Machine learning driven design of high-performance Al alloys

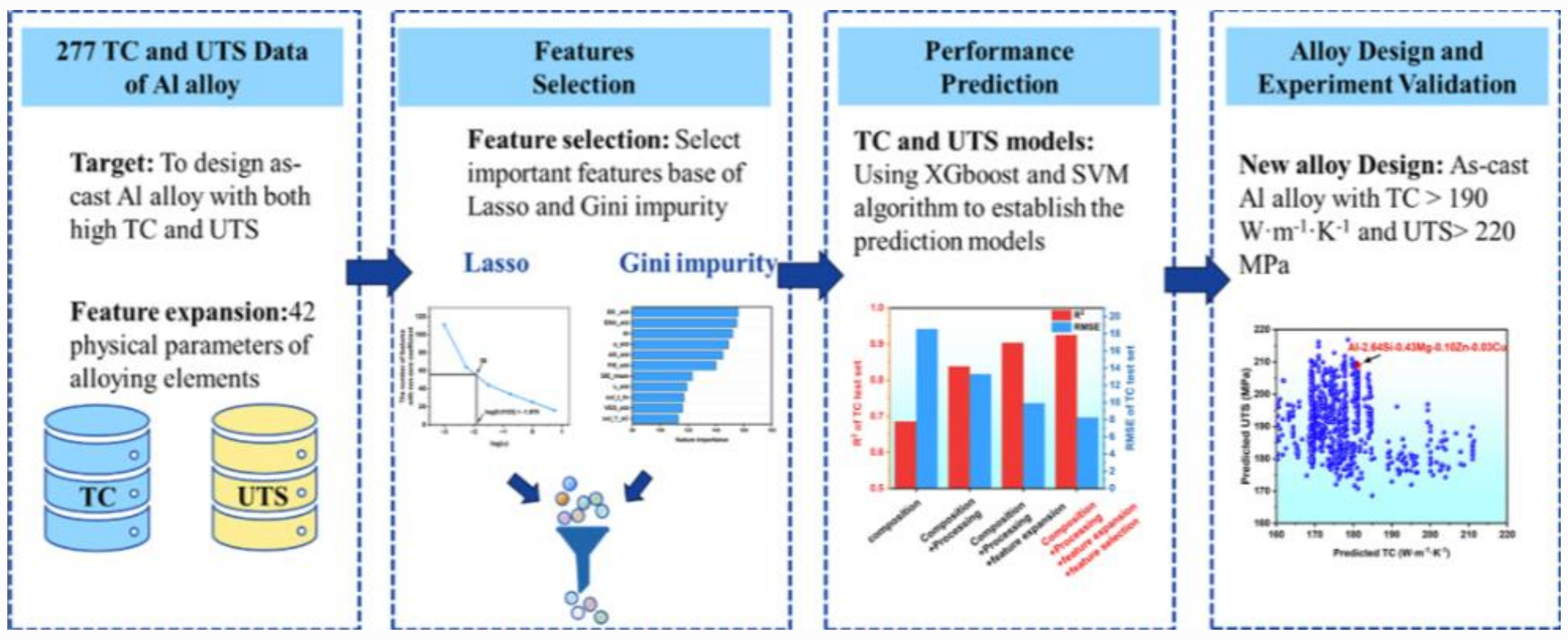
Ziliang Lu, Ishwar Kapoor, Yixiang Li, Yinghang Liu, Xiaoqin Zeng, Leyun Wang

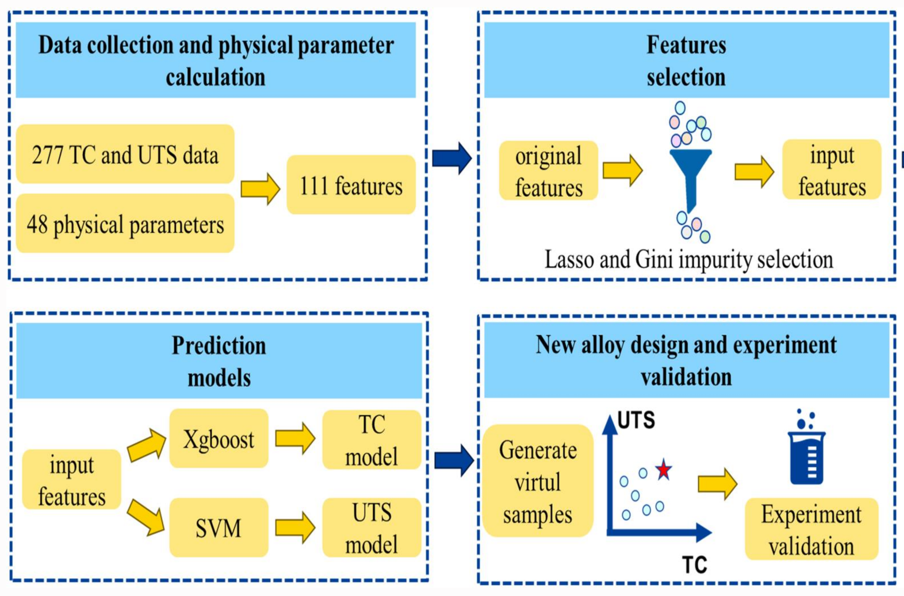
Introduction (problem)

