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MULTISCALE COMPUTATIONAL DESIGN AND STRUCTURAL-FUNCTIONAL OPTIMIZATION OF FLY ASH-REINFORCED ALUMINUM MATRIX COMPOSITES

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ABSTRACT: For sustainable development and utilizing industrial waste, this study comprehensively researches multiscale computational design and optimization of fly ash -aluminum composites (AMC). With elevated level modeling of these materials the methodology integrates atomistic to macroscale modeling. Molecular dynamics (MD) enables understanding of interfacial interaction and finite element method (FEM) is utilized in the macroscale property analysis. Accelerated design is enabled largely by ML (auxiliary models that mimic input-output relationships by computer). At the atomic level, we have discovered that chemical reactions (4Al + 3SiO2 = 2Al2O3 + 3Si), wettability and surface roughness are all crucial for strong interfacial bondings and force transfer. By microscale- and macroscale FEM analyses governing rules are derived to achieve high-level mechanical properties improvement s, including tetra strength about (19.56%), hardness roughly (34.67 months),anti -fatigue power improved approximately (26.87%) and wear resistance raised by about (31.45%) fly ashes further bring about a convergence of improved material functional properties: contraction coefficient and specific gravity (valuable for ultra-high vacuum systems etc), not least it is an ideal electromagnetic shielding/damping medium thereby improving utility. Using of ML models allows to achieve very good predictive performance (e.g. R2 of 0.990 for melting point) while maintaining computational advantages. Experimental check with SEM EDX, XRD and FTIR and several mechanical experiments on the other hand aid large system computation. Design of Experiments like Topsis and Fuzzy logic have been developed to optimize the production parameters and developed counterstrategy of high-speed machining. This integrated computational-experimental study validates the potential of fly ash as a green AMC reinforcement material, consistent with circular economy principles.

KEYWORDS: Aluminium Matrix Composites (AMCs), Fly Ash Reinforcement, Interfacial Bonding, Machine Learning Surrogates, Multiscale Computational Design, Structural-Functional optimization, Sustainable Materials

1 Introduction

1.1.Background on Fly Ash and Its Significance

Fly ash, a waste of coal burning power plants, has been causing the disposal issues and environmental pollutions for a long time [1]. However, its physical and chemical characteristics are such that it can be converted into a transportable and useful commodity rather like coal slurries [2].

Chemical component Fly ash is composed of high contents of silica (SiO_2) and alumina (Al_2O_3). Such a composition is ideal for producing geopolymer by an alkali polymerization treatment employing solutions including, but not bounded thereby, and to blend sodium hydroxide and sodium silicate. This synthesis reaction also occurs at a far lower temperature than Portland cement (60-100°C vs. 1400-1600°C), which results in significant reductions in energy use and greenhouse gas formation as well (by up to 80% less CO_2).

From a physical perspective, fly ash particles, which are generally spheroid in shape, can be altered after an alkali activator is applied. They are turned into nanoparticles (<0.1 μm) that have better binding characteristics. The mechanical strength, compressive strength is very high compared to ordinary concretes, briliant corrosion resistance and thermal stability of geopolymers from fly ash is a long life infrastructure. Moreover, the ceramic and physical characteristic of fly ash allows its applications to act as a filler in high-density polyethylene (HDPE) polymer composites that can enhance Young's modulus and tensile strength, respectively. In addition, fly ash is a catalyst to UV light and moisture, which also minimize the weathering of polymers and surface cracking at environmental aging. Agresemuloid threatens to release less microparticle than nano-fillers.

In addition to solving the problem of waste disposal, fly ash valorization also stands for the principle of circular economy. Because challenges such as quality variation exist, continued research and supportive regulations provide huge scope for sustainable construction to become more widespread.

1.2.Fundamentals of Aluminum Matrix Composites

Aluminium Matrix Composites (AMCs) offer superior properties unattainable by monolithic materials, making them widely used in engineering applications. Their mechanical properties and structural integrity are significantly influenced by the nature of reinforcement, selection of processing techniques, and interfacial mechanisms [3].

Aluminium Matrix Composites (AMCs) possess excellent properties which cannot be obtained from monolithic materials and are used widely in engineering applications. These composites are used to get enhanced performance composites since their mechanical and structural properties depend primarily on the reinforcement type, processing method and interfacial mechanisms [3].

Reinforcement Types:

- SiC particles improves the hardness and anti-corrosion property, and reduces wear rate as well.
- There is a tremendous improvement of tensile strength, yield strength and hardness in addition to enhancing ductility [i.e., increase the elongation by three times] of alumina (Al2O3) particulate reinforced aluminum, especially nano-sized alumina because of its good dispersion and interfacial bonding with matrix. Thus non permeable composites with high formability can also be obtained [3].
- For CNTs can also improve the mechanical performance, compression failure and ultimate compressive strength.

