur on a process scale into metallurgical simulations, such as thermal gradients, mechanical deformation, and residual 4stresses on components. FEM and Computational Fluid Dynamics (CFD) are commonly used to model casting solidification, heat treatment, and rolling processes [69].

For example, FEM was applied to the estimation of temperature patterns and leftover stress in heat-treated aluminum alloys, and CFD models allow studying the melt flow and inclusion transportation during casting. Nevertheless, when the complexity of the process and level of interdependence of the parameters increase, the traditional deterministic model cannot provide high-quality real-time predictions. Machine learning has been found to be a very useful supplement to FEM/CFD owing to its ability to generate reduced-order models that can be used to quickly predict the outcome of a process with little information. By coupling ML to FEM, also known as hybrid digital twins, it is possible to continuously update the model and optimize metallurgical processes in real time [70].

2.3 Multiscale Integration and Data-Driven Paradigms

2.3.1 Multi-Scale Integration

Multi-scale integration connects atomistic, mesoscale, and macro-scale models to provide a complete picture of the behavior of materials. The strategies to be used to scale-up the material structure and properties address the issue of atomistic to coarse-grained model bridging and stress the status and point of view of multi-scale problems. The metallurgy process is considered through an informed multi-scale Integrated Computational Materials Engineering (ICME) approach that involves the investigation of hot extrusion of AA6063 and relates the accident and process parameters to the formation of the micro-structure [71]. Figure 3 describes the Modeling of the materials and their development with simulation.

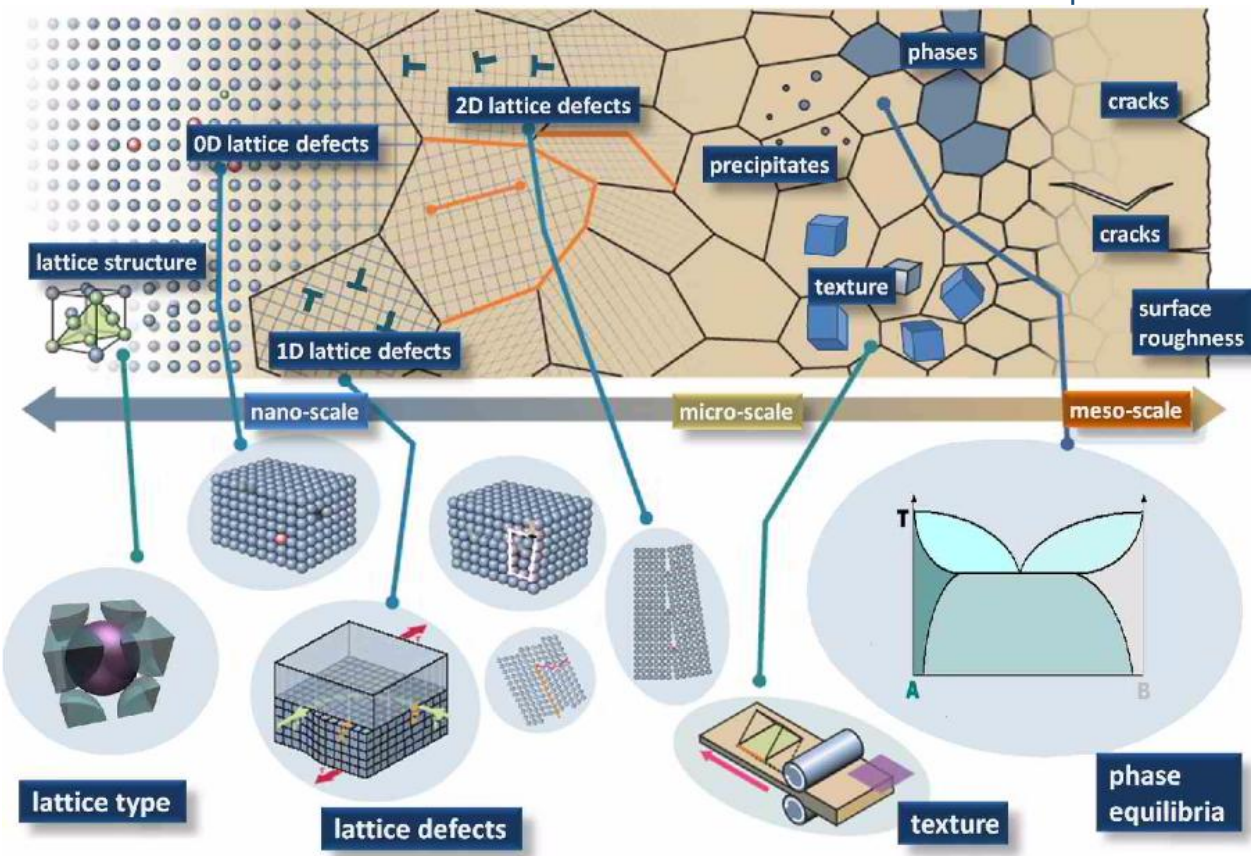

Figure 3 – Modeling of Materials Development with Simulation [138].

Predicting properties between composition and performance prediction between composition and performance can be performed using integration frameworks, a multi-scale approach to the computational design of alloys that combines CALPHAD thermodynamics with ML. Nuclear material multi-scale models are models of the extreme conditions of plasma-facing components. Multiscale Modeling is devoted to bridging the gap between the scales of complex materials. ML and data-driven solvers are used for micro-structure predictions in real-time multi-scale predictions during machining. These problems include the challenge of data transfer at various levels and computational efficiency, and ICME provides answers to sustainable design [72–75].

Metallurgical systems occur in real life, both in multiscale and multi-phase (between a macroscopic and an atomic scale). multiscale modeling is required to obtain appropriate predictions whose results of the low-scale models serve as an input in the high-scale models. As an example, diffusion coefficients obtained with the aid of DFT are applied to inform phase-field simulations, the results of which are, in turn, applied to inform the mechanical property assessment carried out using FEM.

However, the fact that the complication is multiple-scale makes it possible to transfer the data, calibrate the parameters, and propagate uncertainty. Data-driven models, particularly those based on ML regression and Bayesian inference, can offer opportunities to eliminate these problems by training useful scale-bridging correlations between simulation and experimental data [77].

This philosophy of integration can be found in newer projects, such as Materials Genome Initiative (MGI) and Integrated Computational Materials Engineering (ICME), and in fact stimulates the synergy between simulation, experimentation, and informatics. ML is used to complement such schemes with the ability to clean automated data, quantify uncertainty, and explore design space, accelerated, as is needed in the optimization of alloy systems, such as high-alloy Al-Mn-Zr-Ce and Y systems [78]. Chain Data science is used to anticipate the BOF compositions in the steelmaking process to optimize endpoints. Hydrometallurgical gold recovery by simulation

optimizes the leaching parameters. Computer modeling of the metallurgical product chain process cable line simulates complete production lines.

The study of metallurgical process engineering indicates the combined modeling of macro-dynamics operations. Welding is a process in which areas of heat penetration are predicted using thermo-metallurgical simulations [79–80]. All these examples prove that modeling can contribute to the reduction of defects and increase efficiency.

2.4 Limitations of Conventional Modeling

Even though computational modeling is successful, there are a number of limitations:

- Expensive to compute and take a long time to simulate systems of large size.
- Problem with parameter calibration of multicomponent alloys.
- Weak interpretability and extrapolation to non-equilibrium conditions.
- Absence of large and curated datasets of complex alloys.

These difficulties have driven a paradigm shift to machine learning and artificial intelligence, where data-driven models have the ability to learn given experimental and simulated data to predict material properties, phase transformations, and process outcomes without requiring exhaustive tuning of the parameters [81–85]. This evolution is moving away from physics-inspired and hybrid physics-informed ML models, which represent radical changes in modern metallurgy [86–90].

3. Metallurgy and Machine Learning.

3.1 An introduction to Machine learning in Material science.

Machine learning (ML), which is a subdivision of artificial intelligence (AI), has transformed the way materials scientists comprehend, model, and design complex systems. Unlike traditional modeling, which explicitly expresses the physical laws in equations, ML obtains prediction relationships directly based on data using algorithms that discover underlying patterns and correlations.

ML is currently used in all stages of the material development cycle in metallurgy: alloy design, process optimization, property prediction, and failure analysis. The original potential is that it can deal with data of high dimensionality, non-linear dependencies, and noisy experimental data, which are typical of metallurgical data.

The combination of ML and physical modeling is the core of the new Materials 4.0 paradigm, where data science, computation, and experimentation are merged to support faster material discovery and digital manufacturing. The ML predictive process allows metallurgists to experimentally investigate thousands of alloy compositions or process conditions in a few minutes, which significantly decreases the cost and time of the experiment [96].

3.2 Core ML Algorithms

Core ML algorithms are the foundation for applications in metallurgy, where the study of complicated datasets (such as smelting, alloying, and heat treatment) is possible. The most common learning algorithms (supervised learning algorithms) include artificial neural networks (ANNs) and support vector machines (SVMs), which are more common owing to their capacity to take inputs (e.g., composition and temperature) and produce outputs (e.g., mechanical properties). an extensive overview of ML applications in materials science, such as property prediction, regression models, and defect classification.