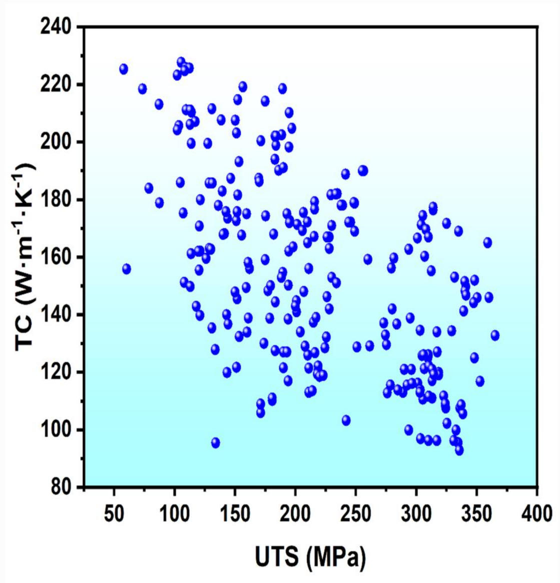
Engineers face a core challenge: making aluminium both strong AND thermally conductive — improving one usually harms the other

Trade-off comes from material physics (lattice distortion + particle structure)

This is difficult for humans to optimise manually → too many interacting variables





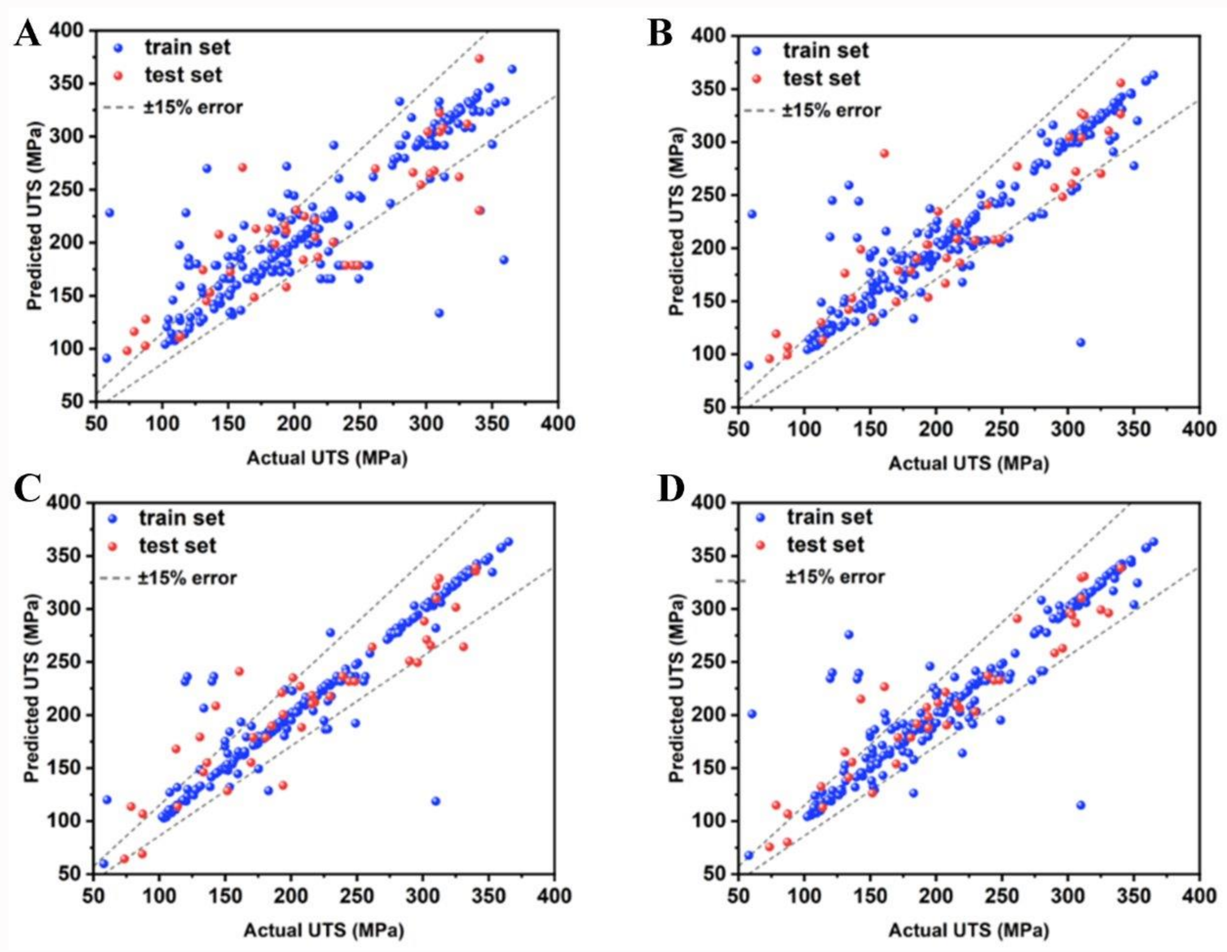


Methods (Human vs AI setup)