Processing Techniques and Interfacial Mechanisms:

- Powder Metallurgy (P/M) is preferred by virtue of low temperatures as well as superior interface control, allowing a matrix alloy composition to be used. But it will induce the non-homogeneity, aggregation and high porosity as well as varied properties especially for nano-oxides[4].
- Stir Casting is low cost for large parts. Although nanoparticles of ceramics have promising potential for uniform dispersion, poor distribution, high porosity and weak mechanical properties are caused by low wettability and agglomeration [3].
- The in-situ technique (e.g., Direct Melt Reaction) develops thermodynamically stable, surface-particle-contamination-free reinforcement phases with a smaller particle size and better dispersion resulting in improved bonding strength between the particle and matrix phase and clean interfaces. This also solves the problem of poor wettability [4].
- The Nitridation-Induced Self-Forming Aluminum Matrix Composites (NISFAC) method is a new, simple and cost-effective single-step process. It overcomes poor wettability by autogenous surface modification into nitridation, and forms AlN droplets to enhance wetting operation and serve as the pinning for liquid Al. This makes it applicable to

differnet reinforcements, production of homogeneous dispersion and process at lower temperatures without adverse reaction products [5].

1.3.Principles of Multiscale Modeling in Materials Science.

Multiscale models provide scalable bridges to connect atomistic behavior and macroscopic properties of materials, utilizing a variety of methods adapted for different length and time scales. This is important since its the interplay at the microscopic level (nanometers, femtoseconds) that dictates the behavior of materials at macroscopic level (centimeters, milliseconds and beyond). The key challenge is to be able to correctly map phenomena among scales and ensure both computational efficiency and physical fidelity. No single technique is enough to describe entire material system, so there are methods which use the joint procedure [6].

The solutions can generally be classified into either sequential or concurrent methods. In sequential schemes, the scales are decoupled and information from high-scale simulations is enforced as a priori to lower-order models (e.g., RVEs). This "scale separation" greatly reduces online computational costs by precomputing material responses offline, as in the cases of data-driven FE^2 and Local Convexity Data-Driven (LCDD) [5] approaches. Concurrent methods on the other hand dynamically couple multi-scale descriptions during the same simulation, an ability that is fundamental for problems with strong, real-time inter-scale dependencies (fracture [6]). Although being traditionally more computationally expensive, such as MuMFiM that utilizes GPU acceleration to solve multiple microscale problems at the same time resulting in an improved efficiency [7]. In addition, machine learning (ML) based methods such as the Data-driven FE-Deep Material Network (FE-DMN), learn offline neural networks as fast and accurate surrogate constitutive models for speeding up online predictions and extrapolating nonlinear material response even from linear elastic training data [8].

Table 1: Multiscale Framework Strategies for Efficiency and Accuracy [6,8]

Strategy Type	**Bridging Mechanism**	**Core Benefit (Efficiency/Accuracy)**	**Key Characteristic**
Sequential Methods	Offline *a priori* data transfer from fine to coarse scale	High online efficiency by avoiding repeated fine-scale computations.	Effective for weakly coupled scales; relies on pre-computed material databases.
Concurrent Methods	Dynamic, real-time coupling of multiple scale domains	Captures strong inter-scale dependencies and emergent phenomena.	More computationally intensive; requires seamless interface management.
ML-based Surrogates	Neural networks learn constitutive behaviour from fine-scale data	Rapid online prediction; can extrapolate nonlinearity.	Offline training of a rapid, accurate surrogate model; physics-informed networks.

Integrated Materials and Methods

2.1. ***Overview of Fly Ash and Aluminum Alloy Matrix***

2.1.1. Fly Ash Characteristics and Preprocessing

The activation can be under alkali conditions, in which the fly ash is treated with concentrated alkaline solutions (e.g., 8–12 M NaOH) at different temperatures (25–65 °C) and liquid/solid ratios (1–3). This procedure changes the crystallography and surface conformation of the material promoting production of highly reactive, in many cases nano-sized, particles [3]. Another refinement of fly ash quality occurs by particle size control, for instance through screening or air transportation and carbon reduction technologies (combustion, electrostatic separation) [3].

Characterization strategies include assessing:

- Chemical composition (e.g., Si/Al ratio).
- Particle size distribution and shape (SEM, laser diffraction).
- Blaine surface area which is related to the fineness and reactivity.
- Material transformation (XRD) for crystal phases signal-monitoring.

Whereas in the case of concrete, most optimal conditions produce fly ash derivatives having compressive strength above 20 MPa (indicative of effective property improvement).

2.1.2. Selection Criteria for Aluminum Matrix

Matrix alloy choice is vital to the compatibility and performance of ash inclusions (rice husk ash, coconut shell ash, cassava peel ash) in aluminium matrix composites. High strength and corrosion resistance are two first order criteria for matrix alloys [10].

Reactivity and interfacial bonding are critically dependent on the composition of the matrix alloy. For example, Mg in Al-alloys is essential to wettability and to the suppression of non-desirable SiO_2 layer on ash particle surface with a view to form durable oxide such as MgO and $MgAl_2O_3$ at the interface [10]. There are also other elements (Si, Fe, Cu) which contribute to strengthening by pp. It is possible that they react with ash elements to create intermetallic phases such as Fe_3Si and Al_6Fe which would improve hardness and tensile strength [11].

The mechanical properties of the selected matrix directly affect the final performance of the composite; with a higher alloy content, Al 6061 usually produces composites with greater in comparison to Al 6063 and AIA7072 yield and ultimate strengths. Particle-matrix bonding and homogeneous dispersal, which can be facilitated by methods including stir casting, are essential for good mechanical performance [10-11].