Pattern discovery in microstructural data is provided by unsupervised learning, such as clustering algorithms, such as k-means, and principal component analysis (PCA) forms a dimensional reduction of spectral data of converters, which helps in predicting temperature and carbon content. Deep learning, based on also proposes

architectures such as recurrent neural networks (RNNs) of time-series data of continuous casting, wherein real-time predictions change a parameter to reduce defects.

Reinforcement learning (RL) is an emerging in-depth method of optimization, similar to annealing furnace adaptive control under constraints. Challenges in overfitting, which are solved by regularization methods, and balance in the data in metal casting industries, where GANs (generative adversarial networks) can potentially generate synthetic data, are described in the context of failed learning experiments. Explainable AI (XAI) techniques, such as SHAP values, are more interpretable and are essential for industrial acceptability.

Future directions also involve the Bayesian optimization of hyperparameter optimization of ML models used to process minerals, which reduces the issues of extractive metallurgy. An example of the use of algorithms, such as gradient boosting, over traditional methods in multi-outcome ML to predict the mechanical properties of alloys can be seen in the examples below. Critiques report that, although ML is more useful in data-rich settings, sparse datasets in niche alloys necessitate transfer learning. Overall, core algorithms can be scaled to provide solutions, and reviews indicate that graph neural networks (GNNs) are seven times more accurate in making predictions compared to classical algorithms [97].

3.3 Property Prediction and Alloy Design.

The prediction of properties and design of alloys are critical uses of ML that will hasten the process of finding materials with specific properties. An example of neural networks using nickel-based superalloy design to predict creep resistance based on composition information is a general-purpose ML model of inorganic materials, where random forests are used to predict properties such as hardness with an R2 of over 0.9.

hybrid ML-genetic algorithms for superalloy design, optimizing for high-temperature performance.ML for high-strength materials, and emphasizing ensemble methods for robust predictions. A detailed analysis shows ML reduces design cycles by 50-70%, as in a rapid alloy design method via transfer learning. Unsupervised learning for pattern recognition in alloy design and cluster compositions for novel discoveries. Challenges include extrapolation beyond the training data addressed by physics-constrained models.

Expansion covers mathematical foundations, such as loss functions in regression for property prediction and critiques of bias in datasets. ML for Mg alloy design combined DFT and ANNs for elastic properties. Overall, ML transforms alloy design from empirical to predictive, with evidence leaning toward integrated frameworks for sustainable materials [98].

3.4 Microstructural Analysis with CNNs

CNNs have revolutionized microstructural analysis in metallurgy by automating image classification and segmentation, demonstrating advanced steel microstructural classification using deep learning, and achieving 93% accuracy across phases such as ferrite and martensite. pioneer computer vision for automated microstructural image analysis, thereby laying the groundwork for CNN applications. link structure properties using 3D CNNs for volumetric data. CNNs for micro-structure recognition in ceramics, extensible to metals. The CNN-based method quantitatively assesses the steel micro-structures in welded zones and offers scalability over manual methods. For thermal spray coatings, CNNs extract features for porosity analysis.

Beyond core uses, ML is applied to failure prediction, energy efficiency, and process monitoring in metallurgy. hybrid ML for hot-rolled steel properties. ML algorithms in metallurgy and the basic cases related to the algorithms.AI for failure prediction in metallurgy optimizes the chains. In mining, ML aids in mineral processing [99].

3.5 Physics-Informed and Hybrid Models.

Hybrid methods combine conventional physics-based simulations with ML to overcome the weaknesses of pure data-driven methods, for example, lack of interpretability and emphasize the application of PINNs in solving phase-transformation differential equations, which are also used in welding and solidification. For example, thermomechanical laws have been integrated into structures, such as metal additive manufacturing, to forecast distortions.

Additive manufacturing (AM) applications in Additive Manufacturing and Additive manufacturing take place at every stage of product development, including the final product. <|human|>Uses in Additive Manufacturing in Additive Manufacturing, Uses in Additive manufacturing Applications in Additive manufacturing occur at each developmental stage of a product, including a final product.ML is changing metal AM because it allows in-situ monitoring and optimization of parameters. CNNs are used to detect anomalies in melt pool images to predict mechanical properties using process data, and hybrid models are used to reduce failures in the manufacturing process. Visual representation: The diagrams of ML workflows in AM are shown in Figure 4.

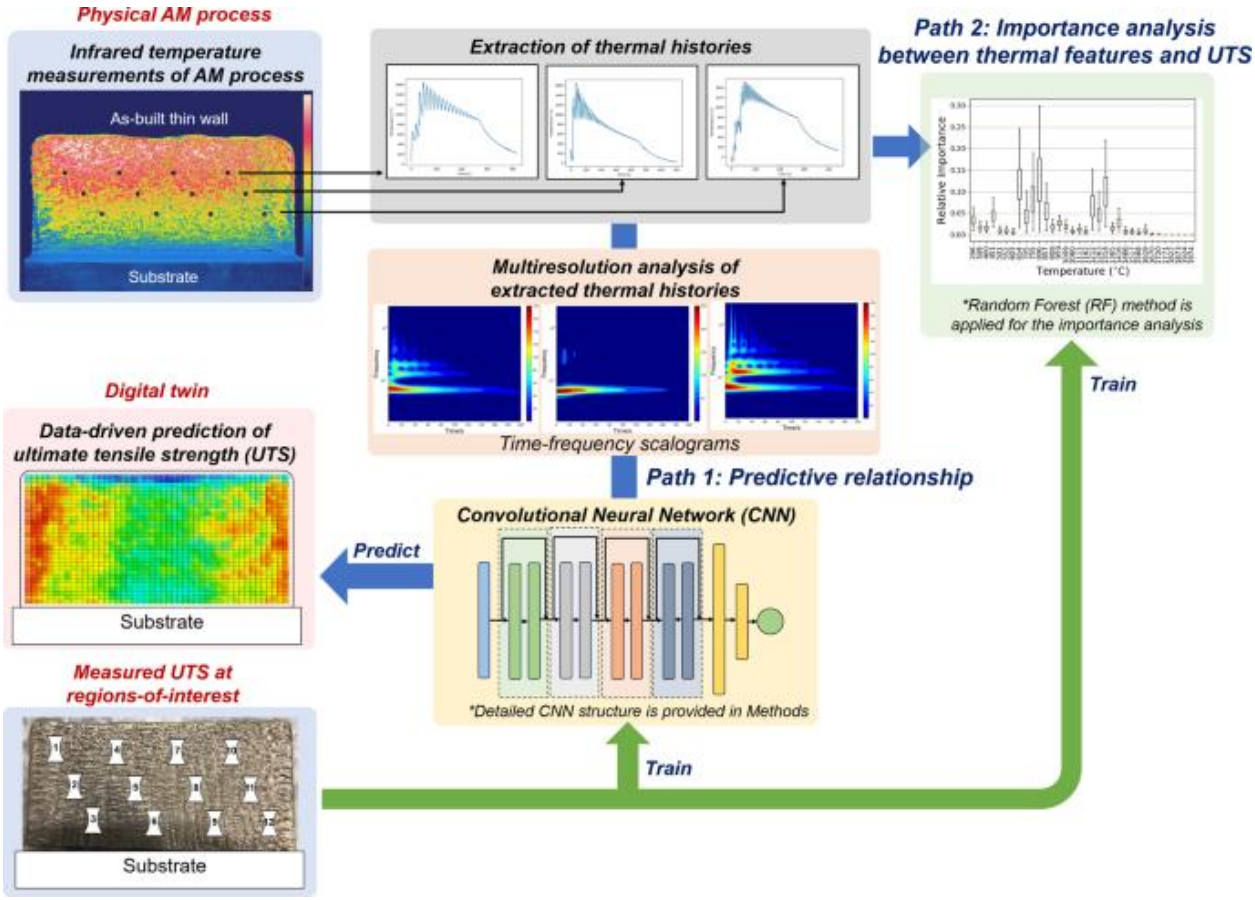

Figure 4 – Mechanistic data-driven prediction of as-built mechanical properties in metal additive manufacturing [141]

3.6 Process Optimization and Control.

In metallurgy, ML is used to provide real-time control, for example, in BOF steelmaking, predicting carbon content based on flame characteristics using algorithms. Dynamic adjustments are performed using optimization tools, such as LSTMc networks with time-series data. Examples of cases describe the saving of energy in annealing furnaces using neural predictive models. Supporting evidence:

ML is implemented practically for defect prediction in continuous casting (when algorithms analyze process data streams and minimize inclusions). This indicates that two-stream networks are used to predict multiple defects and temperature field dynamics in real time [100].

