AI-Driven Exploration of Cost-Effective Fe-Based Shape Memory Alloys: Bridging the Gap Between Prediction and Processability

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Nickel-Titanium (Ni-Ti) alloys dominate the shape memory alloy (SMA) market, but high costs limit their expansion. While iron-based SMAs (Fe-SMAs) offer a cheaper alternative, discovering competitive compositions is challenging. This study leveraged Deep Research AI and Google's GNoME database to hypothesize a novel, low-cost Fe-Mn-Al-Si-Ni-C SMA. We evaluated the "reality gap" between AI predictions and physical processability by comparing this alloy against the established Fe-Mn-Al-Ni (Omori) benchmark. The AI-hypothesized alloy underwent arc melting, hot rolling, cold drawing, and Abnormal Grain Growth (AGG) heat treatments. Although the AI identified a thermodynamically stable composition, experiments revealed severe processing brittleness and a persistent dual-phase microstructure. Cyclic tensile testing and Synchrotron X-ray Diffraction (XRD) confirmed the absence of a stress-induced martensitic transformation; the alloy instead accommodated stress through irreversible dislocation slip. Conversely, testing the Omori benchmark across variable strand-annealing speeds disproved established literature requiring massive "bamboo" grains for superelasticity. Data proved that faster feed rates (20 FPM) producing smaller grains yielded vastly superior pseudoelastic strain recovery compared to slower rates (0.8 FPM). Ultimately, these findings demonstrate that while current AI models generate stable compositional heuristics, they lack the crucial process-structure-property context to predict physical manufacturability. Furthermore, this small-grain paradigm establishes a highly scalable manufacturing pathway for mass-producing low-cost Fe-SMAs.

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