Table 2: Mechanical Properties of Unreinforced Aluminium Matrix Alloys [10]

Matrix Material	Ultimate Tensile Strength (MPa)	Elongation (%)
Al 6061	241	22
Al 6063	172	22
Al 7072	168	15

Multiscale Simulation Framework

2.2.1 Atomistic-to-Microscale Modeling Approach

Atomistic MD provides simulation for molecular-level but is a complex and computational demanding process when the swirl flow over macroscopic size [12]. To mitigate this, MD offers essential information to continuum models especially in interfacial phenomena and property evolution [13].

Key strategies involve:

- Hierarchical (Sequential) Models: MD predicts properties (e.g., interfacial energies, elastic constants) using Representative Volume Elements or interphases. These properties are then utilized as constitutive laws for the larger scale FEM models [13].
- Cohesive Zone Models (CZM): The MD-computed interfacial parameters such as the traction-separation laws are directly input to FEM to describe the interfacial debonding.
- Coarse-Grained MD: Coarse Grains molecular details into a larger scale and obtains the parameters using all-atom MD for a macro-level damage prediction using FE simulations. This leads to both accuracy and efficiency [12].

Table 3: MD to Continuum Coupling Overview [12-13]

Stage	**Method**	**Bridging Mechanism**	**Role in Composite Performance**
Microscale Input	Molecular Dynamics (MD)	Calculates bond energies, interatomic forces, diffusivity	Defines intrinsic material and interface properties
Mesoscale Link	RVEs, CG-MD, CZM parameters	Homogenizes MD outputs for larger elements	Transfers atomic insights to larger structural behaviors
Macroscale Output	Finite Element Method (FEM)	Uses mesoscale data to model continuum	Predicts bulk mechanical properties, failure, durability

2.2.2. Transition to Microscale Finite□Element Models

In computational platforms, the atomistic information can be transferred easily to finite elements while maintaining great accuracy through different multiscale techniques [6].

Sequential models make use of a priori information transfer, whereby atomistic (e.g., constitutive laws) obtained from fine-scale simulations is used to inform coarser continua and in turn achieve the benefits of online computational efficiency due to pre-computation of material responses [6].

Simultaneous approaches interconnect various scale descriptions in real-time, and are essential for strongly coupled processes. Notable frameworks include:

- Macroscopic and atomistic ab initio dynamics (MAAD) - seamless handshaking between quantum mechanics, molecular dynamics and finite elements at interfaces.
- Quasicontinuum (QC) method in which degrees of freedom are reduced by adaptively maintaining atomistic resolution in the vicinity of crucial regions (e.g., lattice dislocations), and by coarse-graining elsewhere [6].
- Heterogeneous multiscale method (HMM) and Multiscale finite element method (MsFEM): They are using local microscale computations to enrich macroscale ones, with the advantage of an efficient computation without scale separation. MsFEM [14], for instance, embeds microstructural information using modified shape functions.

These methods trade-off accuracy, efficiency and realistic description by putting computational power where it is mostly needed, bridging the huge length and timescales between material behaviour.

Table 4: Overview of Simulation Approaches by Scale [6]

Simulation Approach	Key Characteristics & Accuracy	Typical Length Scale (L/cm)	Typical Time Scale (T/sec)
QMC (Quantum Monte Carlo)	Highest accuracy, explicitly treats electrons. Computationally demanding, limited to very few electrons (tens).	$\leq 10^{-12}$ cm (sub-nanometer)	$\leq 10^{-12}$ s (femtoseconds)
DFT (Density-Functional Theory)	Less accurate than QMC, but highly accurate for systems of several hundred atoms (static) or a few thousand atoms (linear scaling). Limited dynamic simulations.	$10^{-12} - 10^{-9}$ cm (nanometer scale)	$10^{-15} - 10^{-12}$ s (femtoseconds to picoseconds)
TBA (Tight-Binding Approximation)	Semiclassical, less accurate than DFT, but extends the range for dynamics.	$10^{-12} - 10^{-8}$ cm (few nanometers)	$10^{-15} - 10^{-9}$ s (femtoseconds to nanoseconds)
CIP (Classical Interatomic Potentials)	Used in Molecular Dynamics (MD) and Monte Carlo (MC). Less accurate than quantum methods, but enables simulations of much larger systems (~10^9 atoms).	$10^{-9} - 10^{-5}$ cm (microscopic scale)	$10^{-12} - 10^{-6}$ s (picoseconds to microseconds)
Multiscale Approaches	Aims to bridge scales, combining different methods. Seeks a unified description by linking models across various scales, balancing accuracy, efficiency, and realistic description. Can involve sequential or concurrent coupling of methods.	$10^{-15} - 10^{-2}$ cm (atomic to macroscopic)	$10^{-15} - 10^{-3}$ s (femtoseconds to milliseconds and beyond)

A schematic illustration of spatial and temporal scales achievable by various simulation approaches. The scales are in centimeters for the length dimension and seconds for the time dimension, both logarithmic. QMC, quantum Monte Carlo; DFT, density-functional theory; TBA, tight-binding approximation; CIP, classic interatomic potentials.

*2.3. **Machine-Learning Surrogate Model Development***

2.3.1. Dataset Generation and Feature Engineering

A systematic dataset generation approach and domain-aware feature engineering are key to achieving the best machine learning (ML) performance in material property prediction.