3.7 Classical/Quantum Mechanics.

To fill the gap in standalone methods, hybrid models are based on a combination of physics-based simulation frameworks and ML to obtain results in the form of powerful predictive instruments to predict the metallurgical process. Loss functions: Physics-informed neural networks (PINNs) incorporate equations governing the process (e.g., heat transfer or Navier-Stokes) as loss functions, which are then learned based on data. physics-informed ML models of accelerated simulations in AM combined supervised ANNs with variational autoencoders (VAEs) to predict micro-structure evolution, which saves 10x simulation time with no performance loss. These models are also utilized in the welding field of metallurgy, where they rely on deep learning and phase-field integration to predict the evolution of titanium alloys. This generalized to multi-scale modeling of composites, which can be applied to multi-phase alloys, with the aid of ML, to help with the calibration of parameters on different scales to predict micro-structure, assesses techniques in metal AM, and finds that PINNs perform better in low-data regimes, as they adhere to conservation laws, than pure data-driven models. In the case of hot-rolled steel, a physics-informed NN predicts the temperature using a combination of process data and heat-transfer equations, with a minimum error of 5%. The economic advantages of PIML (Physics-Informed Machine Learning) in AM, as presented in business, include reduced cost due to interpretability and fewer iterations. Some challenges include the scales of hyperparameter tuning, physics-data weights, and dynamic loss functions[101].

3.8 Additive Manufacturing Applications.

ML use in metal AM is directed toward defect reduction, optimization of parameters, and quality control , with catalysis by simulations to create closed-loop) ML challenges, in which anomaly detection algorithms are applied in laser powder bed fusion. ML in AM discusses design evaluation and process innovation, where DL is used to predict the spatiotemporal thermal evolution. Tapia and early requirements of models in monitoring and multi-scale CNNs when classifying autonomously detected defects. Mechanistic data-driven prediction of as-built mechanical.

Rapid AM development uses AI to combine high-throughput characterization with ML for alloy discovery. In AM, deep learning includes in situ monitoring, where sensor data are analyzed using CNNs to predict porosity. Hybrid models with their integrations and outcomes with ML to prediction and optimization in AM specifies the methods of mechanical property prediction. Artificial intelligence-driven material development is a technique that targets metals, where bioinks and polymers are processed with the help of ML but can be applied to alloys. Some of the challenges are over fitting in sparse AM datasets, which are offset by transfer learning in simulations [102].

3.9 Metallurgical Application of Machine Learning Workflow.

The construction of a powerful ML model for use in metallurgical studies is normally a step-by-step procedure that includes six major steps.

- Data Collection and Curation: Release of superior quality experimental, simulation, or literature information, such as thermodynamic, microstructural, and mechanical properties.
- Engineering of features: Convert projected metallurgical variables (composition, temperature, cooling rate, etc.) into numerical forms that can be used as inputs in the model.
- Data Preprocessing - Processing the missing data, scaling the data, and dividing the data into training, validation, and test data.
- Selection of models: Selecting the right algorithms (linear regression, random forests, neural networks, etc.) depending on the type of data and the desired property.
- Training and validation: Minimization of model parameters through the use of iterative processes to reduce prediction error, and by R2, RMSE, or MAE.

- Model Interpretation and Deployment - Learn to interpret features, learn to handle uncertainty, and use the model to perform either predictions or optimization problems.

The quality, variety, and representativeness of the data are crucial determinants of the accuracy of any ML model used in the metallurgy industry. Metallurgical data are typically sparse, heterogeneous, and incomplete, unlike the more conventional datasets used in computer vision or text analysis, and may need to be preprocessed with specialized methods, including feature normalization by alloy composition or prior information, either with physics models or via information augmentation.

3.10 Metallurgy in Terms of Data Sources and Descriptor Generation.

In metallurgical ML, the Feature engineering or description generation is essential in metallurgical ML. Descriptors can be described as quantitative models of material composition, structure, and process state.

There are common categories of descriptors, which are:

- Separating descriptors: atomic fraction, electronegativity difference, atomic radius, valence electron concentration (VEC), and mixing enthalpy.
- Thermodynamic descriptors: Gibbs free energy, enthalpy of formation, diffusion coefficients, and phase stability measurements based on CALPHAD.
- Microstructural parameters: grain size, phase fraction, dislocation density, and precipitate morphology.
- Rolling reduction, annealing time, sintering temperature, and cooling rate were used as descriptors.

Tightly coupled algorithms are offered in automated tools, including Matminer and Pymatgen, and generate descriptors and data repositories, such as Materials Project, AFLOW, and Open Quantum Materials Database (OQMD), which emerge with millions of computed material entries. Domain-specific datasets, including Thermo-Calc, ICDD XRD, and experimental alloy property databases, have also been employed in metallurgy-specific applications. Principal Component Analysis (PCA), t-SNE, and autoencoders are often used as dimensionality reduction methods to improve the generalizability of models. These algorithms reveal low-dimensional manifolds that reflect key physical trends obscured by high-dimensional metallurgical data [103].

3.11 Metallurgical Modeling Supervised Learning.

The most common ML paradigm used in the field of metallurgy is supervised learning, in which algorithms are trained with labeled datasets to predict a given target property.

3.11.1 Regression-Based Models

Continuous material properties predicted by regression algorithms include the hardness, yield strength, corrosion rate, and diffusion coefficient. Classical models include the following.

- Linear and polynomial regression: Composition-property correlations are commonly used for binary or ternary alloys.
- Support Vector Regression (SVR): Suitable with limited amounts of data and non-linear property prediction.
- Decision Trees and Random Forests (RF): Resistant to noise, they can model complex interactions and are widely used in micro-structure-property prediction.

- Gradient Boosting Machines (GBM, XGBoost): Gradient boosting machines are highly accurate in predicting the mechanical or thermal properties using limited data.

The Al-Mg-Si alloy yield strength and ductility in 500 alloy compositions were successfully predicted using a Random Forest model that was trained on 500 alloy-based compositions; this is better than traditional regression models. In addition, SVR models have been used to predict microhardness in Al-Mn-Zr alloys under different annealing conditions and have shown prediction ability within plus or minus 5 per cent experimental values. Figure 5 shows a diagram of the regression-based machine learning

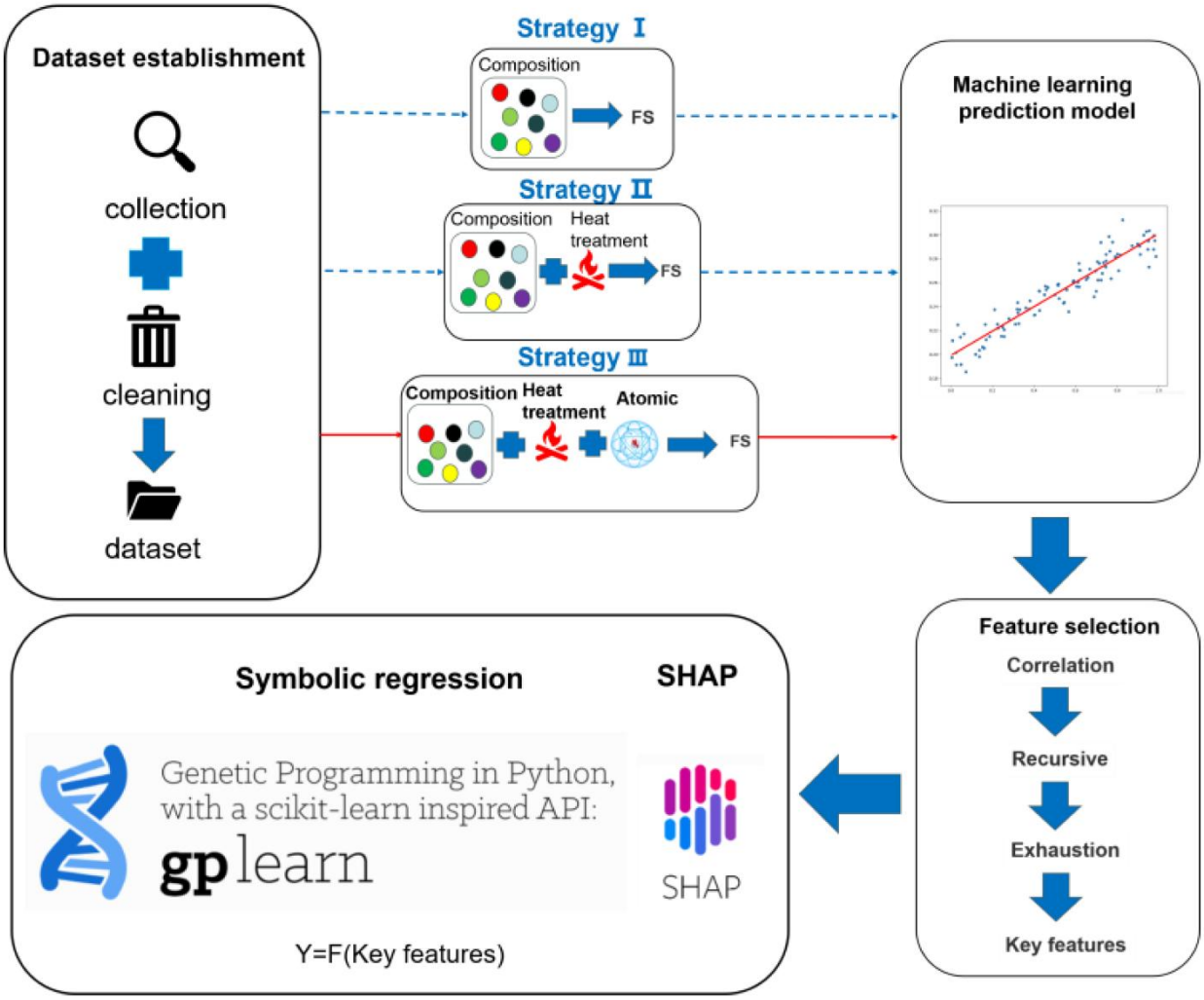

Figure 5 – Diagram of regression-based machine learning models for property prediction in metallurgy, such as linear regression or random forest for hardness prediction [2]

3.11.2 Embryo classification-based models.

Classification models are used to predict discrete values such as the type of phase, type of failure, or type of process. Popular algorithms include k-Nearest Neighbors (kNN), Logistic Regression, Support Vector Machines (SVM), and Neural Networks.

