Research Campaign: Advanced Manufacturing in Space: Properties, Structure and Simulations to Pioneer New Applications

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Abstract:

This topic underpins synthesis of, and in many cases manufacturing of, value-added materials via liquid phase processing. Materials and processes range from cast metals and optical glasses through exploration-relevant technologies such as additive manufacturing, casting and in-situ resource utilization to support human space exploration. A recurring theme is the need for accurate thermophysical property and atomic structure data for relevant materials and the exploitation of reduced convection/sedimentation in microgravity to enhance the quality of data and to develop new and transformative technologies for materials processing.

Advancements of metallic and non-metallic materials additive manufacturing (AM) processing depends heavily on high resolution numerical simulations. The role of these simulations become more important for in-space manufacturing where process optimization by trial and error is costly, time consuming, and may not be practical in some cases. However, the validity of these models are under question, primarily due to a lack of accurate thermophysical properties.

Both ground-based and microgravity programs are complementary to each other in terms of capabilities and accessibility. A progression of research is recommended, starting with a strong ground-based program that will provide a strong foundation for flight-based experiments that exploit the additional quiescence of liquids that is needed for the most precise measurements.

NASA's advanced manufacturing and space exploration efforts have a strong interest in additive manufacturing for spacecraft components and for the construction and maintenance of components while in space and for future habitats. The data provided by the tools and techniques in this white paper can be used with the MGI approach to advance and accelerate the TRL advancement needed and infuse AM products for these needs.

This topic underpins synthesis of, and in many cases manufacturing of, value-added materials via liquid phase processing. Materials and processes range from cast metals and optical glasses through exploration-relevant technologies such as additive manufacturing, casting and in-situ resource utilization to support human space exploration [1]. A recurring theme is the need for accurate thermophysical property and atomic structure data for relevant materials and the exploitation of reduced convection/sedimentation in microgravity to enhance the quality of data and to develop new and transformative technologies for materials processing.

The Materials Genome Initiative (MGI) was launched in 2011 to accelerate the discovery, design, development, and deployment of new materials, at a fraction of the cost, by harnessing the power of data and computational tools in concert with experiment. Significant advancements have been made; in November 2021, a new strategic plan was released describing an approach to increase the impact and realize the full potential of the initiative [2]. The work proposed in this white paper would provide critical contributions to support the implementation of the MGI approach to advance the needs of NASA exploration. The plan identifies three goals to expand the impact of MGI.

2021 MGI Strategic Plan Goals to expand impact	How this work supports goals for NASA applications and enhances impact for NASA
1) Unify the Materials Innovation Infrastructure (MII), a framework of integrated advanced modeling, computational and experimental tools, and quantitative data	Quantitative data sets for a wide range of materials needed by NASA exploration can be provided by the experimental tools described in this white paper. Unique NASA data needs can be addressed using the techniques in this topic: <u>ultra-high temperatures</u> for extreme environments and nuclear thermal engines, <u>vacuum environments</u>, and <u>reduced gravity</u>.
2) Harness the power of materials data	Develop and provide open source materials data for NASA materials needs for research community. Provide opportunities for MGI work on these data sets, for example via the NASA Physical Sciences Informatics (PSI) database and support for MGI work using data sets via the PSI program and leverage work by OGAs.
3) Educate, train, and connect the materials research and development workforce	Academic-led research teams funded by BPS grants supporting graduate and undergraduate researchers interacting with NASA and International Partners to connect teams with unique expertise and develop workforce focused on NASA space exploration materials needs.

Advancements of metallic and non-metallic materials [3] additive manufacturing (AM) processing depends heavily on high resolution numerical simulations. It is important to understand processes on the small time (μs) and length (μm) scales that are relevant in AM. The role of these simulations become more important for in-space manufacturing where process optimization by trial and error is costly, time consuming, and may not be practical in some cases.