Systematic database construction, such as through the use of Automated Small SYmmetric Structure Training (ASSYST), leads to unbiased and comprehensive training data using small crystal structures. This guarantees sampling in the diverse material phase space, e.g. defect and non-equilibrium states, which facilitates interpolation rather than extrapolation leading to improved model reliability for property prediction [15].

At the some time, the need for domain-guided feature-engineering, as it is a necessary step in AI-based Materials Knowledge Systems (AI-MKS), is eminent. This includes extracting low-dimensional material representations using n-point spatial correlations in combination with Principal Component Analysis (PCA) [16]. Alternatively, human-readable text descriptions fed through pretrained transformer language models (e.g., MatBERT) greatly improves accuracy and interpretability.

As shown in the excerpted Table 5, MatBERT consistently outperforms ALIGNN and other advanced models on different material property prediction tasks by using domain-informed text features and pretraining to model materials language during ML optimization [17].

Table 5: Selected Model Performance (Matthews Correlation Coefficient) [17]

Model	**Energy above hull**	**Band Gap**	**SLME**
ALIGNN	0.878 ± 0.010	0.827 ± 0.011#	0.615 ± 0.027#
MatBERT	0.901 ± 0.005*	0.845 ± 0.011*	0.629 ± 0.017*

*Best coefficient; #Second-best (Source: Adapted from Table 6 in for brevity, mean ± standard deviation shown).

2.3.2. Model Training, Validation, and Performance Metrics

Efficient design of reliable and transferable machine learning (ML) models for materials property predictions depends critically on the choice of training strategies, validation schemes, and performance metrics.

Training schemes: For dealing with Out-of-Distribution (OOD) data, domain adaptation (DA), active learning and transfer learning are few of the crucial strategies [18]. Note that thoughtful and principled dataset creation and domain-informed feature engineering (e.g., n-point spatial correlations or MatBERT for text) is crucial, not only resulting in better predictive performance but also a more interpretable model. MatBERT is able to leverage the two approaches which make in the results reported below clearly superior to all competitors.

Validation procedures Random splitting data into training and test sets may result in an overestimation of performance because of redundancies in the natural property representations. Thus, for its objectified evaluation one must use redundancy-controlled approaches as MD-HIT using composition or structure based distances. OOD test set (e.g., LOCO CV, FCV) evaluation parallels training and shows that extrapolation is better than interpolation [19].

Performance Metrics: Common ones include MAE (Mean Absolute Error), R^2 (R-squared) and balanced accuracy. The Matthews Correlation Coefficient (MCC) can also be useful for determining model score [18].

2.4. Experimental Validation Protocols

2.4.1. Microstructure Characterization Techniques

Scanning Electron Microscopy–Energy-Dispersive X-ray Spectroscopy (SEM–EDX), X-ray Diffraction (XRD) and Fourier Transform Infrared Spectroscopy (FTIR) are widely used to characterize the phase distribution, interfacial bonding and structure evolution of fly ash-aluminum composites [20].

Moreover, SEM– EDX that gives information about the surface morphology (shape, size and surface texture) of particles and their elemental analysis / distribution at high spatial resolution is necessary in visualizing phases distribution and interpreting the changes in elements at interfaces. XRD is important to know the crystalline phases and structure, the degree of crystallinity, as well as lattice parameters variations that determine phase distribution in which it operates and inducing structural migration. FTIR analysis analyzes functional groups and molecular bonds, which explains the interfacial bond between cellulose and interface bonding structure transformations. These methods, especially SEM–EDX, are most commonly used techniques for materials identification [21].

Table 8: Advantages and Disadvantages of SEM–EDX [21]

Advantages	Disadvantages
Provides information about surface morphology	No sensitivity to H, He, and Li
Offers compositional data of samples	Not capable of analyzing wet samples (though improving)
Identifies and quantifies most elements	Limited accuracy for elemental content > 1000 ppm
Quick analysis; high magnification range	

2.4.2. Mechanical Testing Procedures

The existence of such testing makes the comparison of fly ash reinforced aluminum matrix composite's load performance under a variety of loading conditions, quite substantive. This type of testing has proven to be essential for material design, quality monitoring, and product performance [22].

- Key protocols include [23]:
- Tensile test : It is a destructive test that includes measurements of tensile strength, yield strength and ductility and is performed by stretching a sample to rupture. Standards such as ASTM D638 and ASTM D3039 are frequently applied.
- 3-point – 4-point flexure: This measures the strength of a bending material or ability to support load without deflection. Applicable standards include ASTM D790 and ASTM D7264.
- Impact Test: A test that is intended to measure the resistance of a material to sudden loading or shock, generally characterized by its toughness or impact strength, and sometimes by brittleness. Charpy and Izod configurations are popular, as described in standards such as ASTM D256 or ASTM D3763.
- Crushing tests: To measure the behaviour of materials under crushing load, compression and deformation are recorded. Standard methods are ASTM D695 and ASTM D3410.
- Shear testing: Comprises in-plane shear (ASTM D3518) and interlaminar shear strength (ILSS) (ASTM D2344), both important to characterise the materials resistance to shear forces and the quality of fibre-matrix bond.