3.12 Unsupervised Learning and Clustering in Metallurgy.

Unsupervised learning finds latent structures in unlabeled data vital to exploratory alloy design and micro-structure analysis. Alloys have been grouped based on composition or performance similarity by alloy techniques, including k-means clustering, hierarchical clustering, and Self-Organizing Maps (SOMs) [104].

4. Deep Learning and Neural Networks in Metallurgy

One of the subfields of ML, deep learning (DL), a subfield of ML that relies on multi-layered neural networks, provides unprecedented capabilities in identifying non-linear relationships and analyzing unstructured data, such as micrographs or diffraction patterns.

4.1 Full-Connected Neural Networks (ANNs).

Artificial Neural Networks (ANNs) are widely used for the prediction of properties. For example, ANN models trained with thermomechanical data can be used to predict the yield strength, hardness, and creep rate of alloys operating under various conditions [105]. Figure 6 illustrates that the neural network architecture for deep learning in materials science ANNs is also better at predicting the solidification of Al-based alloys compared to the traditional regression models.

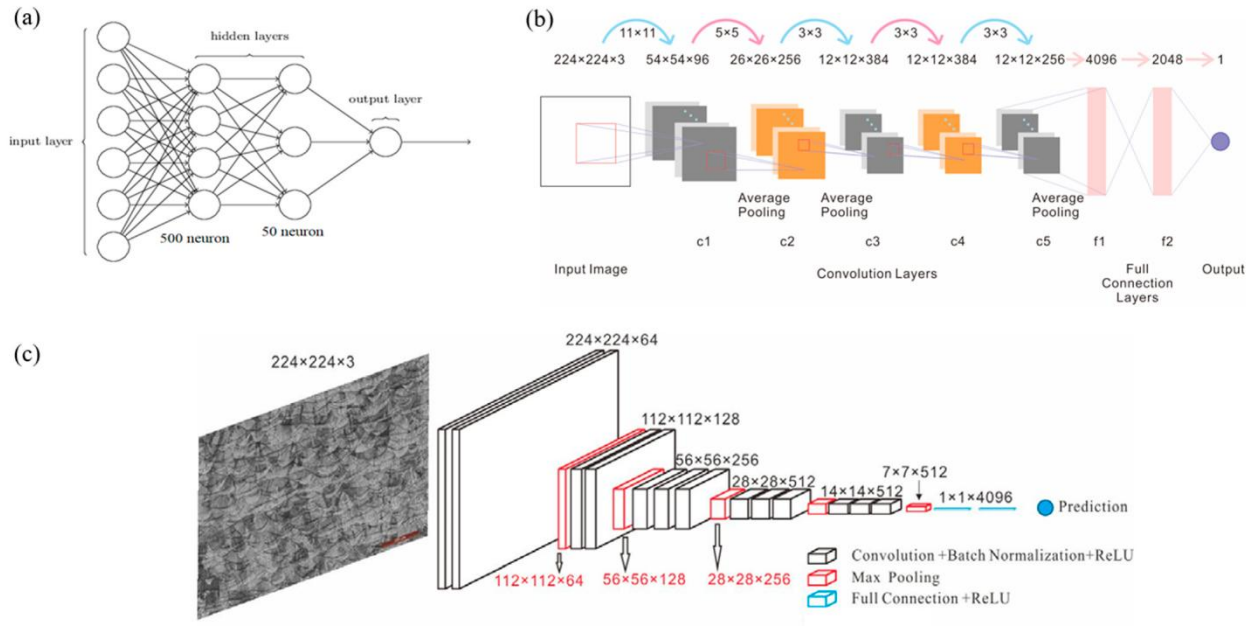

Figure 6 – Neural network architecture for deep learning in materials science, focusing on metallurgy applications [5]

CNNs can be used to identify faces in photographs. <|human|>Convolutional Neural Networks (CNNs) can be applied to recognize faces within photographs, and CNNs have been largely utilized on image-based data, including scanning SEM, Transmission Electron Microscopy (TEM) and EBSD micrographs, and make it possible to extract backscatter diffraction. Examples include:

- Determining precipitates and grain boundaries in aluminum alloys.
- Surface classification of fractures and morphological matching mechanical failure modes.
- Direct prediction of phase volume fractions as directly measured by SEM images.

Microstructural quantification based on CNN facilitates real-time microstructural quality control of metallurgy and avoids the necessity of manual analysis.

4.2 Graph Neural Networks (GNNs)

GNNs model materials as graphs with the atoms and chemical bonds forming a node and an edge, respectively. Such models can directly estimate the formation energies, elastic constants, and diffusion coefficients through atomic connectivity [106].

4.3 Additive Manufacturing and Solidification Processes.

Additive manufacturing (AM) offers a great platform for ML because it is data-intensive and has layer-by-layer characteristics. ML is now being applied to forecast melt pool behavior, porosity formation, and micro-structure evolution based on process parameters and sensor data. ML applications in metal AM have been used for defect prediction, powder quality analysis, and in situ process monitoring. Multi-scale CNNs were used to detect defects in laser powder bed fusion], and process monitoring was introduced as an innovative way to control the adaptive process. Modeling of solidification based on data has enhanced the accuracy of prediction of micro segregation and solidification front velocity, which is important in the quality of castings. Recent computational fluid dynamics (CFD) simulations have also been performed with deep learning surrogate models with similar accuracy at a fraction of the computational cost. Figure 7 shows a Diagram of ML applications in additive manufacturing for solidification processes.

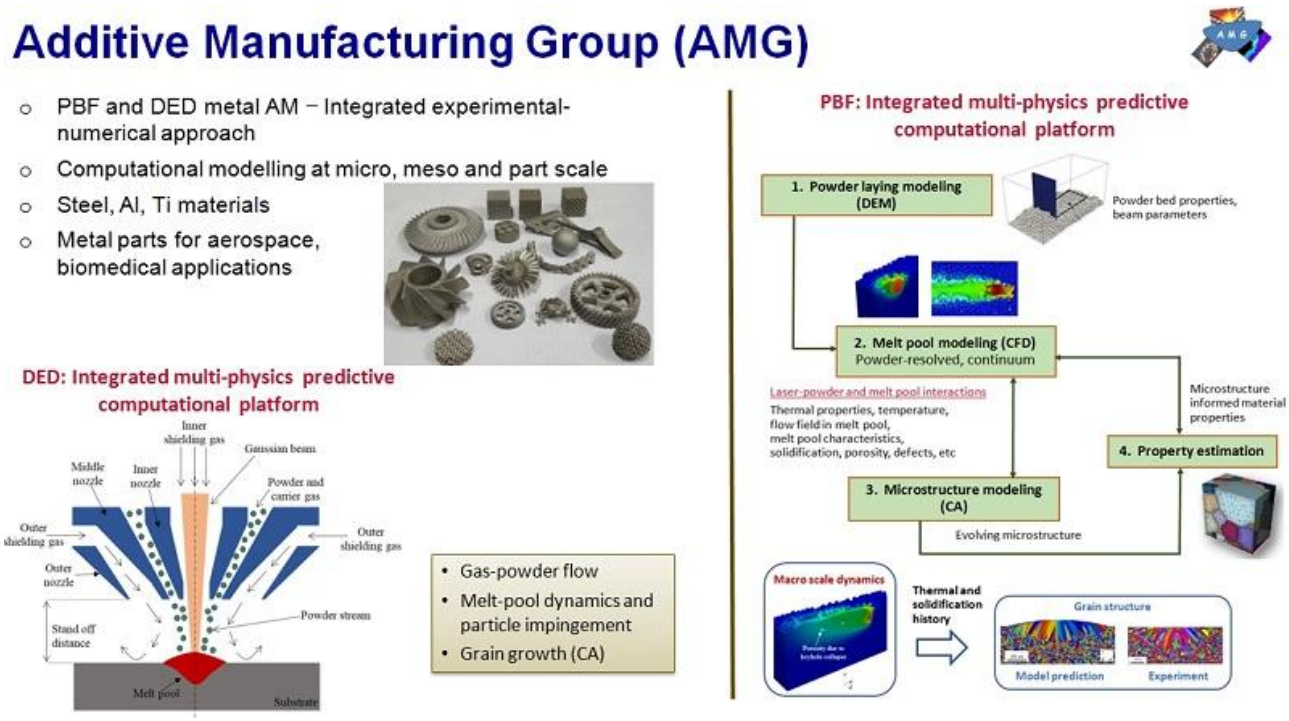

Figure 7 – Diagram of ML applications in additive manufacturing for solidification processes [9]

Regression models were also found to be quite accurate in predicting changes in microhardness at varying annealing times (15-120 minutes) and temperatures (350-400 Degree Centigrade) in the case of Al-Mn-Zr-RE alloys to assist in the design of heat treatment.ML applications in predicting high-strength materials with a focus on the interpretability of the feature contributions, e.g. solute strengthening and grain size refinement.