Humans: 277 past alloys compiled and understood using physics + domain knowledge

AI: builds models using composition + physical descriptors (atomic properties)

Hybrid approach: Human knowledge → features, AI → prediction + optimisation



Results (What AI achieved)

AI screened **hundreds of virtual alloys** and proposed anew composition

Real-world testing showed**~5% error → very close to prediction**

Key insight: AI can **reliably guide real material design, not just simulations**

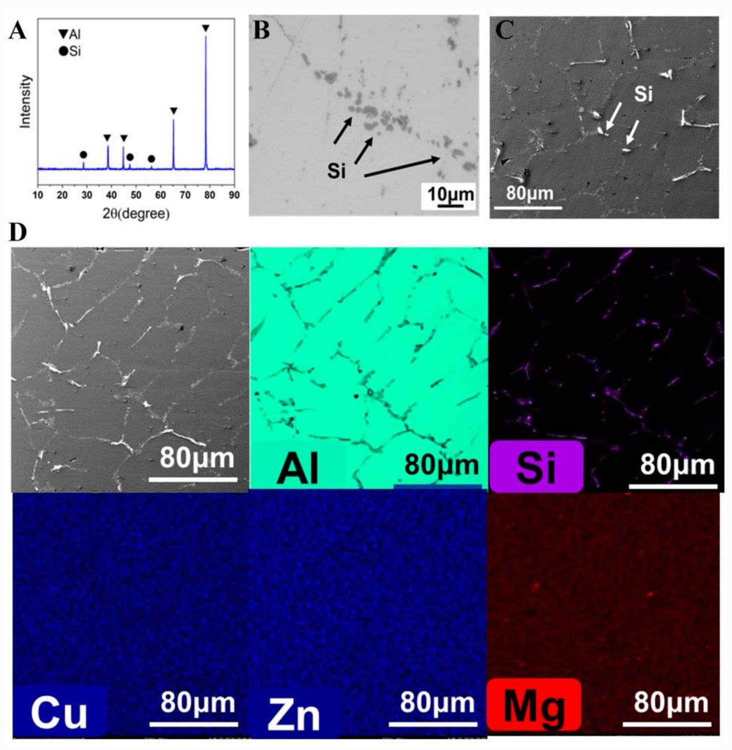


Figure 11. (A) XRD patterns (B) OM (C) SEM micrograph (D) EDS maps of the Al-2.64Si-0.43Mg-0.10Zn-0.03Cu alloy. XRD: X-ray diffraction; OM: optical micrograph; SEM: scanning electron microscopy; EDS: energy-dispersive X-ray spectroscopy.

Why it worked (Insight)

Success linked to **microstructure control (spherical, fragmented Si particles)**

These structures allow both:

- **Good heat flow (less scattering)**
- **High strength (precipitation strengthening)**

Shows AI didn't just guess — it found **physically meaningful solutions**

Conclusion (Theme: Human vs AI)

AI does not replace engineers — it **amplifies human decision-making**

Humans define the physics & data → AI explores the design space faster

Key takeaway: **Engineering intelligence is now hybrid —human insight + AI search power**

Human engineers define the rules — AI explores the possibilities.

UNIVERSITY OF WARWICK

AI-Driven Early Detection of Neurodevelopmental Disorders Using Serious Gaming in Children

M.F. Shaikh · Dr D. Piaggio

Background (Problem)

Neurodevelopmental Disorders (NDDs) affect 5–11% of children *(ADHD, Dyslexia, Dyscalculia, Dysgraphia)*