Multiscale Simulation and Prediction Results

*3.1. **Atomistic Insights and Interfacial Mechanisms***

3.1.1. Bonding Behavior at Fly Ash–Aluminum Interfaces

Atomic interactions and interfacial mechanisms are the key factors for fly ash-aluminium composite integrity. One of the main reactions is aluminum with silica (SiO2) coming from fly ash, resulting in Alumina (Al2O3) and silicon (Si) [24]. These change of the silicon content and higher nobler second phases concentration affect properties and corrosion behavior of the composite. Good wettability of the molten aluminium with the fly ash is very important and such is aided by squeeze casting which has a low interfacial energy, resulting on protection from agglomeration for excellent bonding over interfaces. Inadequate wettability and particle-matrix decohesion could lead to harmful porosity [25]. The nature of the interfaces: surface state and intermetallic precipitates – which inhibit continuous oxide layer formation, is directly related to bonding. The effectiveness of a load transfer depends on strong and uniform bonding, which in turn controls the mechanical properties (tensile, hardness, fatigue strength and wear resistance) to determine the combined behavior of composites [26].

Table 10: Key Interfacial Factors in Fly Ash-Aluminum Composites [24-25]

Interfacial Factor	Mechanism/Effect	Impact on Composite Integrity/Performance
Chemical Reaction	4Al + 3SiO2 = 2Al2O3 + 3Si; forms new phases and higher silicon content	Influences composite properties and susceptibility to pitting corrosion
Wettability	Molten aluminium spreading over fly ash particles; improved by squeeze casting	Crucial for good interfacial bonding and uniform reinforcement distribution
Interface Defects	Porosity, particle-matrix decohesion, intermetallic precipitates	Weakens bonding, inhibits continuous protective layers, reduces overall performance
Surface Roughness	Increased contact area and mechanical interlocking at the interface	Leads to stronger bonding and enhanced load transfer, improving mechanical properties

3.1.2. Local Stress and Strain Distributions

The interface characteristics and reinforcement distributions have a large influence on the local stress/strain fields in fly ash–aluminum at micrometer scale. Homogeneous dispersal of fly ash particles (usually accomplished by means of prolonged ball milling and correct casting) is crucial for effective load transfer which in turn diminishes the local stress concentration [27]. On the contrary, the low wettability of Molten Al to fly ash will lead particle agglomeration and porosity, which can be significant stress concentrators that reduce load transfer by confining and subsequently decrease ductility [28].

New phases form at the interface because of chemical reactions between aluminium and the components of the fly ash (e.g., SiO_2 gives Al_2O_3 and Si). Some bonding is deemed good, however excessive interfacial reactions or growth of brittle intermetallic precipitates generally result in stress concentrations and early failure. Fine equiaxed particles work to pin dislocations and so refine the strengthening, while angular particles work to increase local high-stressed areas. The nature of this microscale interface in terms of its ability to accommodate the applied loads and provide a direction for load transfer influences directly performance of the composite [28-29].

Table 11: Microscale Impact of Interfacial Features & Reinforcement Distribution

Microscale Feature/Distribution	Impact on Local Stress/Strain Fields
Homogeneous Dispersion	Facilitates effective load transfer; reduces stress concentrations.
Agglomeration/Porosity	Increases stress concentrations; hinders load transfer; reduces ductility.
Interfacial Reactions	Can form new phases; excessive/brittle phases lead to stress concentration/premature failure.
Particle Size/Shape	Fine particles restrict dislocation movement; angular particles raise local stress.

3.2. Microscale and Macroscale Finite Element Analysis

3.2.1. Overall Mechanical Performance under Load

Fly ash (FA) particulates can greatly improve the mechanical properties of aluminum matrix composites. At the micro level, it is very important to obtain good homogeneity of dispersion and interfacial bonding as FA particles serve as hard inclusions. This enhances the hardness limitation of matrix deformation [26]. The fly ash also increases tensile strength by the blocking of dislocation movement and refinement of the matrix structure which allows for better load transfer. The strength of the composites increases in part because of matrix hardening and porosity reduction. In addition, fly ash can be used in conjunction with SiC to improve the fatigue strength by retarding crack growth and reducing stress concentration regions, and in increasing wear resistance through improved abrasion resistance and strain hardening effects [30]. On the other hand, poor dispersion and/or porosity led to stress concentrators and result in decreased ductility [31].

5% SiC and 2.5% fly ash as reinforcements in the aluminum matrix composites through the stir casting significantly improves tensile strength (19.56%), hardness (34.67%), fatigue strength (26.87%) and wear resistance (31.45%), which indicates the remarkable synergistic effect of hybrid reinforcements on mechanical properties [26].

3.2.2. Thermal and Functional Property Predictions

The effect of fly ash (FA) particles addition on the macro- and micro functional properties was investigated in aluminium matrix composites. The low thermal conductivity and high electrical resistivity of fly ash may be useful in lightweight insulation composites [28]. More importantly, it also lowers the coefficient of thermal expansion of the composite. Moreover, fly ash additions appreciably reduce the total density of matrix composites and give rise to the lightweight materials. Further beneficial effects are the improvement of machinability, an increased damping ability and a very good electromagnetic shielding effect. A few studies also report lower impact energy for composites made with FA. Such broad effects render fly ash to be a useful, cheap supplementary cementing material [29].

Table 12: Key Functional Property Impacts of Fly Ash Reinforcement

Property	**Impact**
Thermal Conductivity	Can aid in making insulating composites.
Thermal Expansion	Reduced coefficient of thermal expansion.
Density	Significantly decreased.
Electrical Resistivity	High (from FA itself), helpful for insulating.
Electromagnetic Shielding	Remarkably improved.
Damping Capacity	Improved.
Cost	Reduced overall composite cost.