For the past decade, national-level efforts have been conducted to model metal AM processing with an objective of reasonably-accurate predictions of the microstructure and mechanical properties of as-built AM metals. Various numerical models have been proposed to simulate the melting, solidification, and other phase transformations during cooling, and the associated residual stress formation [4-6]. However, the validity of these models are under question, primarily due to a lack of accurate thermophysical properties. For an accurate numerical prediction, thermophysical properties are needed over a representative range of temperature, chemistry, and flow conditions. However, measurements of these properties are extremely scarce and practically non-existent for low gravity cases.

Using reliable thermophysical property data in numerical simulations is a necessary condition for the accurate prediction of phase transformation and thermal evolution in and near a melt pool, which should lead to valid estimation of the microstructure, defect, and residual stresses in as-built parts. This capability is of critical importance for optimizing process parameters and reducing post processing steps for in-space manufacturing. Further, building material properties databases will provide a pathway to rapid qualification of components and contribute to the development of new alloys optimized for additive manufacturing (AM) processes.

Surface tension, or more generally speaking surface energy, is crucial to in-space manufacturing (ISM). For example, in the case of laser powder bed fusion (LPBF), the temperature varies within a small (~100s μm) melt pool from close to the melting point at the solidification front to potentially >3,000 K at the region directly heated by a laser or other heat source [7]. Such a large temperature gradient (10^7 K/m) induces a violent turbulent flow driven by the surface tension gradient (Marangoni flow) and affects the solidification and resulting microstructure [8]. The Marangoni flow is dominant in space due to the absence of gravity. Similar phenomena also occur during welding and to a much lesser extent casting. Beyond LPBF, AM processes in consideration for ISM, including wire+arc additive manufacturing, directed energy deposition, and bound metal deposition, all include melt pool or liquid phase evolution whose dynamics are driven by surface and interfacial energies.

Due to the high reactiveness of almost all molten materials, the surface tension must be measured by containerless methods such as electrostatic levitation (ESL) or electromagnetic levitation (EML). Both methods, when used on the ground, have limitations due to field effects, buoyancy-driven convection, and sedimentation. To avoid arcing between the electrodes, the ESL processing chamber must be evacuated. In a high vacuum condition, substantial mass evaporation occurs at high temperatures, which can shift the composition of the tested alloy due to selective evaporation of constituents that have a high vapor pressure. This can lead to a uncertainty in the measured properties. The maximum temperature that can be used for the studies is therefore limited. In addition, with ground-based ESL, it is very difficult to process silicate, aluminate, and titanate glasses and metal oxides as they need stronger electric fields which promotes arcing. For EML, a sample is deformed and stirred significantly by a strong magnetic field, which complicates data processing and adds uncertainty to the measured properties. Microgravity overcomes the above-mentioned roadblocks as it allows for processing molten materials in various ambient gases and under controlled pressure. In this case, the interfacial tension between a molten material and different gases can also be measured, which is needed for controlled high-precision manufacturing of semiconductor crystals. In microgravity EML, the amount of stirring in the sample can be controlled, which can be utilized to study the effect of convection on the thermophysical properties and solidification of molten materials.

For these reasons, it is essential and advocated to have novel technical methods and associated facilities that will provide accurate measurements using low gravity platforms that include the ISS, low orbit vehicles, and, in some cases, parabolic flights [9]. Methods could include continued use of levitators with better and more versatile infrastructure, electrochemical methods for measurement of surface energy, and resonance techniques for measurement of interfacial tension.

Aside from measuring thermophysical properties, the same facilities and skill sets can be extended in diverse directions. Oxidation of molten materials is common in several manufacturing processes such as welding and AM. It has been reported that oxygen affects the thermophysical properties of molten materials significantly. For example, the surface tension of molten iron decreases by 40% near its melting temperature as the oxygen partial pressure increases from 3.6×10^{-14} Pa to 7.6×10^{-9} Pa [10]. The oxygen effect on the thermophysical properties of many other molten materials still remains to be explored [11]. Thermochemical property data information including partial pressures and chemical activities relative to alloy composition and temperature, aid in the understanding and development of phase data important in the material design process.