Early signs routinely missed due to resource-intensive clinical assessments

Significant societal & academic burden if undetected

Need: scalable, non-invasive, school-based screening tools

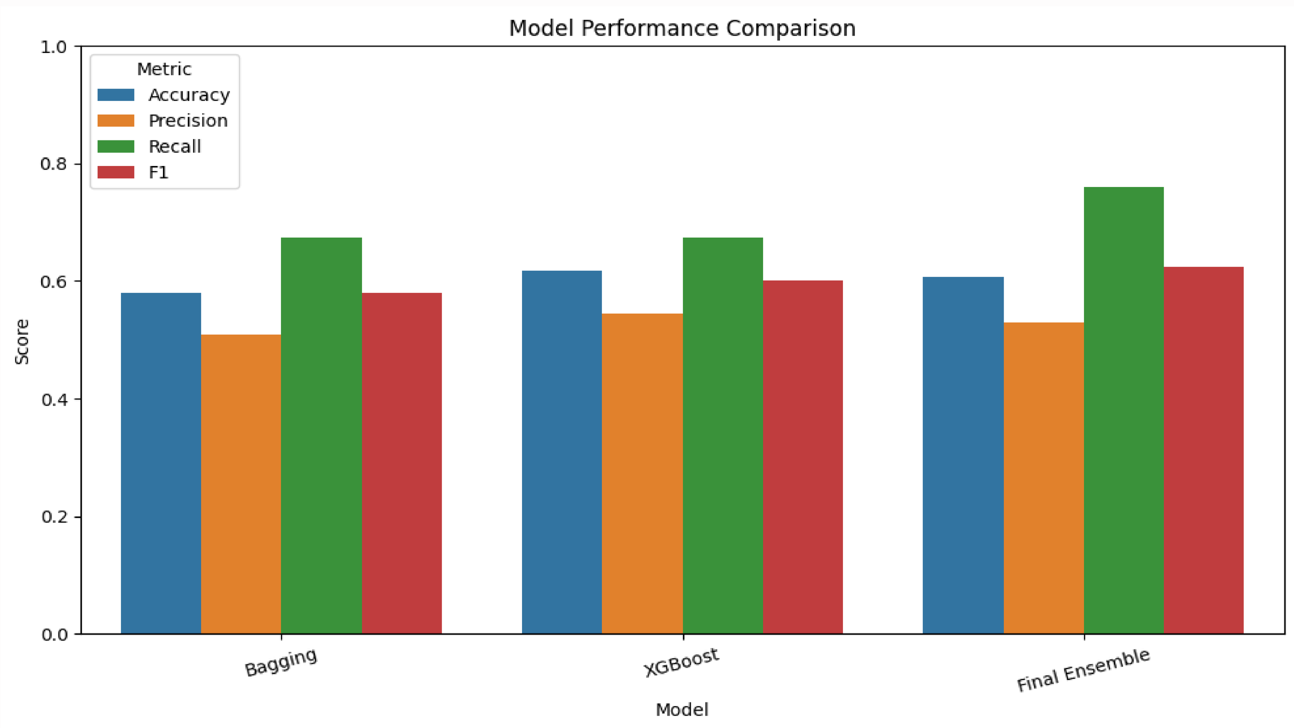
Serious gaming platform deployed in 3 Birmingham primary schools

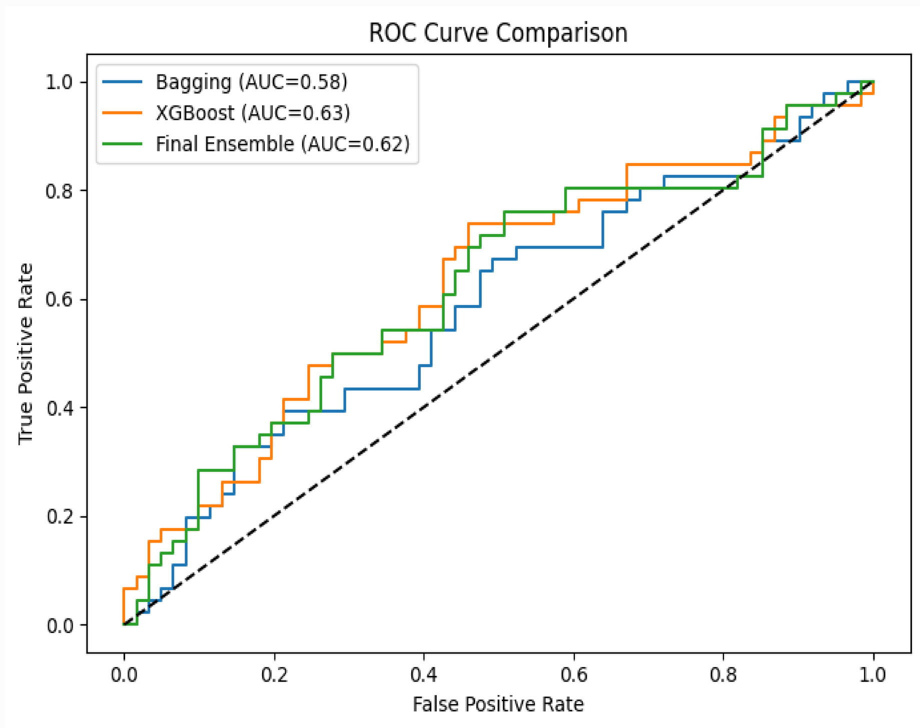
12 games across Reception, KS1, KS2 capturing performance, attention & mood