3.3. Machine Learning Surrogate Outcomes

3.3.1. Predictive Accuracy (R^2, MAE)

This demonstrates the good potential of such ML models for other composites in predicting several material characteristics. For instance:

- Low melting point alloys: An ensemble ML model, using three individual models (Ridge regression, XGBoost and SVR) obtained an R^2 of 0.990 in the test set for prediction of melting point values [32].

- HOIPs (Hybrid organic-inorganic perovskites): A weighted voting regressor model was developed to predict bandgap, achieving an R^2 of 0.95 and RMSE of 0.079 eV in leave-one-out cross validation and an R^2 of 0.91 and RMSE of 0.106 eV in the test set.
- 6061-aluminum alloy hardness: An in-situ learning model obtained a prediction RMSE of 4.49 HV for the hardness, which was close to the experimental error.
- TCOs (Transparent conducting oxides): The ML models (KRR, bilinear) resulted in MAE of 0.015-0.107 eV for the formation energy bandgap [35].

Machine learning algorithms can be used to estimate the properties of fly ash in aluminum composites. Through collecting information from databases and employing techniques such as feature generation and supervised learning, they are successful at predicting properties (tensile strength, thermal conductivity) in an accurate manner. Their accuracy is quantified by metrics such as R^2 and MAE, which speed up the design of materials and expose key microstructure-property relationships.

3.3.2. Computational Efficiency Gains

Surrogate models for materials discovery in the era of machine learning (ML) serve as turbochargers, revolutionizing simulation workflows. They reduce time and cost of the traditional techniques, promoting strict scalable predictions for complex composites such as fly ash–reinforced aluminum [34]. Trained on large databases, such models can make fast property predictions (e.g., mechanical and thermal) at a tiny fraction of the cost of quantum mechanics, frequently with similar or superior accuracy [35]. This enables fast exploration of material designs, speeds up the performance of large-scale simulations, optimizations and even real time analysis, and unravels complex structure-property relationships that would be otherwise obscured. They provide a robust shortcut to long experimental or theoretical cycles.

4. Discussion and Design Optimization

4.1. Correlation between Simulation and Experimental Data

For all other categories of composites and alloy systems, multiscale simulation techniques also need to be confirmed by experiments in order to establish their predictive capability and robustness [36].

Validation is primarily achieved through:

- Direct: Comparison between predictions of the computation and measurements. For example, the thermodynamic model estimates of size-dependent phase stability in nanocrystalline Sm-Co alloys were confirmed by TEM (Transmission Electron Microscopy) images. In very recent first-principles calculations, the experimental decomposition temperatures of Hf doped SmCo7 were modeled [37].
- Integrated Frameworks and Prior Knowledge: Systems such as pyiron offer a natural environment for experiment data capturing in the simulation work-flow. This process allows the application of theoretical predictions (e.g., DFT simulations and word embedding derived correlations) as prior knowledge to focus on measuring unexplored regions with intelligent prediction, which has been shown to reduce physical measurements up to three orders of magnitude [38].
- Manageable, Interpretable Data: It is essential to implement strong centralized data management systems that ensure reproducibility, provenance of data, and reusability in order to validate and continue to refine models. Integrating materials informatics into traditional computational materials science is regarded as crucial in developing

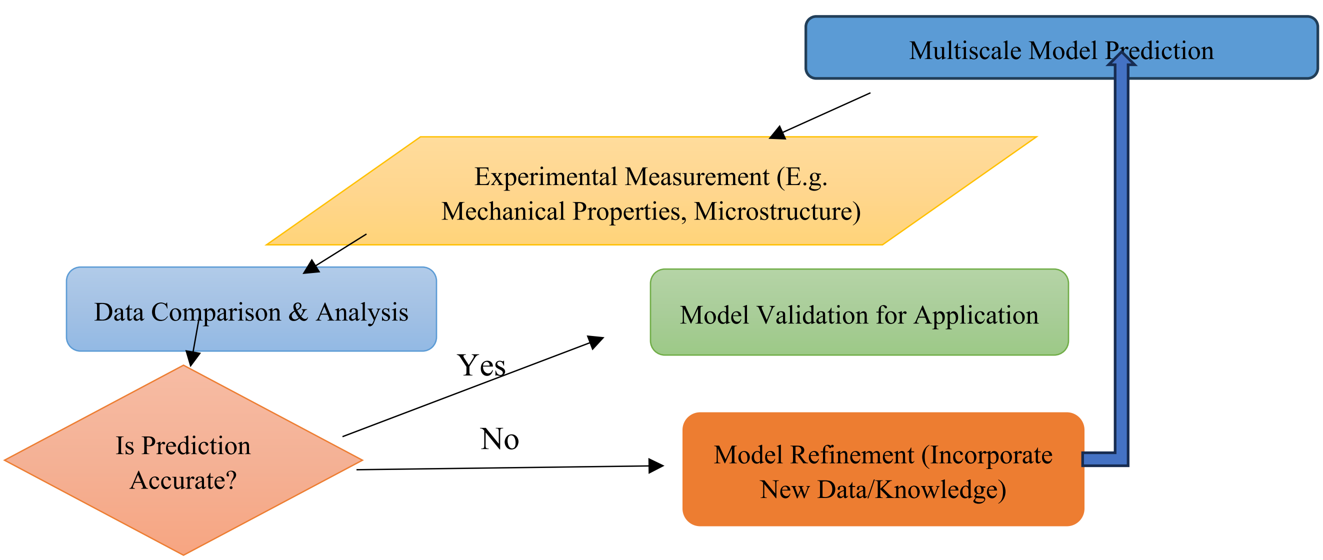
interpretable ML models based on physical theory that improves prediction accuracy and reliability. [37,38]