4.4 Corrosion, Wear, and Fatigue Behavior Prediction.

Important degradation processes in metals are corrosion and wear, which can have complex non-linear relationships with environmental, compositional, and microstructural factors. ML models can predict the corrosion rates and wear coefficients under different conditions with a high level of accuracy. Two types of models trained on compositional and electrochemical data (Random Forest and Gradient Boosting models) have been shown to predict the pitting potential and corrosion current density in aluminum and stainless steels with high levels of generalization. Near-real-time corrosion data can be obtained using deep learning techniques that combine electrochemical impedance spectroscopy (EIS) data. Hybrid models based on fatigue crack growth have also been developed by combining the parameters of Paris' law with deep learning networks. These systems are used to aid digital twins in predicting the lifetime of structural materials.

4.5 Analysis of Failure and Defect Detection.

ML-based computer vision methods have enabled the automatic detection of defects in metallurgical parts. Convolutional and transformer-based models can be used to identify porosity, cracks, inclusions, and delamination based on high-resolution images and ultrasonic data [107].

4.6 Combination and Hybrid Models.

The future of metallurgical modeling is hybrid models that integrate machine learning with physics-based imagery, such as the finite element model (FEM), which proposes a multiscale model based on machine learning to predict the mechanical behavior of composite metals to enhance fidelity and lower the cost of computing. combined phase-field modeling with deep learning to forecast the transformation of welding phases of titanium alloys to obtain near-experimental precision. Physics-informed neural networks (PINNs) incorporate thermodynamic and kinetic constraints, facilitating the transition between black-box ML and physics-based modeling. Figure 8 shows a hybrid model diagram combining ML and physics-based methods in metallurgy, which represents the Digital Metallurgy Era, when virtual simulations are improved indefinitely with the help of ML to reproduce the complexity of the real world.

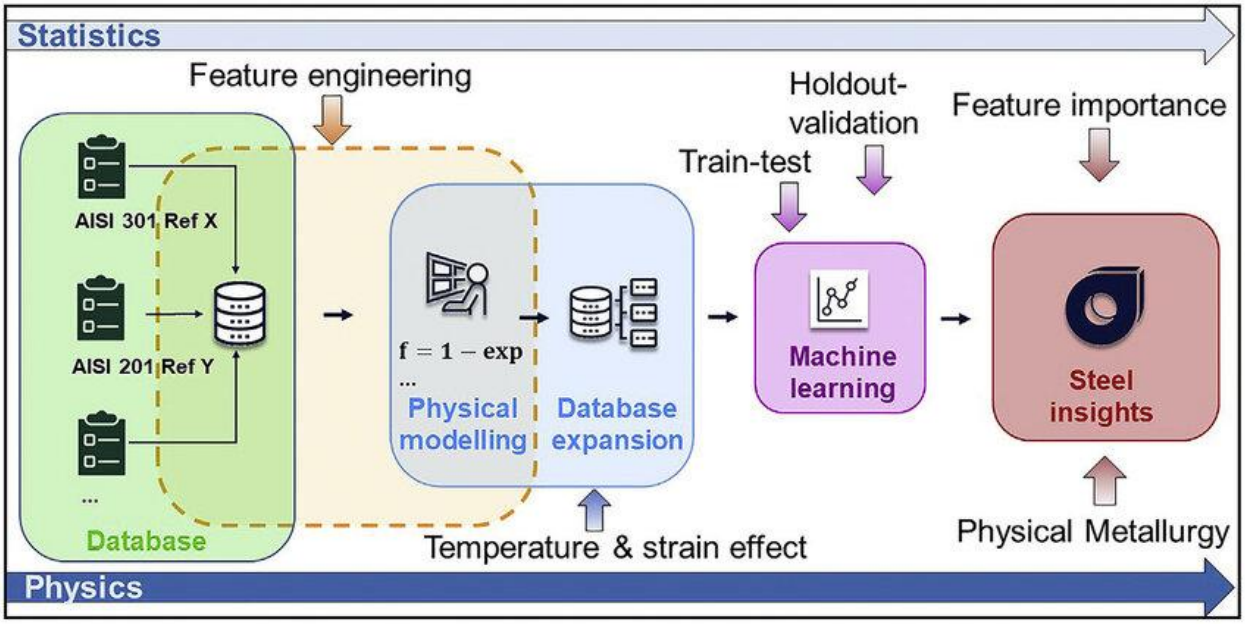

Figure 8 – Hybrid model diagram combining ML and physics-based methods in metallurgy [12]

The introduction of ML into metallurgical studies has made it possible to improve the design of alloys, cutting processes, predict microstructures, and detect defects. With data-driven intelligence and physics-informed modeling, there is now a new method of analyzing and optimizing metallurgical systems. Alloy design and composition optimization are the primary advantages of finite element analysis in metallic engineering applications. ML models have been employed to forecast the precipitation hardening behavior, microhardness, and grain refinement responses to small amounts of Zr, Sc, and rare-earth elements (Ce, Y, La) in an aluminum-based alloy. The further addition of ML-assisted CALPHAD databases also increased the accuracy of the predictions by incorporating both thermodynamic and kinetic characteristics into the training of the model [108].

4.7 Phase Diagrams: Prediction and Thermodynamic Modeling.

Phase diagrams are the basis of metallurgical design and determine the microstructure and properties under different processing conditions. The conventional methods for constructing phase diagrams are based on thermodynamic calculations performed using CALPHAD, which have become more complicated with multicomponent systems. ML is an effective alternative to phase equilibrium prediction and is used to construct pseudo-binary or pseudo-ternary diagrams using data. A neural network system trained on a thermodynamic

database to accurately predict the liquidus and solidus temperatures in multicomponent Al-based alloys with impressive precision. In addition, Gaussian process regression (GPR) was used to predict the phase stability in HEAs, allowing the quantification of uncertainty and active learning-based data collection in unexplored compositional spaces.

4.8 Process Modeling and Optimization.

Process modeling has also been transformed through machine learning, which has provided effective frameworks for the optimization, control, and prediction of metallurgical operations, including casting, rolling, extrusion, sintering, and heat treatment. Reinforcement learning and genetic algorithms have also been used to optimize heat treatment to generate time-temperature profiles that maximize hardness or strength. a reinforcement learning model that automatically came up with the most optimal aging parameters with 7xxx series Al alloys that enhanced the yield strength by 8-10 percent over the traditional schedules.ML can be used to predict densification behavior and residual stress formation in powder metallurgy and additive manufacturing (AM). CNNs trained on process monitoring data (e.g., melt pool images and laser power profiles) can learn to predict the porosity and roughness of the surface in real time; thus, AM processes can be controlled in a closed-loop manner. These smart manufacturing systems based on the combination of ML models and in-situ sensors represent a new paradigm of smart metal production, and Figure 9 shows a Flowchart of ML in process modeling for casting or rolling in metallurgy [which complies with Industry 4.0, objectives of automation, and sustainability.