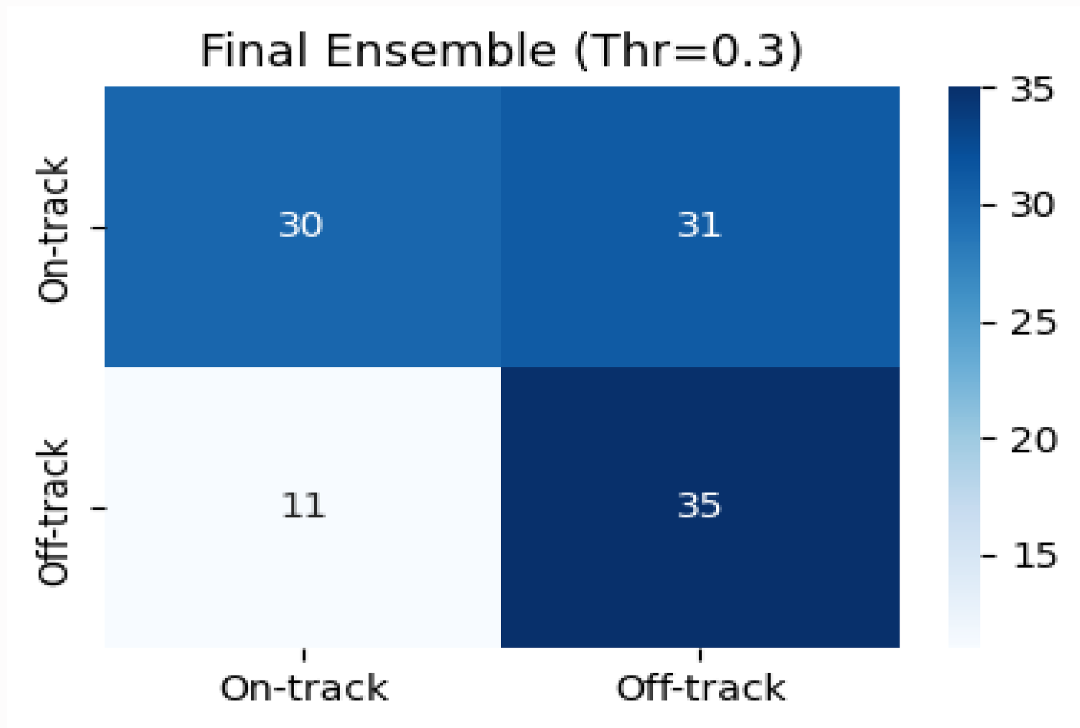
Multi-game signals (G1–G4): errors, attention (mean/var/trend), reaction time, task completion

R = f(G1,G2,G3,G4, Attention, Behaviour) Threshold tuned 0.30–0.80 via cross-validation

Screening must catch at-risk kids. A missed case (FN) is far costlier than a false alarm (FP)







Results

Little Wandle (systematic synthetic phonics) used as external benchmark, maps to Game 2 (phonics) only

Dino screens 4 cognitive domains, comparison beyond LW is essential to capture the full NDD picture

Results reflect an initial subset **(100–120 records)** from one school, data from the remaining schools is still being collected and cleaned, so these are preliminary/proof-of-concept findings, not final performance.

Why Precision is not enough, Recall is the priority:

A missed at-risk child (False Negative) denies timely intervention. Model optimised to minimise FN, even at cost of more false alarms.

Semantic Intelligence in Metallurgy: A Dual-Stage Language Model Framework for Processing-Aware Magnesium Alloy Design

UNIVERSITY OF WARWICK

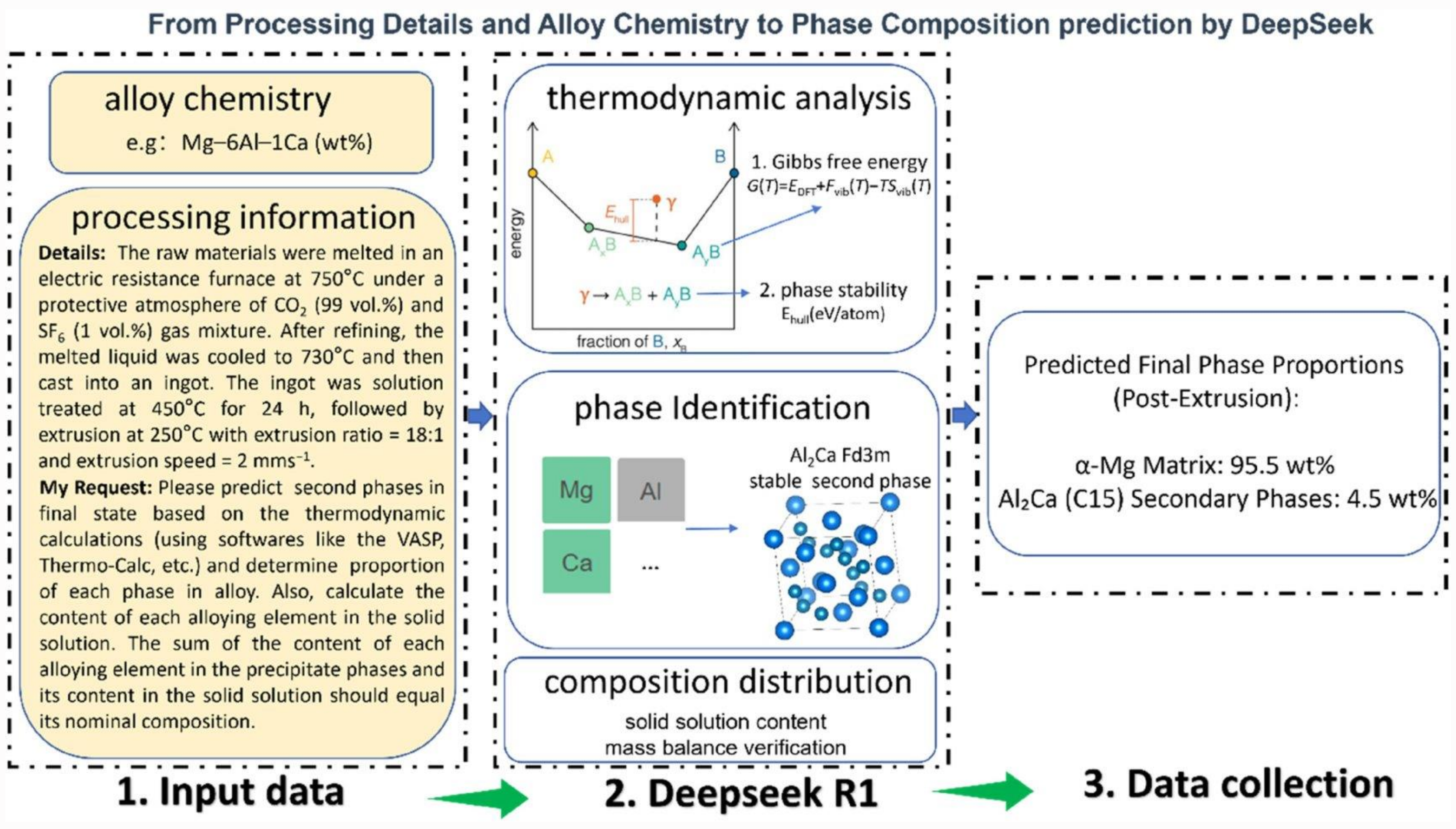
Ziliang Lu, Ishwar Kapoor, Takeru Araki, Lu Chen, Tao Song, Yixiang Li, Yang Su, Xiaoqin Zeng, Leyun Wang