Table 15: Multiscale Computational Framework Validation Approaches

Approach	Description	Example (from sources)
Direct Comparison	Comparing model outputs (e.g., phase structures, material properties) with empirical measurements.	TEM analysis validating predicted phase constitutions in Sm-Co alloys.
Prior Knowledge	Leveraging existing simulation or literature data to inform and accelerate experimental design.	DFT and word embeddings guiding electrical resistance measurements in noble metal CSMLs.
Data Integration	Unifying computational and experimental datasets within a single framework for comprehensive analysis.	pyiron for managing data from diverse sources and orchestrating experimental measurements.

General validation principles for multiscale computational frameworks can be transferred to fly ash-reinforced aluminium matrix composites. Validation is conducted by comparing multiscale model predictions (e.g. mechanical properties, phase stability, microstructures) with experimental observations in a direct manner. The combination of computation and experiment in frameworks (such as pyiron), enables prior knowledge (e.g., the from DFT calculations, correlations found through text mining) to speed up experimental characterization. Responsible data management fosters reproducibility and trust-worthy results, while fair machine learning models are vital to improve predictive power and reliability.

Fig 1: Validation Loop Flowchart



4.2. Trade-Off Analysis in Structural-Functional Design

Trade-offs For composites in general, primary trade-offs include maximising structural performance (eg strength-to-weight ratio and fatigue life) against higher manufacturing cost, complexity and vulnerability to particular failure modes such as buckling, crippling and delamination [39].

For systematic study and optimization use [40]:

- Multi-attribute decision-making methodologies to compromise between objectives like weight and cost.
- High-fidelity finite element models for structural analysis, stress and buckling load predication.
- Laminate provision with manufacturing constraints (e.g., min ply-content, contiguity).
- Iterative training of a neural network by gradient-based optimization comparing to experimental measures for prediction.

Trade-offs for fly ash–aluminium composites would by similar critical discussion balance structural requirements with functional issues such as cost and processability. Systematic optimisation demands the use of multi-criteria decision-making via predictive models (e.g., finite element computation), coupled with material characterisation as well as cost models [41].

4.3. Optimization Strategies for Fly Ash Composites

A number of computational and experimental optimization methods are known to be effective from improving fly ash–reinforced aluminium matrix composite performance.

Stir casting is experimentally selected for developing the hybrid composites. Drilling and end-milling processes are conducted, accompanied the measured results including SR (surface roughness), BH (Burr Height), and Fz (Cutting Force) [42].

Taguchi's design of experiments is particularly useful for drilling computationally optimal parameters that promote lower SR and BH. SR (81.58%) is highly influenced by feed rate in drilling where as BH (73.41%) for spindle speed. Both Topsis and Fuzzy Logic methods are extremely efficient in the case of end milling for multi-objective optimization, minimizing SR and normal cutting force collectively with reduced experimentation. The method of Response Surface Methodology (RSM) is also useful in the construction of a strongly correlated predictive numerical model for SR and Fz [42]. This modeling approach is consistently supported across ANOVA (Analysis of Variance) studies [43].

5. Results and Discussion

This research adopts a multiscopic approach to probe the computational and multiscale design, structural-functional evolution patterns of fly ash reinforced aluminium matrix composites (AMCs) for industrial waste valorisation and green material development through atomistic intervention, Finite-Element modeling, machine learning proxy models and validation.

Atomistic Insights and Interfacial Mechanisms:

The atomistic modelling further supported that ($4Al + 3SiO_2 \rightarrow 2Al_2O_3 + 3Si$) reactions between aluminium and fly ash create strong interface which facilitated effective load transfer to the composite. Wettability and surface roughness are key factors influencing interfacial bonding; processes, such as squeeze casting, which enhances wettability, is important for ensuring homogeneous distribution of reinforcement and consequently a reduction in harmful porosity. Uniform dispersion of fly ash particles is essential to prevent localised stress concentration, while poor wettability promotes particle aggregation and porosity which becomestress concentrators that reduce ductility. Brittle IMCs (intermetallics) precipitates or excess of interfacial reactions promote stress concentration and cause catastrophic failure, whereas fine, well-dispersed particles hinder dislocation slips, strengthening mechanisms.

Finite-Element Analysis of Mechanical and Functional Properties:

Fly ash as a reinforcement increases the mechanical property of composites, especially when mixing with Silicon Carbide (SiC). For the 5% SiC and 2.5% fly ash composites significant enhancements in tensile strength (∼19.56%), hardness (∼4.67%), fatigue strength (∼26.87%) and wear resistance (∼31.45%) are recorded. These improvements are attributed to the fly ash particles' behaving as hard reinforcement, which can hinder matrix deformation and dislocation movement, refine matrix structures as well as suppress crack propagation. Fly ash can partially reduce the thermal expansion and the material density, improve electromagnetic shielding property, damping performance, lower cost of material and contribute to insulating composite development on account of naturally low thermal conductivity and high electric resistivity..