Phase separation in liquids provides unique opportunities to synthesize new types of composite materials ranging from tough glasses to photonic crystals. An understanding the kinetics and the spatial distribution of phase separation in the absence of liquid stirring and convection is of critical importance. Furthermore, understanding the role of buoyancy and flow on the kinetics and resulting morphologies of the products is essential to exploiting these materials full potential. Ultimately, transformative processes such as combining controlled phase separation with additive manufacturing can lead to new types of materials with superior properties. A second phase can be organized in a controlled way to enable new materials. This will require knowledge of buoyancy issues (density, viscosity) and understanding of the chemical behavior of the two-phase fluid system.

To a large extent, the quality and integrity of AM parts is determined by their microstructural characteristics such as solute micro segregation, grain size and shape, porosity, etc., which develop during the dendritic solidification process. Work can be conducted investigating cooling rates and solidification of molten alloys, using ESL to study dendritic solidification of undercooled alloys. This data could identify optimal processing windows, validate models, and support part and process qualification – all vital AM needs.

Both ground-based and microgravity programs are complementary to each other in terms of capabilities and accessibility. A progression of research is recommended, starting with a strong ground-based program that would include pushing the limits of the most promising approaches, such as ESL, to establish performance benchmarks. Ground-based research will provide a strong foundation for flight-based experiments that exploit the additional quiescence of liquids that is needed for the most precise measurements. Research done utilizing NASA labs and/or Investigator's labs would feed into free-flyer missions, such as parabolic and suborbital flights. These would finally feed into experiments that can only be performed in long duration microgravity.

Other ground-based facilities, such as synchrotron X-ray and neutron beamlines (typically supported by the DOE), are required to study the structure of materials, and funding for investigators to use these facilities should be supported as part of the compliment of research. Ultimately, with accurate knowledge of atomic pair potentials, many thermophysical properties can be derived from first principles. However, for this approach to be viable, a considerable database and empirical testing are needed to validate methods. Additionally, viscosity, surface tension, and chemical activity are properties sensitive to characteristics of the sample surface (composition within 10 μm of the surface). Understanding and quantifying surface composition, the presence of chemical gradients, segregation, and diffusion plays an important role in bulk property measurements and can be facilitated by ground-based beamline experiments. Structural characterizations, including in-situ, dynamic analysis would provide important quantitative data important in understanding the processing and evolution of AM materials via laser and e-beam processes,

Furthermore, a synergistic approach that includes teams of researchers could help to provide solutions to NASA's exploration missions. For example, a team consisting of an Investigator modeling physical phenomena in an in-space manufacturing process, a thermophysical properties Investigator to ensure that the modeling has the necessary properties, and an Investigator to perform model validation experiments could streamline the development of materials and processes.

Another example flows from the Materials Genome Initiative, which has led to a focus on the importance of bringing together computation, experiment, and data (both experimental and computational) to develop materials more rapidly than by Edisonian approaches. This effort also dovetails well with the intense interest in machine learning (ML) for discovering new materials, since data fuels machine learning algorithms. An adaptive ML framework, combined with a closed-loop learning strategy that integrates experiments and databases, can be used to continuously improve the prediction models with increased data and guide data generation at hyperspace locations (hyperparameter optimization) that most efficiently reduce the uncertainty of ML predictions and reduce the number of experiments. Ultimately, ML can guide the efficient search for candidate alloys in a compositionally extended space. This confluence of data, computation, and experiment can be used to rapidly develop materials and processes.

NASA’s advanced manufacturing and space exploration efforts have a strong interest in additive manufacturing for spacecraft components and for the construction and maintenance of components while in space and for future habitats. The data provided by the tools and techniques in this white paper can be used with the MGI approach to advance and accelerate the TRL advancement needed and infuse AM products for these needs. In addition, the techniques can be used to accelerate the discovery of new materials and provide an opportunity for NASA to participate in the emerging Materials Innovation Infrastructure.

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