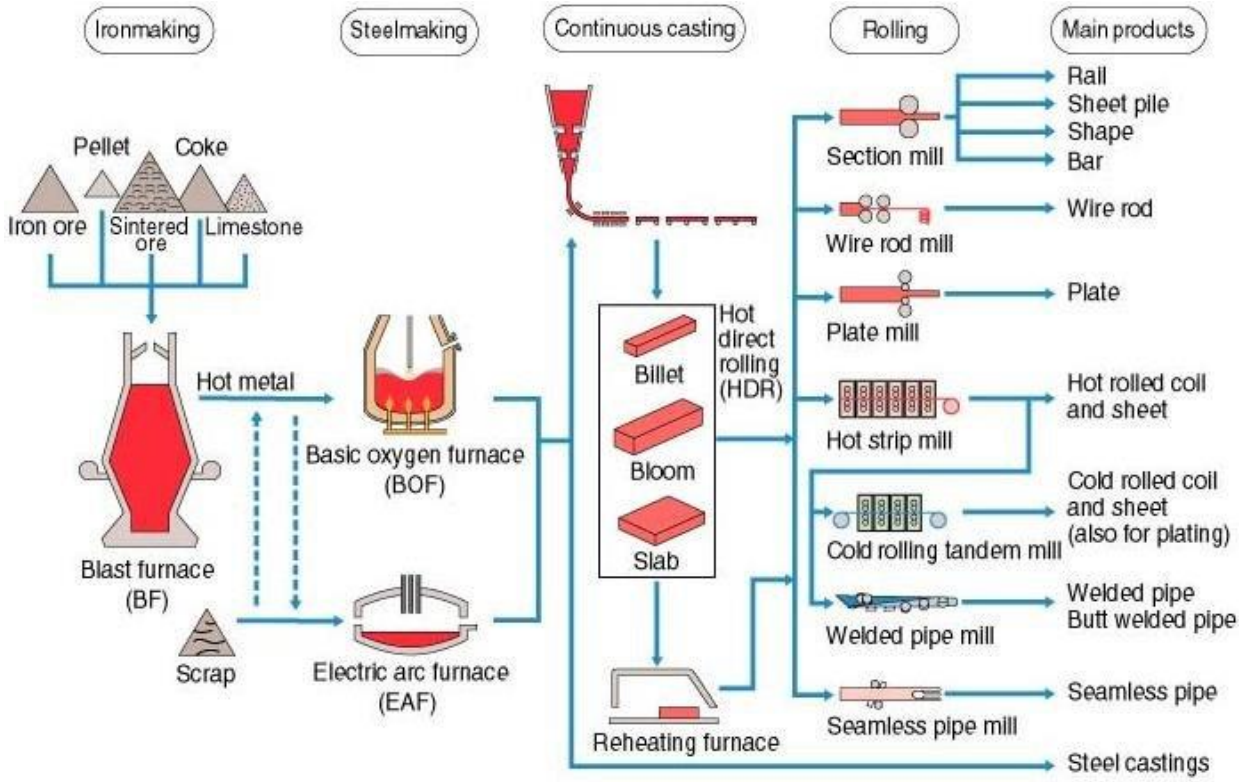

Figure 9 – Flowchart of ML in process modeling for casting or rolling in metallurgy [14]

4.9 Characterization and Prediction of micro-structure.

The evolution of microstructures, which is a key area in metallurgy, is the subject of understanding and prediction. ML has been especially effective in deriving quantitative data on microstructures obtained using scanning electron microscopy (SEM), electron backscatter diffraction (EBSD), and transmission electron microscopy (TEM).

Transformer-based vision models and CNNs can extract grains, precipitates, dislocations, and voids in complex images at superior rates compared with manual or threshold-based segmentation techniques. [109].

5.Combination of Artificial Intelligence and Advanced Metallurgical Systems.

5.1 AI-Integrated Metallurgical Ecosystems.

The transition of metallurgy to a data-driven, intelligent field represents one of the major periods of the Fourth Industrial Revolution (Industry 4.0). Machine learning (ML), deep learning (DL), and reinforcement learning (RL), which are part of Artificial Intelligence (AI), have taken center stage in this change. Combined with computational modeling, digital twins, and intelligent manufacturing systems, AI can form the basis of a paradigm shift toward autonomous metallurgical ecosystems that are adaptive, self-learning, and predictive. In metallurgical engineering, the combination of AI and sophisticated modeling frameworks has resulted in real-time monitoring, predictive control, and optimization at various scales of material production, all the way up to component performance analysis. Digital twins of the action process Casting, rolling, heat treatment, and additive manufacturing (AM) are now an intelligent feedback mechanism, with AI algorithms constantly updating simulated models based on real-time sensor and experimental data. Such AI-based systems minimize human interaction, enhance reproducibility, and allow closed-loop control of the process, in which the model automatically optimizes its process parameters to attain target properties. This smart integration enables metallurgy to be more consistent with the larger objectives of the smart design of materials, sustainable production, and resource efficiency. [110].

5.2 Metallurgical Processes Digital Twin.

A digital twin (DT) is a computer-generated copy of a real-world system that is updated in real time with a physical system through data exchange. Digital twins have been applied in metallurgy to combine FEM, CFD, CALPHAD, and ML models to develop dynamic, multi-fidelity modeling of manufacturing and material evolution processes. For example, DTs are used in aluminum alloy casting, where thermal-fluid simulations are coupled with ML-based defect prediction models to track solidification dynamics and automatically control cooling rates to avoid shrinkage porosity. In rolling and extrusion, reinforcement learning is applied to determine the optimal strain paths and forecast surface defects before the occurrence of the DTs. The concept of DT is not limited to the control of processes but covers the entire life cycle of materials, including design, fabrication, and recycling. This autonomous digital twin system is a closed-loop digital twin platform that reflects the philosophy of Integrated Computational Materials Engineering (ICME), in which real-world experiences continuously feed multiscale simulations. A good example is the digital twin of hot-press sintering of Al-Mn-Zr-RE alloys, where pressure, temperature, and densification rate data are combined in real time with ML models to predict the microstructure and hardness development. These systems allow tuning processes to immediately attain optimum performance [111].

5.4 AI-Improved Materials Informatics Systems.

The current state of material discovery depends on a combination of high-throughput computational screening and data mining. AI is a key component of the Materials Informatics (MI) ecosystem, which integrates databases, simulations, and experimental workflows on a platform of automated learning. International efforts, such as the Materials Genome Initiative (MGI) and Open Quantum Materials Database (OQMD), have generated large datasets of available thermodynamic, structural, and mechanical properties. However, conventional database queries are fixed and confined to known materials. AI supplements MI with dynamic knowledge retrieval, visualization and backward design. Predictive Maintenance and Intelligent Metallurgical plants 5.5 Predictive Maintenance and intelligent metallurgical plants. The scope of AI is not restricted to material design but rather to optimization at the plant level, predictive maintenance, and optimization, which convert traditional metallurgical factories into intelligent production facilities. With the adoption of Internet of Things (IoT) sensors, including AI-powered anomaly detection, equipment (furnaces, molds, and presses) can be constantly monitored. Maintenance systems can forecast failures ahead of time and proactively plan maintenance using time-series forecasting systems, such as long short-term memory (LSTM) networks. Predictive AI systems have been

reported to reduce unplanned downtime by up to 40% in steelmaking and aluminum extrusion plants and improve energy efficiency and equipment life.

5.5 Circular Metallurgy, Sustainability, and Green AI

One of the new challenges in the field of modern metallurgy is to be sustainable, reduce carbon emissions and waste, and increase the precision of recycling. AI has become a key catalyst for green metallurgy through the efficient use of energy in processes, scrap recycling, and alloy design, which can be used in a circular economy. Machine learning can be used to recognize energy-consuming operations and suggest alternative routes with less impact on the environment, which have been trained on historical process data. ML is useful in the process of recycling aluminum to categorize scrap compositions, forecast melting loss, and refine conditions to enhance yield and purity. Furthermore, life cycle assessment (LCA) models integrated with AI can predict the environmental footprint of alloy systems before manufacturing, allowing designers to prioritize sustainability alongside performance. Figure 10 shows the Circular Metallurgy and Green AI diagram. Circular Metallurgy 5.0 envisions a fully digital, data-driven, and sustainable ecosystem where materials are tracked, recycled, and remanufactured through AI-guided decision-making. AI also contributes to Green AI principles, emphasizing energy-efficient computation through model compression, transfer learning, and federated data-sharing approaches, ensuring that the computational sustainability of AI aligns with the broader goals of metallurgical sustainability [112].

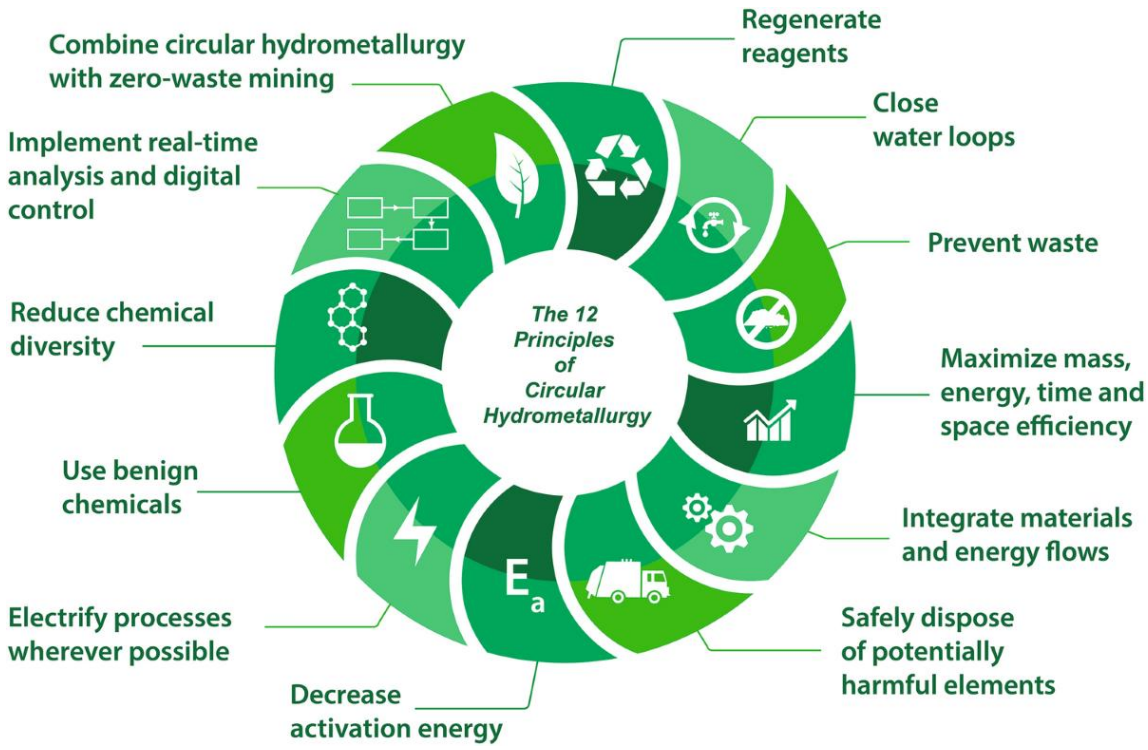

Figure 10 – Circular metallurgy and green AI diagram [23]

5.6 Problems with AI Integration.

Despite impressive developments, there are several technical and operational obstacles to the full implementation of AI in the metallurgy industry: -

- Data Sparsity and quality: Experimental data in metallurgy are usually small, noisy, and heterogeneous, which hampers model generalization.
- Interpretability of models: Most ML models, particularly deep neural networks, are black boxes that are difficult to understand mechanistically.

