



WPI

MATERIALS SCIENCE & ENGINEERING

Derek Tsaknopoulos Optimization of Coupled Computational Modeling and Experimentation for Metallic Systems

PhD Thesis Defense

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Abstract

Additive manufacturing technologies place materials at the direct point of need of the warfighter, enabling the development of optimal, situation-specific means to produce and repair parts of Army and DoD weapons systems. Systems. In the case of solid-state AM, a full understanding of the metallic powder is critical with producing ideal consolidated material properties reliably and repeatably. By way of iteratively coupling computational models with supportive experimental testing, one can rapidly archetype differences in processing methods, alloy compositions, and heat treatments for metallic powders that serve as feedstock for these AM technologies. Through the combination of thermodynamic models, advanced characterization, and dynamic nano-indentation, representative correlations are established between microstructural features and mechanical properties, enabling the development of enhanced feedstock materials that can achieve the specific needs of the warfighter efficiently without forfeiting quality. This represents both a holistic and a materials by design approach to AM through the deliberate use of computation to drive down the discovery process and allow feedstock powders to be engineered with specific properties dictated by Army requirements for performance.

In a case study of Al-6061, unique observations were made through the combination of modeling and experimentation. It was discovered that the precipitation kinetics were greatly accelerated in powders and therefore, typical heat treatment processes used for cast-aluminum alloys were not valid. Due to this shift in precipitation sequences, high-temperature treatment was limited to discourage precipitate and grain coarsening. Additionally, when compared to typical cast Al-6061, the main precipitation hardening phase shifts from Mg₂Si to Al₄Cu₂Mg₈Si₇, changing how aging mechanisms were accounted for. These conclusions were supported by both the computational models and experimental results. Through the generation of numerous data, the models were calibrated, enabling more efficient and precise development of tailored material characteristics from specific microstructural features to serve as an input in a holistic through-process model for a solid-state AM process and guide future experimentation.

