Grain Boundary Engineering: AM 2.0

In 2011 the Materials Genome Initiative, which is a federal multi-agency program, defined a vision for discovering, manufacturing, and deploying advanced materials twice as fast and at a fraction of the cost compared to traditional methods. In 2021, the Materials Genome Initiative marked its first decade of operation by developing a strategic plan that identified three goals for the next five years. Those goals were (i) unify Materials Innovation Infrastructure (MII) to include advanced modeling, computational tools, experimental tools, and quantitative data; (ii) harness the power of materials data; and (iii) educate, train, and connect materials research with workforce development [**1**].

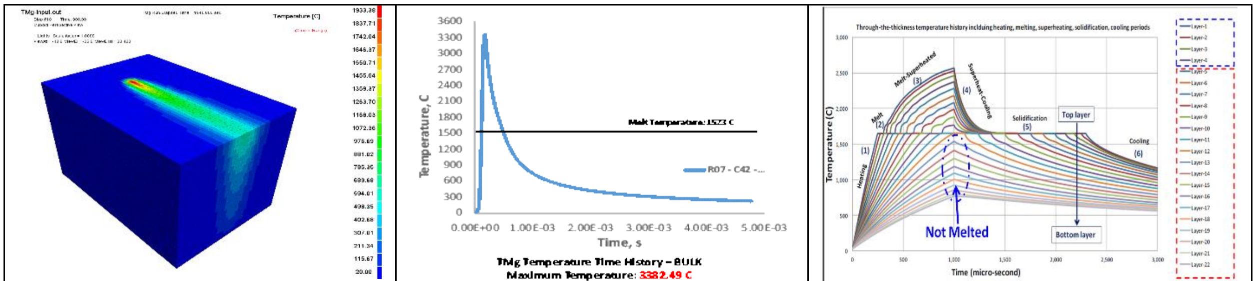
The blending of Integrated Computational Materials Engineering (ICME) technology with Additive Manufacturing (AM) has similar objectives. ICME seeks to integrate materials information, manufacturing-process simulation, engineering product performance analysis within a computational multiscale environment. In that manner, ICME relies heavily on computational physics and informatics with systematic experiments to optimize design and performance. AM uses data from computer-aided-design (CAD) software or 3D object scanners to direct hardware to deposit material, layer upon layer, in precise geometric shapes. As its name implies, AM adds material to create complex objects with fewer independent parts [**2**]. When coupled together, AM and ICME can not only improve part quality but also improve part microstructure, performance, reliability, and explore optimization in areas previously never considered.

Looking back over the previous two decades, AM technologies have transformed our concept of fabrication; yet the primary goals of researchers have been limited to qualification, certification, netshape. While most teams pursue pedestrian challenges, others are exploring next generation technologies, AM 2.0 in the current vernacular. Specifically, the Defense Logistics Agency (DLA), think DOD Supply Chain, is seeking technologies and processes in AM that can predetermine the microstructure of AM parts with “tailored” grain boundaries to produce predictable mechanical properties including mode of failure. Grain boundaries influence the mechanical properties of metals; hence, certain grain boundaries are preferred over others. For example, coincidence site lattice (CSL) grain boundaries and low angle grain boundaries (LAGB) support increased resistance to stress, corrosion, and cracking. Accordingly, it is assumed that grain boundary engineering (GBE) techniques can improve material properties, secure desired microstructural outcomes, and provide DoD with more reliable parts.

A team led by AlphaSTAR Technology Solutions (ATS) that includes General Electric Research Center (GERC), the University of Michigan and Quadrus Corporation, has taken on this challenge and achieved several impressive breakthroughs. First and foremost, the team has developed and validated algorithms, modules and integrated tools for AM metal that can predict AM build outcomes in terms of alloy compositions, presence of precipitates, use of nano/micro material inclusions, and alteration of process parameters to exploit thermal cycling within the AM platform [**3**]. These capabilities have resulted in improved material properties, desired architectures in terms of grain size and boundary angle; and the capability to optimize and ultimately customize build outcomes. In practice this translates into a detailed understanding of the dynamics of AM meltpool behavior including the full thermal cycle common to LPBF and EBM platforms, specifically heating, melting, melt superheating, superheated cooling, solidification, and cooling process associated with laser interaction (**Figure 1**). Information extracted from meltpool is used to generate thermal process and density maps which identify stable/unstable print regions and is the first step on the road to optimization (**Figure 2**).

