Physics-Aware Multi-Agent AI Framework for Property Prediction and Design of Aluminium Alloys

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Abstract

A major frontier in aluminium alloy discovery is the development of intelligent systems that can automate complex material modelling and design tasks leveraging diverse knowledge, tools and capabilities. Such systems are very crucial for generating novel insights into aluminium alloy properties by iteratively refining the alloys prediction and discovery strategies, merging insights across the discipline to converge towards optimal physics compliant solutions. Large language models (LLM) have demonstrated significant potential in complex reasoning, strategic planning, coding, and workflow orchestration showing promising capabilities in materials analysis and property prediction including hypothesis testing, knowledge retrieval and multimodal reasoning. However, they face challenges in new alloy design and discovery due to out-of-domain knowledge, inability to perform physics-based simulations, restricted access to external sources, and reliance on potentially outdated knowledge.

In this work, we propose physics aware multi-agent LLM framework designed to address the unique challenges for property prediction, design, and discovery of aluminium alloys. The framework utilises an orchestrated network of LLM agents that performs automated knowledge retrieval and reasoning on integrated multi-modal data of heterogeneous nature of the process, experimental and simulation material dataset. To ground the models on physics laws and to support advanced simulation capabilities, the LLM agents are synergistically combined with Large Atomic/Molecular Massively Parallel Simulator (LAMMPS) for atomistic simulations.

Our work presents a series of experiments to demonstrate how our agentic system addresses various task in the aluminium alloy design, particularly through generating new physics via atomistic simulation, substantially reducing the need for human intervention. Specifically, we show that the model can integrate material properties from diverse sources, tackle multi-modal problems and solve multi-scale problems connecting microscale features to macroscopic properties.

Keywords: Large Language Model (LLM), Aluminium alloys, Agentic framework, Physics simulation.

1. Introduction

Aluminium alloys play an indispensable role across diverse industries, including aerospace, automotive, and renewable energy, owing to their favourable strength-to-weight ratio, excellent corrosion resistance, and versatile mechanical properties. Despite their broad application, the systematic design and optimisation of novel aluminium alloys remain challenging due to the complexity of alloy composition spaces and the extensive computational and experimental effort required. Conventional alloy design approaches frequently rely on iterative experimentation and

atomistic simulations, which are inherently labour-intensive and pose difficulties in scalability and reproducibility. Consequently, there is an increasing need for innovative methodologies capable of streamlining and automating these complex workflows, facilitating rapid and reliable exploration of alloy chemistries.

Recent advancements in artificial intelligence (AI), particularly the emergence of multi-agent orchestration systems and sophisticated machine-learning models such as Graph Neural Networks (GNNs), offer promising solutions to overcome traditional limitations. In this work, we present a novel multi-agent orchestration framework designed specifically for aluminium alloy modelling and simulation, leveraging autonomous computational agents specialised in research, simulation planning, molecular dynamics execution, data processing, and visualisation tasks. The proposed approach is demonstrated via agent-based simulations performed with Large-scale Atomic/Molecular Massively Parallel Simulator LAMMPS [1] and interatomic potential predictions derived from GNNs which was constructed and trained autonomously through agentic orchestration. We substantiate our methodology through targeted case studies that demonstrate its capabilities across multi-scale property prediction, structure–property relationship modelling, and atomistic visualisation, thus highlighting significant improvements in efficiency, reproducibility, and speed of discovery in aluminium alloy design.

2. Literature Review

Atomistic modelling with the LAMMPS remains the core for probing aluminium alloys at the nanoscale. Recent studies, such as the MD analysis by Wu and Zhang on Al-4 wt% Cu single crystals, have clarified orientation-dependent plasticity by correlating dislocation activity and stacking-fault evolution with macroscopic anisotropy [2]. Comparable LAMMPS investigations across Al-Mg, Al-Li and Al-Cu chemistries have mapped solute segregation, grain-boundary stabilisation and temperature-controlled precipitation, underscoring the simulator's ability to link atomistic events to bulk properties. Nevertheless, exhaustive sweeps over composition, temperature or defect space remain computationally prohibitive, and the heavy manual effort required for script preparation and data post-processing hampers throughput and reproducibility.

Addressing these constraints, the materials community is rapidly adopting AI-driven multi-agent orchestration frameworks that automate literature mining, simulation planning, execution and analysis. The MULTI-agent autonomous facilities scalable framework (MULTITASK) developed at NIST demonstrates how heterogeneous machine-learning agents can co-ordinate experiments facility-wide, optimising resource use while allowing researchers to "fail smarter" and learn faster [3]. Extending this concept to alloy discovery, the recently proposed AtomAgents platform integrates large language models with physics-aware agents that retrieve knowledge, generate LAMMPS inputs, launch simulations and analyse outputs, all within a closed-loop environment [4]. These frameworks highlight the transformative potential of agentic systems to standardise complex workflows, scale exploration across vast compositional spaces and ensure transparent provenance for every computational step.

Parallel progress in graph neural networks (GNNs) has furnished highly accurate, data-efficient interatomic potentials that can be embedded within autonomous pipelines. The E(3)-equivariant NequIP model, for example, attains near first-principles accuracy with up to three orders of magnitude fewer training structures than earlier ML potentials, enabling long-time, large-system molecular dynamics at minimal cost [5]. When coupled with multi-agent planners, such GNN surrogates serve as rapid predictors that flag high-uncertainty regimes and trigger targeted high-fidelity simulations only, when necessary, thereby optimising computational budgets while preserving reliability. Together, LAMMPS-level physics, AI-orchestrated autonomy and GNN-powered surrogacy define the contemporary frontier in aluminium-alloy modelling, offering an unprecedented route to scalable, reproducible and accelerated materials discovery.

6. References

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