Project Title: AI-Driven Exploration of Cost-Effective Fe-Based Shape Memory Alloys
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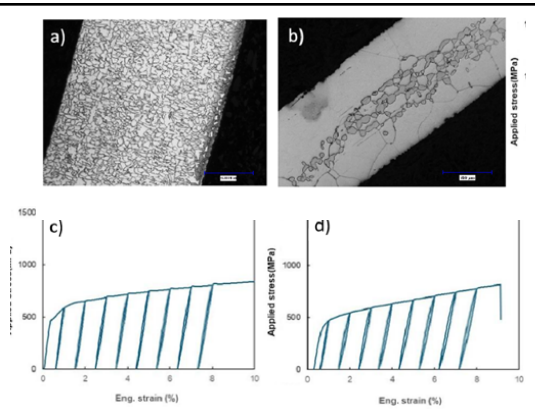
Q1: Rationale & Goal

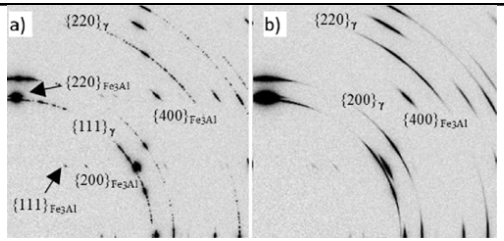
- The Problem: Nitinol is a great shape memory alloy but is prohibitively expensive.
- The AI Promise: AI can predict millions of stable crystals, but struggles to predict real-world manufacturability.
- Goal: Use an AI Large Language Model to design a low-cost iron-based alternative (Fe-Mn-Al-Si-Ni-C) and physically test it.
- Hypothesis: AI will predict a thermodynamically stable composition, but it will fail to achieve superelasticity due to unforeseen processing and ductility barriers.

Q2: Methodology

- AI Discovery: Prompted an LLM to balance pseudoelasticity with cost-efficiency by minimizing expensive elements like Cobalt and Nickel.
- Physical Synthesis: Arc melting, hot rolling (850°C), and cold drawing down to 0.014” wire.
- Heat Treatment: Abnormal Grain Growth (AGG) cycling (1200°C → 900°C) sealed in quartz tubes to prevent oxidation.
- Characterization: Cyclic Tensile Testing and Synchrotron X-Ray Diffraction (XRD).

Q3: Results





- [Fig 1a & 1b] Microstructure: AGG heat treatments failed to create the necessary single-phase matrix, retaining an undesirable dual-phase morphology.
- [Fig 1c & 1d] Mechanics: Open hysteresis loops with significant residual strain. No "flag-shaped" superelastic plateau occurred.
- [Fig 2a & 2b] Synchrotron XRD: Spectra before and after 8% strain remained identical (FCC γ-phase). This definitively confirms no stress-induced phase transformation occurred

Q4: Conclusions

- Experimental Failure: The alloy achieved ~0% recoverable strain, deforming via irreversible plastic slip rather than superelasticity, and suffered from severe brittleness.
- The AI "Reality Gap": AI successfully optimizes for theoretical thermodynamic stability, but currently lacks the "process-structure-property" context to predict functional manufacturability.
- Final Takeaway: AI is a revolutionary high-speed hypothesis generator, but human-led physical experimentation remains absolutely essential to bridge the gap between digital discovery and industrial application