Introduction

Traditional magnesium alloy design is slow because engineers must balance **strength, thermal conductivity, and processing history** all at once.

Existing ML models often miss the **order and context of processing steps**, even though these strongly affect microstructure and final performance.

This paper frames AI as a partner to engineering: **LLMs read the literature, ML predicts properties, and thermodynamic reasoning adds physics awareness**.



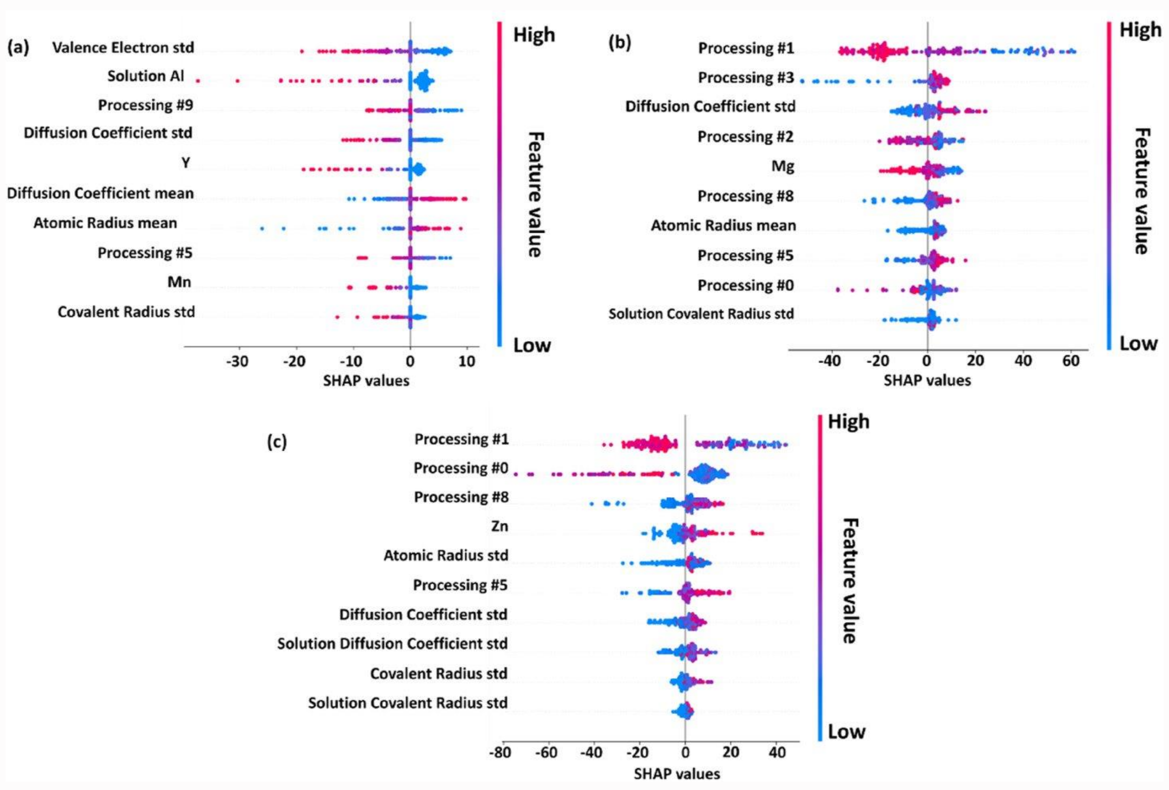
Workflow of the DeepSeek framework for phase prediction in Mg alloys.