- Integration complexity: The interoperability and standardization of AI systems must be high to integrate AI systems with legacy process control and simulation software.
- Computational cost: The training of deep models or digital twins, such as multiscale simulations, can be computationally expensive and energy-intensive.
- Security and ethical issues: Responsible data ownership, cybersecurity, and algorithmic bias must be addressed in industrial AI applications.

These issues require a cross-disciplinary approach that unites the knowledge of metallurgy, materials science, computer science, and systems engineering to realize the potential of AI-assisted metallurgy.

5.7 Future Prospects

Hybrid intelligence, that is, the combination of physics-based simulations, experimental data, and machine learning operating on common frameworks, is the future of metallurgy AI. Physics-informed neural networks (PINNs) and knowledge graph-based reasoning enable interpretable and reliable predictions to enhance the discovery and deployment of novel alloy systems.

In the near future, quantum machine learning (QML) can be used to predict material properties directly at the quantum level, eliminating the constraints of DFT and molecular dynamics simulations. With autonomous laboratories, robot experimentation, and cloud-based collaboration, metallurgy is on the verge of entering an era of self-optimizing, sustainable, and intelligent material innovation.

6.Difficulties, constraints, and outlooks of AI-Driven Metallurgy.

6.1 Overview

Although artificial intelligence (AI) and machine learning (ML) have made major advances in the modeling, optimization, and predictive analysis of metallurgical systems, several technical, methodological, and infrastructural issues remain. These issues complicate the reproducibility, interpretability, scaling, and generalization of AI models for alloy systems and processing routes. It is critical to address these issues to achieve the long-term objectives of autonomous, sustainable, and data-driven metallurgy [113].

The adoption of AI in metallurgical processes, including ore fine-tuning, smelting, solidification, heat treatment, and recycling, requires a profound synergy of domain knowledge, computational simulation, and strong data environments. However, obstacles such as a lack of data, model ambiguity, and resource availability continue to hinder industrial implementation. This section reviews these issues and provides an understanding of the current solutions and future development of artificial intelligence-based metallurgy.

6.2 Data Heterogeneity and Scarcity Issues

A key weakness in the metallurgical domain is the unavailability of large, well-organized, and labeled datasets for training generalizable artificial intelligence (AI) algorithms. In contrast to image recognition or language processing, where large standardized datasets exist, metallurgical data are fragmented, non-homogeneous, and proprietary.

Metallurgy data are provided from a variety of sources, such as experimental characterization (SEM, TEM, XRD, EDS), process monitoring systems, and computational simulations (finite element method (FEM), computational fluid dynamics (CFD), molecular dynamics (MD)). The unbalanced characteristics of these collections, coupled with the lack of or inconsistent metadata, create a lot of noise, which affects the performance of ML. Initiatives such as the Materials Project, Open Quantum Materials Database (OQMD), and AFLOW have enhanced the accessibility of data, although they focus mostly on crystalline structures and thermodynamic properties. Real-world metallurgically relevant systems such as non-equilibrium processing, additive manufacturing, casting, and mechanical alloying are underrepresented. New solutions, such as federated learning and transfer learning

models, which allow AI models to be trained on distributed data without sharing data, can be used to solve confidentiality and data ownership challenges. Moreover, worry quantification and active learning methods can address high-value data regions, in which specific experiments can be targeted to maximize the value of limited datasets.

6.3 Model Interpretability and Physical Transparency

The black-box nature of most machine learning models, particularly deep neural networks, is one of the most straightforward criticisms of AI applications in metallurgy. Although these models are very good at recognizing patterns and predicting them, they do not usually provide physical information about what happens behind the scenes in material behavior. Metallurgical processes, such as precipitation hardening, recrystallization, and phase transformations, are governed by well-known thermodynamic and kinetic principles. Without the inclusion of these physics-based constraints in AI models, the models may exhibit non-physical correlations and overfitting. Recent developments have attempted to address this drawback using Physics-Informed Neural Networks (PINNs) and hybrid ML-physics models. The governing equations, boundary conditions, and conservation laws were directly integrated into the structure of the neural network, and the neural network was guaranteed to make physically consistent predictions. Moreover, explainable AI (XAI) methods, including Shapley Additive Explanations (SHAP) and Local Interpretable Model-agnostic Explanations (LIME), are increasingly being applied to identify the microstructural features or process parameters that have the greatest effect on the material results, which increases the accuracy of the model results and provides practical suggestions to metallurgists.

6.4 Computational Costs and Efficiency.

Such high-fidelity metallurgical simulations, including molecular dynamics (MD), phase-field, and finite element (FEM) simulations, can be computationally intensive. When combined with a deep learning architecture or multi-scale digital twins, the computational cost increases exponentially. Deep neural networks may be prohibitively expensive to train on large datasets or to perform high-throughput simulations in a multi-dimensional parameter space owing to energy or time costs.

To solve these issues, studies are underway to research the following:

- Surrogate modeling: In surrogate modeling, ML predicts the results of simple-to-code physics-based simulations with nearly the same precision as the actual simulations.
- Transfer learning and model reuse enable pre-trained models to be fine-tuned to new alloy systems with minimal retraining.
- Parallel and quantum computers can significantly accelerate training and simulation convergence for large-scale metallurgical problems. Such approaches are leading to a new direction in Green AI, including energy-efficient computations and sustainability in data-driven metalworking.

6.5 Standardization and Interoperability.

Data standardization and interoperability among experimental, computational, and AI platforms have become major challenges for the metallurgical community. Various laboratories use different measurement procedures, software packages, and metadata standards, which make data integration and model reproducibility challenging.

The absence of standard metadata, such as standardized names to denote grain size, dislocation density, or impurity concentration, prevents the consolidation of information into holistic learning systems. New efforts, including FAIR data principles (Findable, Accessible, Interoperable, and Reusable (FAIR) data principles, propose systematic data management and are slowly being adopted in metallurgical informatics. It is necessary to develop ontology-based data schemas, common data exchange protocols to support cross-platform AI processes, and coherent metallurgical databases.

6.6 Ethical, Environmental, and Security Issues

The rapid development of AI in the metallurgical industry raises ethical and security concerns. Issues such as data privacy, algorithmic bias, and unfair access to computational resources should be handled with care. AI-controlled industrial machines can be hazardous when it comes to safety in the case of failure of algorithms or data stream corruption of furnaces, casting, or rolling mills. Therefore, cybersecurity, model validation, and human-in-the-loop control are key to effective AI-based metallurgy. Training AI models on a larger scale may require considerable energy on the environmental front, negating manufacturing efficiency gains. This has resulted in sustainable AI frameworks that focus on model compression, hardware usage efficiency, and data center carbon neutrality. Lastly, the implementation of AI should be in accordance with ethical governance systems, which should have transparency, accountability, and fair benefit distribution among metallurgical sectors worldwide.

6.7 Future directions in AI-driven Metallurgy.

Autonomous, interpretable, and sustainable systems will form the next generation of AI-enabled metallurgy system. Several disruptive trends have emerged: -

6.7.1 Physics-ML Hybrid Structures.

The combination of domain knowledge and data-driven learning is maintained at its core. First-principles simulations are used with machine learning inference to create hybrid models that produce predictive systems that are both accurate and physical. These structures will improve the prediction of the microstructure, control of the processes, and modeling of defect formation in complex alloys, such as Al-Mn-Zr-RE and Ni-based superalloys. Figure 11 shows the challenges of deep neural network hybrid structures, including balancing λ weights; however, evidence from computational methods for magnesium alloys shows that hybrids outperform pure ML by 15-20% in terms of accuracy for microstructure predictions.