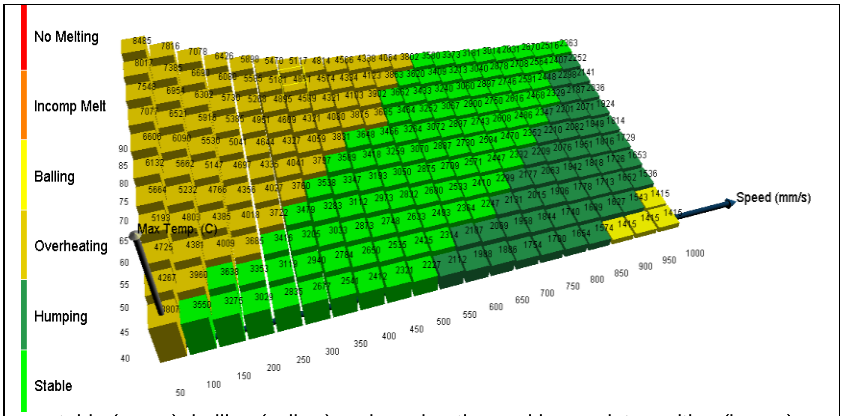
The list of predictive capabilities includes (i) generation of process and density maps to identify stable/unstable print regions; (ii) prediction of meltpool size distribution: absorption, heat flux; (iii) prediction grain size; (iv) prediction void versus X-ray computed tomography (XCT); (v) prediction of macro void, i.e., effect of print orientation/hatch spacing on defects and degraded material properties; (vi) generation of multiple carpet plots (% defects versus volumetric energy density) for multiple preheat temperature to minimize bend and cracks; (vii) prediction of strength and scatter: effect of machine modality and precipitates on scatter; (viii) prediction of post heat treatment: assessment of all effects including damage to grains; (ix) prediction of fracture toughness per thickness and fatigue crack growth rate towards

SN curve; (x) prediction of surface roughness effect on fracture and fatigue life; (xi) assessment of grain crystallization : Low Angle Grain Boundary (LAGB), Coincident Site Lattice (CSL); (xii) analysis of multipart fabrication with focus on heat trap; and (xiii) thermally driven powder to part new alloy design.



a) TMg temperature predictions b) Temperature-time history c.) thermal history

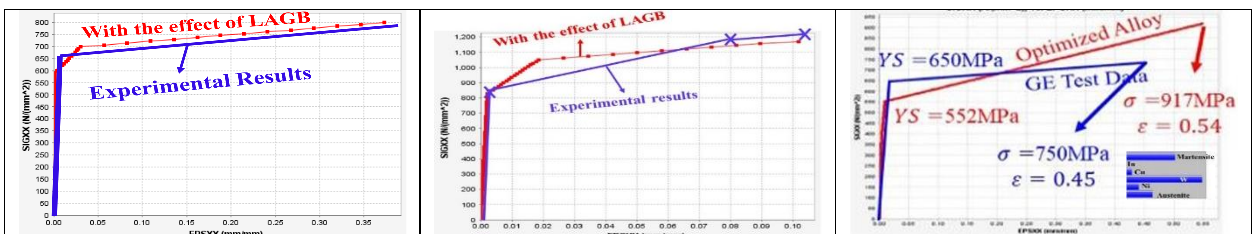
Figure 1. Temperature distribution and meltpool size variation with time.



stable (green), balling (yellow) and overheating and incomplete melting (brown)

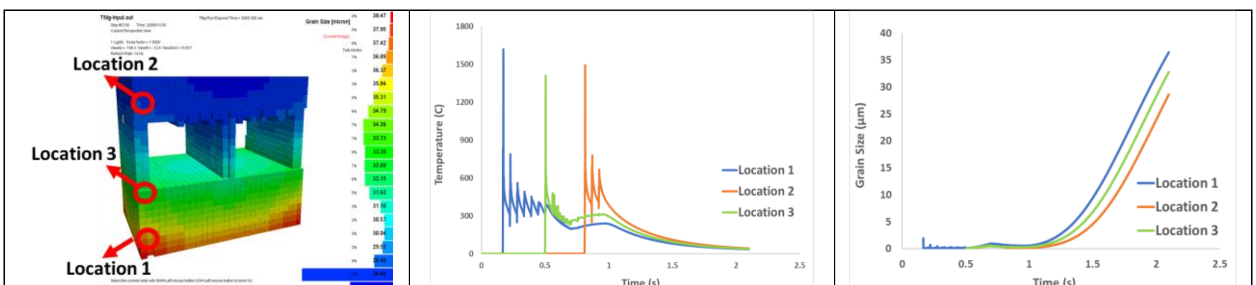
Figure 2. Process Map for Inconel 718 LPBF Machine Parameters