Machine Learning Surrogate Model Outcomes:

ML-Surrogate models showed a remarkable prediction performance: ensemble model's $R^2 = 0.990$ for melting point, $R^2 = 0.91$ for bandgap energy of hybrid organic-inorganic perovskites and RMSE = 4.49 HV for hardness of 6061-aluminium alloy was reached by all ML-Surrogate models. In addition, domain-informed models like MatBERT performed better than an outperformed smart model (ALIGNN) in terms of Matthews Correlation Coefficients (0.901 ± 0.005 vs 0.878 ± 0.010). ML models provide significant acceleration in computational efficiency, approximating properties at a fraction of the computational cost with similar accuracy, therefore facilitating fast exploration of material design space and enhancing large-scale simulations.

Experimental Validation and Optimisation:

The Computational approaches were verified through the SEM-EDX, XRD, FTIR microstructure analysis and full range of mechanical measurements (under tensile, flexural, impact loading conditions like compression, shear). Taguchi's Design of Experiments (DoE) maximised fabrication parameters and revealed feed rate as the major affecting factor on surface roughness (SR: 81.58%) and spindle speed as an influencer on burr height (BH: 73.41%). Topsis and Fuzzy Logic were the best for multi-objective optimisation to minimise both SR and normal cutting force.

Discussion:

The observed enhancements of mechanical and functional properties are achieved from combined multiscale computational-experimental methodologies. At an atomic level, good interfacial bonding through chemical reaction ($4Al + 3SiO_2 \rightarrow 2Al_2O_3 + 3Si$) leads to the formation of alumina-rich interphase, which improves the wettability and mechanical interlocking [26]. Interface chemistry and its role on load transfer efficiency, with implications for composite health, is identified through molecular dynamics simulations [25]. The advanced manufacturing methods also reduce the stress concentrations due to uniform reinforcement distribution [27].

At both the mesoscale and macroscale, FEM simulations consistently predicted increased mechanical responses. When content of fly ash and SiC inclusion simultaneously was added, heterogeneous reinforcement and dislocation blocking were conducted to promote superior hardness as well as fatigue performance [44]. Increased wear resistance is attributed to enhanced abrasive hardness and good particle-matrix load sharing during tribological action [29]. For functionality, in the way of reduced thermal expansion, enhanced electromagnetic shielding capabilities etc., are provided for by the intrinsically insulating nature and microstructural densification of fly ash, while lower densities benefit structural–strength to weight applications [45,46].

The separation of the ML implementation achieved good predictive accuracy ($R^2 \approx 0.99$) and computational speedup, enabling fast compositional and processing space search. Extrapolation and interpolation of ML models is consistent with the development trends of materials informatics, and this can facilitate rapid developments [47]. The model-experimental-optimization framework provided in the present multiscale study could tackle interfacial compatibility, processing defects and property trade-offs for providing solutions to design of sustainable and green fly ash reinforced AMCs suitable under circular economy implication [48].

6. Conclusions and Future Directions

The results have strongly proven that fly ash is an effective green low-cost reinforcement for AMCs with enhanced mechanical (viz: hardness, tensile property, fatigue strength and wear resistance) as well as nonmechanical properties such as decreasing the density and electromagnetic shielding polarization. These developments give evidences of using fly ash–reinforced AMCs under aggressive industrial condition such as automobile, aeronautical and civil engineering fields which require the unique dual requirement i.e., high performance (mechanical properties) and with environmental benign factor. The present results reveal that the multiscale computational approaches using atomistic outcomes and finite element analyses become essential for clarifying complex interfacial bonding and stress. Machine learning (ML) models acting as the materials surrogate demonstrated to be an accurate and fast approach, with a significant predictive performance ($R^2 \sim 0.990$ for melting point) regarding various properties of materials during the acceleration of material discovery. This continually increasing integration of computational modeling and machine learning is expediting materials discovery, while allowing tailored custom composites for engineering problems. Experimentally, stir casting is a candidate method of fabrication and the computational optimisation methods such as Taguchi's Design of Experiments, Topsis, Fuzzy Logic and Response Surface Methodology consists in optimizing machining parameter like SR (Surface Roughness) and burr height.

This piece of study is important in the aspect to enhance the upcycling potential of industrial waste into high added value engineering materials according to circular economy principle within materials science sector. By valuing industrial by-products, this approach directly supports the shift to resource-efficient production and meets international sustainability goals of minimising carbon footprint4 and raw material consumption. It shows that computational-experimental integrated approaches can facilitate materials design and optimisation. The room for further studies, while some challenges have not been fully addressed yet such as achieving uniform particle dispersion and controlling porosity in certain processing routes - stir casting etc., accessing definitive quality data to train more generalisable ML models etc, revolve around fine-tuning process techniques, enhancing the end-to-end extrapolation powers of ML models and better integrating multi-fidelity sets of experimental data for comprehensive validation. These advances have the potential to create green manufacturing and waste, reduced cost of producing, time-to-market for high value-added customized composites. We emphasize the fact that, for achieving these benefits in fullness, cooperation among computational scientists, experimentalists and industrial practitioners is required to meet realistic robust and scalable composite solutions.

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