Results and Discussion

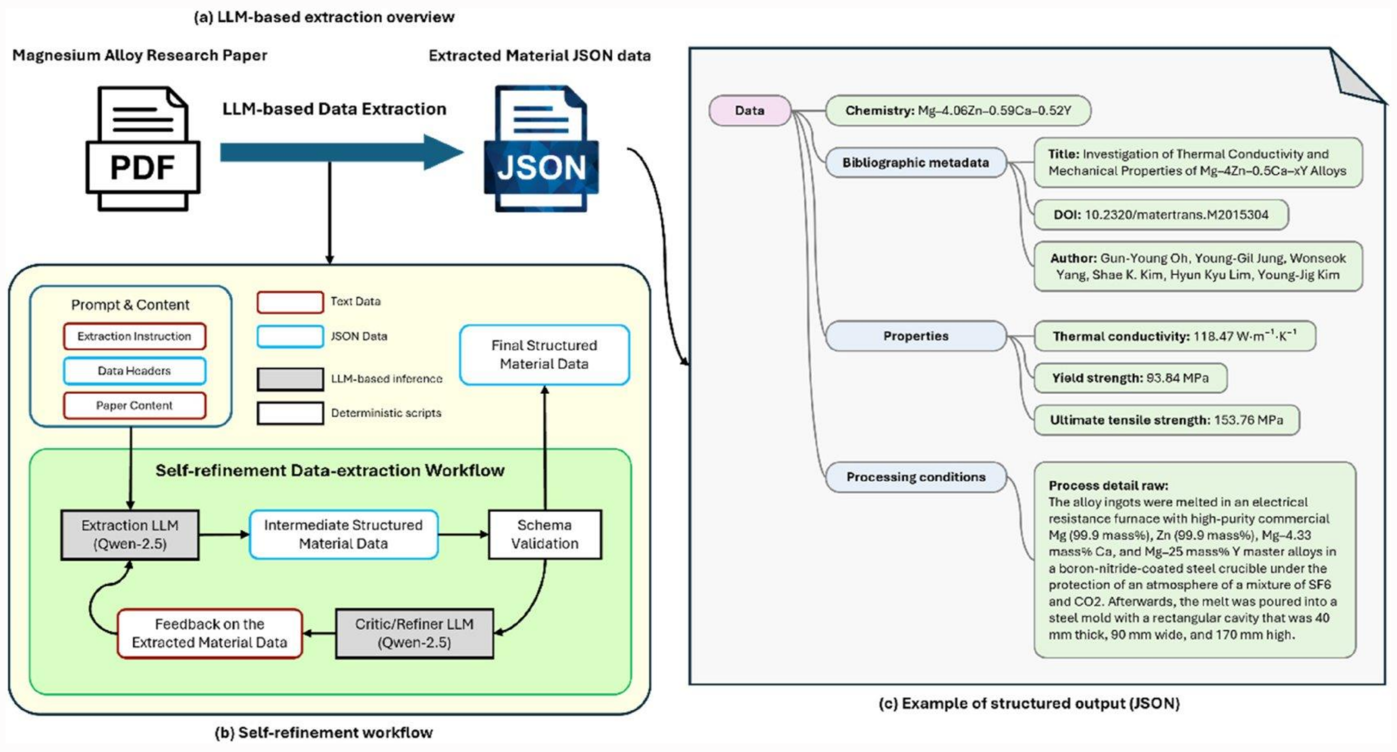
The dataset showed that **strength and thermal conductivity are not linked by a simple trade-off** — they depend on chemistry, processing, and phase structure together.

For **mechanical properties**, processing features mattered most: adding processing information improved prediction of **YS and UTS** much more than chemistry alone.

For **thermal conductivity**, chemistry mattered most, while feature selection helped the model reach its best TC performance of $\mathbf{R^2 \approx 0.80}$.



The SHAP values of the top 10 important features in (a) TC, (b) YS, and (c) UTS models.