In layman's terms this means better parts with increased performance (**Figure 3**) and reliability as envisioned by the DLA, i.e., localized microstructural tailoring or AM 2.0 (**Figure 4**). To date, the team has applied the technology to explore alloy composition, including improving the properties of stainless steel, embarked on a quest to recreate legendary Damascus Steel knives within an AM platform (**Figure 5**), and developing techniques for the repair and retrofit of critical hardware, such as gas turbine engine blades, seals and flaps and other extreme temperature components.



a) Mechanical results of SS316L b) Mechanical results of Damascus Steel c) Proposed Steel Design & Composition

Figure 3. AM Stainless Steel Mechanical Strength Prediction Compared with Test



a) Grain size distribution on model b) Temperature-time history per location c) Grain Size prediction per location

Figure 4. Grain size distribution, Temperature-Time history, and local grain size [6].

More significantly, the full digital twin integration will finally allow end users to predict defects and effect of defects on part performance, while considering, (i) warpage; (ii) net shape (shrinkage, expansion), tolerance, and precision assembly; (iii) heat entrapment; (iv) mechanical properties versus temperature; and (v) cracks and delamination.

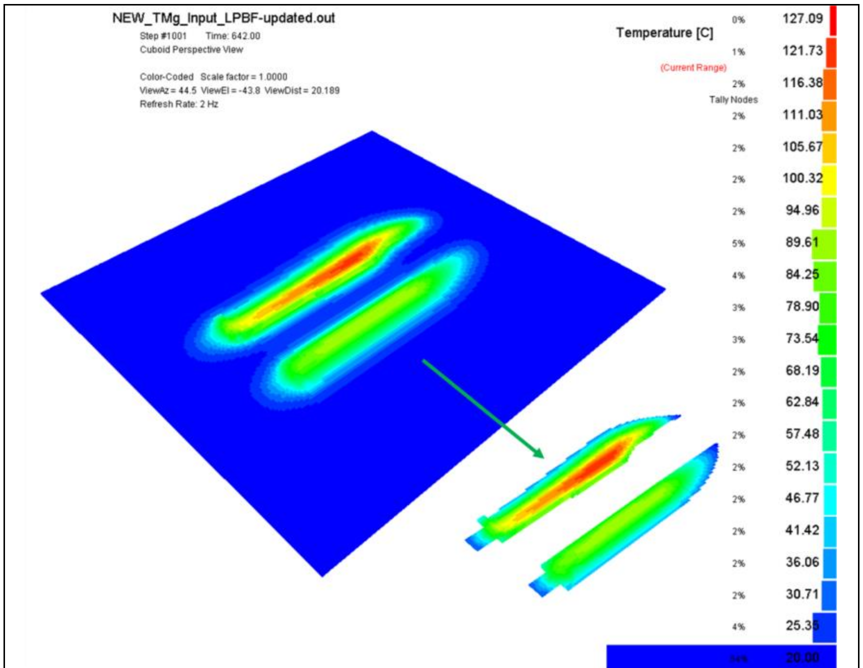


Figure 5. Analysis of Two Knives and Validation of New Alloy Composition

The Department of Defense (DoD) has a need for out-of-production parts to maintain mission readiness of various weapons system platforms is an ongoing challenge. DLA's strategic objective has always been to enable a flexible supply chain that can accelerate repairs and part replacements utilizing AM technology. Understanding the microstructure development and evolution during the AM process of metallic alloys is an important precondition for the optimization of the parameters to achieve desired mechanical properties of the AM builds. DLA is looking to leverage this evolving technology to enable a supply chain that is flexible, scalable, and capable of producing parts that are more reliable. It is now recognized, that improved grain boundary engineering techniques are desirable and may be a viable technology to provide DoD with more reliable parts. In subtractive manufacturing, the grain boundaries are predetermined in the net-shaped parts. In AM, it is now possible to design the grain size and grain boundaries of the net-shaped parts by altering the process parameters or by adding nano/micro particles in a specific localized region during the AM process. Clearly AM 2.0 is here to stay.

[1] https://www.mgi.gov/about
[2] https://www.ge.com/additive/additive-manufacturing
[3] Abdi, Frank, Amirhossein Eftekharian, Dade Huang, Raul B. Rebak, Mohamed Rahmane, Veera Sundararaghavan, Alec Kanyuck et al. "Grain Boundary Engineering of New Additive Manufactured Polycrystalline Alloys." Forces in Mechanics (2021): 100033.