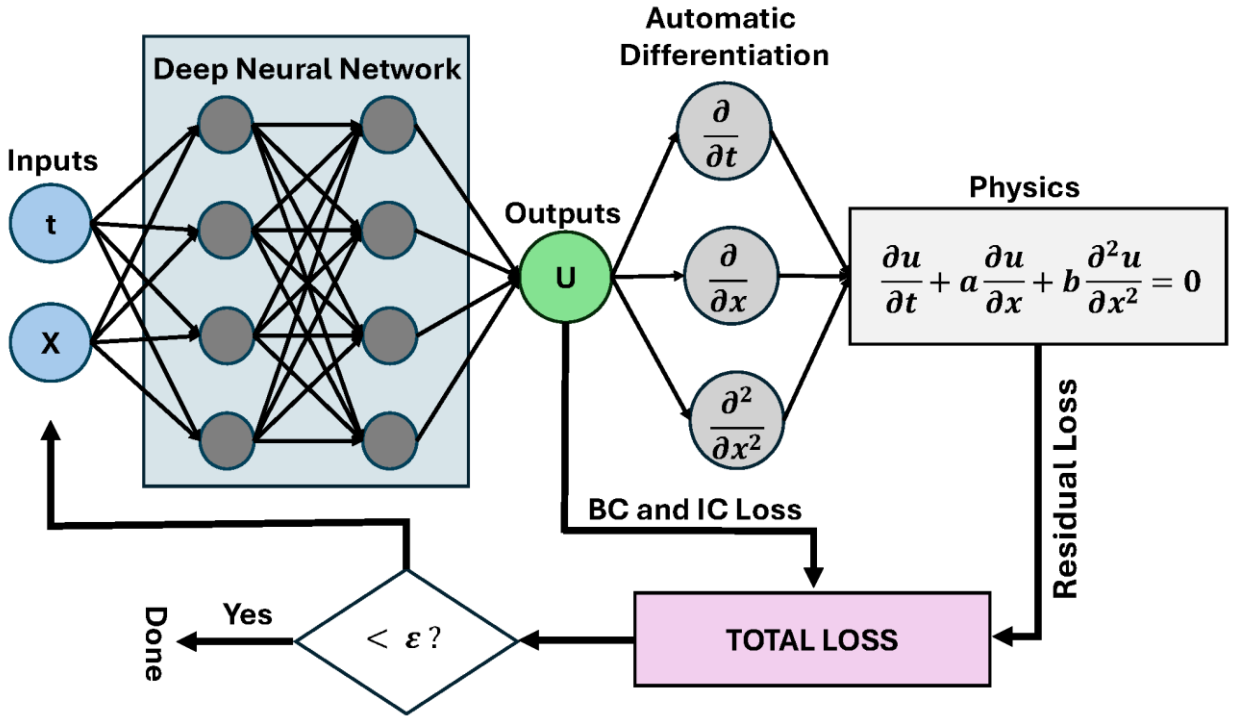

Figure 11: Deep Neural Network Hybrid Structures [140].

6.7.2 Neuromorphic and Quantum Computing.

The development of quantum computing is set to transform material discovery by addressing quantum-mechanical equations of large systems that are solvable only on quantum computers. Self-driving laboratories,

which are based on a combination of robotic experimentation, autonomous synthesis, and AI-guided characterization, are potent tools for accelerating alloy discovery. These systems can be combined with reinforcement learning and active learning loops to explore unexplored material spaces using their own designs. Figure 12 shows the future prospects diagram for AI in metallurgy, while neuromorphic chips, that is, chips that recreate the structure of human neural structures, provide energy-efficient architectures for ongoing metallurgical monitoring and adaptive control.

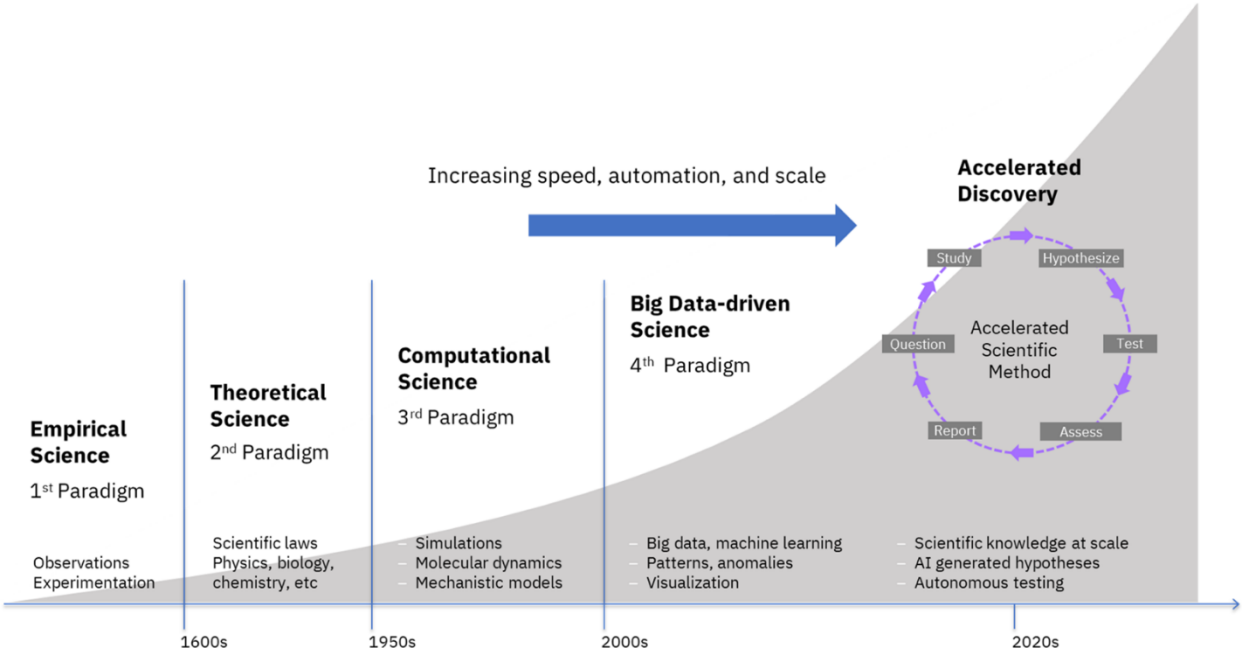

Figure 12 – Future prospects diagram for AI in metallurgy, including quantum computing [25]

6.7.3 Digital Twins and Real-Time Process Optimization

Digital twins will transform into dynamic models instead of mere impersonations, and they will be further upgraded with AI features linked to process feedback, enabling them to learn in real time. Digital twins dynamically optimize parameters in high-temperature processes, such as continuous casting or additive manufacturing, to reduce defects at the expense of reproducibility and energy efficiency. AI-based life-cycle analytics will help metallurgists produce alloys and processes with the lowest waste and recyclability. The creation of Circular Metallurgy 5.0, which incorporates green AI, renewable energy, and smart resource management, will be significant in ensuring that industrial ecosystems are carbon neutral [114].

7.Concluding Remarks

The combination of computer modeling and machine learning with metallurgy is a breakthrough in the data-oriented, predictive, and autonomous design of materials. These methods have shown the ability to overcome more complex alloy systems, not only by accelerating microstructure–property knowledge but also by optimizing processing paths and decreasing experimental loops. Most machine learning models can now forecast mechanical performance more accurately with heterogeneous data, and new algorithms, such as convolutional neural networks, can provide detailed information on microstructural trends that require vast amounts of expert interpretation. Mechanistic and physics-based simulations (phase-field models and physics-informed machine learning) complementarily form a formal basis for establishing the connection between processing variables, microstructure evolution, and end material behavior. Collectively, these instruments provide the context of a strong paradigm whereby metallurgical innovation becomes a process of repetition and discernment, and is very effective.

The shift to AI-driven metallurgy is associated with major challenges, namely data completeness, multiscale integration, model interpretability, and the computational cost of high-fidelity simulations, which remain significant. Nevertheless, a combination of materials science, data science, and computational engineering is rapidly moving towards predictive metallurgical systems and self-optimization. It is projected that next-generation materials processing will focus on merging autonomous testing and multi-physics simulations with adaptive machine learning-based architectures, which will radically change the workflows of alloy design, manufacturing, and sustainability.

Recommendations

Future studies should focus on the logical transition of basic prediction exercises to complete physics-based modeling. The first step involves creating effective regression models that can be used to predict the mechanical properties of alloys and hybrid methods that combine empirical evidence with mechanistic knowledge of dispersion-strengthened systems. Future work should build on microstructure-oriented simulations, convolutional neural networks to analyze quantitative images, machine learning to assess the distribution of precipitates, and data-driven optimization to ease sintering parameters and enhance alloy performance. At the latest stage, one should focus on computational and physics-based models, such as phase-field simulations of microstructure development, models of phase transitions coupled with mechanical responses, and machine learning systems that can predict thermal stability and long-term behavior based on a combined computational-experimental dataset. Together, these directions form a single path toward multiscale, AI-driven, and complete metallurgy.

As a strategic direction, the field must support multidisciplinary research among metallurgists, computer scientists, and systems engineers; create open, high-quality metallurgical databases; and scale up training in materials informatics with concerns over sustainable and ethical AI practices. Collaboration with the industry and public sector can facilitate the faster introduction of AI-based metallurgical technologies, whereas strict validation patterns are necessary to guarantee not only physical fidelity and robustness but also the bias-free behavior of predictive models. Thus, the industry will be able to advance prescriptive intelligence and complete autonomous metallurgical ecosystems as part of Industry 4.0.

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