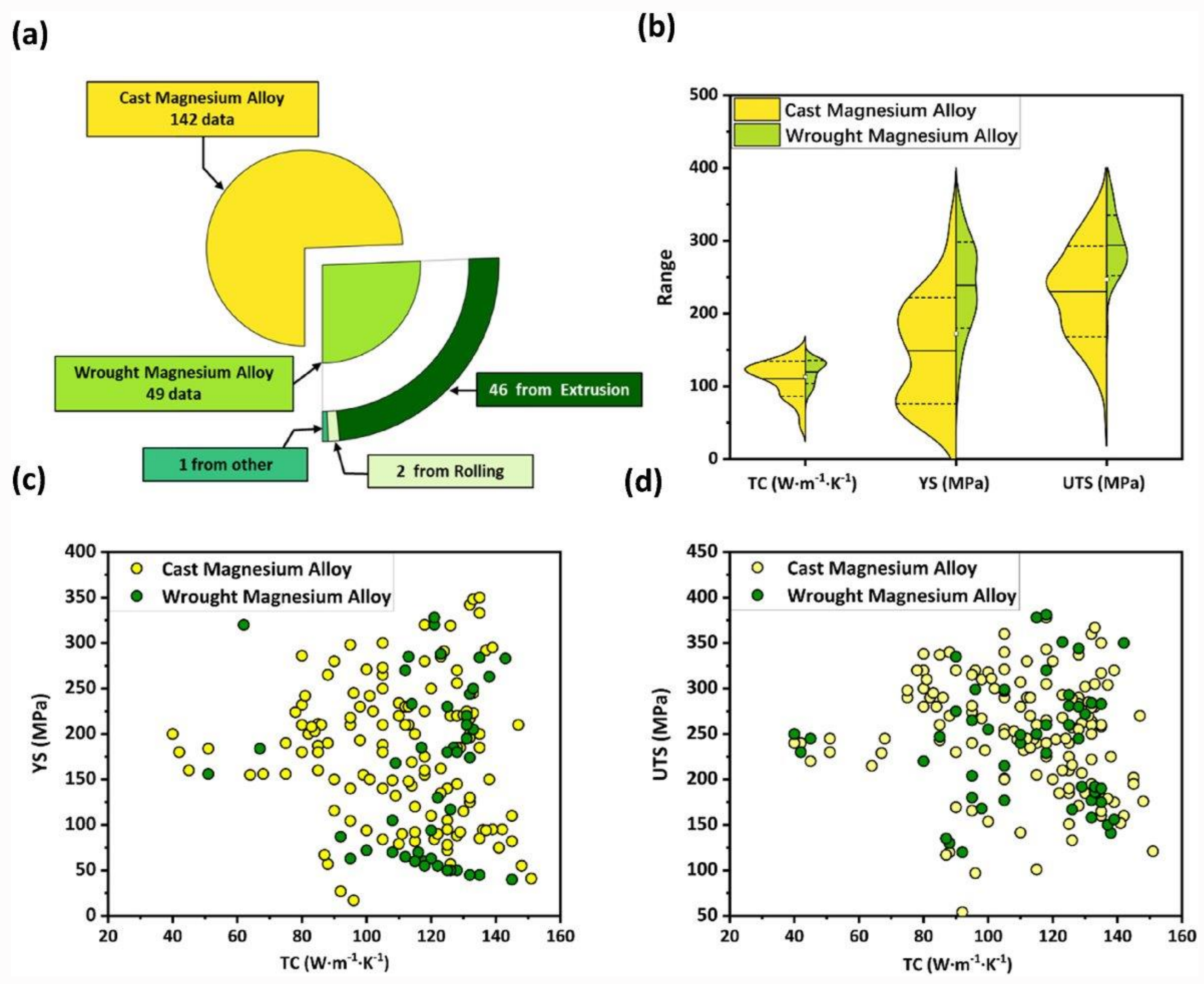
LLM-based extraction for Mg alloy literature (PDF → JSON workflow).

Methodology

Qwen-2.5 was used to read full research papers and extract alloy chemistry, processing details, and measured properties into structured data.

DeepSeek-R1 then estimated thermodynamic phase information, while processing descriptions were converted into numerical embeddings so the model could learn from manufacturing sequences.

These combined features were used to train ML models to predict **thermal conductivity (TC), yield strength (YS),and ultimate tensile strength (UTS)**.



Thermodynamic / AI Insight

DeepSeek-R1 reproduced equilibrium phase fractions **within about 1 wt.% of CALPHAD**, showing that an LLM can support physically meaningful metallurgical reasoning.

This is important because the AI is not just extracting text — it is also helping connect **composition → phase formation → predicted properties**.

In Human vs AI terms: the AI handles **scale, speed, and hidden patterns**, while metallurgy still relies on **human interpretation of phases, mechanisms, and validation**.

Conclusion

The paper shows that **semantic intelligence** can turn unstructured literature into a usable design pipeline for magnesium alloys.

Processing dominates strength prediction, while chemistry dominates thermal conductivity.

AI accelerates metallurgical intelligence, but it works best when combined with human engineering knowledge and physical reasoning.

Problem definition → Sketching → CAD modelling → Prototyping

This work explores how AI-generated 3D models can accelerate early-stage design in engineering education.

In my first-year CAD module, students traditionally follow two tutorial videos (24 min + 9 min) to model a helmet from scratch.

Using Meshy.ai, a comparable concept can be generated in under a minute.

Students then refine the AI mesh into a parametric CAD model, adding details and engineering features while learning both creative ideation and precision.