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FUNDAMENTAL MATERIALS RESEARCH

NON-EQUILIBRIUM MATTER – UNDERPINNING TRANSFORMATIONAL ADVANCES IN MATERIALS FOR APPLICATIONS SPANNING SPACE EXPLORATION TO BIOMEDICINE

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1. Background: Non-equilibrium processes are ubiquitous. Natural and synthetic materials are rarely the result of equilibrium processes. Numerous processes that occur in non-equilibrium conditions [1, 2] have been exploited to achieve novel and often transformational technological advances in optical and aerospace materials, pharmaceuticals, food preservation and others [3]. Much of the underlying science about the relationships between non-equilibrium processing and the resulting properties, structure, and performance remains to be discovered. This campaign will implement a research theme to **identify, characterize, establish and exploit aspects of non-equilibrium processes that provide a foundation for transformational materials research**. "The need for a deeper understanding on non-equilibrium phenomena is nowhere greater than in materials science." [4] The present paper builds on the topical papers that were submitted earlier to this Decadal Survey in the Materials:Fundamental Studies area.

Non-equilibrium processes can be used to develop novel functional materials *via* liquid and liquid-gas phase processing and solidification. **In contrast to equilibrium, the specific route determines the outcome of non-equilibrium processes**. Liquids can enter non-equilibrium states by supercooling below the melting point, supersaturation of solutes, and/or formation of structural or compositional heterogeneities on various length scales. Investigating these states is challenging because precise control of kinetic variables is essential in order to correlate processing with the properties (*e.g*. viscosity, diffusivity, density, thermal expansion, surface tension, interface kinetics, heat of transformation) and structure (*e.g*. atomic bonding, clustering, short-range and meso-scale ordering) as liquids evolve to the final product.

The central problem in many non-equilibrium studies is that process kinetics are strongly influenced by complex heat, momentum, and mass transport. In fluid systems – including molten phases, solutions and supercooled liquids – convection, stirring, fluid motion, sedimentation and flow-induced effects play critical roles in determining the nature of the resulting products. These processes are mediated by the fluid properties and structure and by gravity-induced transport. Microgravity experiments largely avoid the complications of kinetic variables by enabling processes to be performed in quiescent, diffusion-controlled transport conditions [5]. This enables synthesis and *in-situ* characterization of materials in ways that cannot be accomplished on Earth. Knowledge gained can help to advance materials processing on Earth both by optimizing methods and providing benchmark data for validation of models used to develop new products. Understanding how processes occur in different gravity levels is essential for development of space-based fabrication and manufacturing, *in-situ* resource utilization, materials re-use, and in-flight servicing.

2. Benefits: This campaign will establish, develop and build a strong, crosscutting program to investigate non-equilibrium processes in liquid-bearing systems. In addition to enabling significant advances in materials application on Earth, the program will: (i) create and characterize new non-equilibrium material structures that can only be made in the absence of gravity, and (ii) exploit gravity-induced convection (and its absence) to tailor the structure and properties of materials, achieving process control and resultant properties that are not possible on Earth. These achievements will help to advance a robust LEO economy for materials production in space. Non-equilibrium effects span all classes of materials and affect high and ambient temperature, biological and electronic processes. Specific benefits of the research will be:

- To achieve an advanced understanding of:
  - Ways in which non-equilibrium liquid and liquid-gas phase processing can be controlled in the absence of fluid motion, sedimentation and buoyancy-driven convection.
  - How processing of multiphase fluids can be controlled to develop novel structures.
  - How freeze casting can be used to produce hierarchical materials with unique properties.
  - Non-equilibrium processes: glass formation, phase separation, metastable crystallization and bubble formation in supercooled liquids.

- Fundamental non-equilibrium phenomena relating to morphological instability during solidification, electro-deposition, and precipitation.
- Practical issues that affect the types of processing that can be accomplished in different gravity levels where transport rates can differ significantly from Earth-based conditions.

- To make accurate measurement of material properties essential for computational modeling to reduce new materials development time/cost. Modeling areas span materials design (*e.g.*, CALPHAD) to molecular dynamics, multi-physics and multi-scale (*e.g*. for additive manufacturing processes [6]).
- To develop and establish new technology skillsets needed in the workforce. A training pipeline and recruitment of diverse, talented personnel is essential to create innovation based on new knowledge and intellectual property that results from the research.
- To improve U.S. economic and technological leadership in amorphous, glassy and hierarchical materials used in optical, aerospace, infrastructure, energy conversion, food and pharmaceutical technologies among others.

3. Examples: Non-equilibrium states are pervasive across numerous scientific disciplines and classes of materials. Selected overlapping topics (see Fig. 1) are used to highlight high impact research problems in the context of advancing both basic and applied research areas in non-equilibrium materials science. **Emphasis is on liquid phase processes where transport properties largely determine the product outcome**. Microgravity is needed to control transport effects that otherwise obfuscate the answers to research questions. High value research activities will be identified and pursued in a flight- and ground-based program that leverages specialized capabilities for characterization and modeling of materials. Work will be coordinated with needs for application development areas, such as those cited earlier.

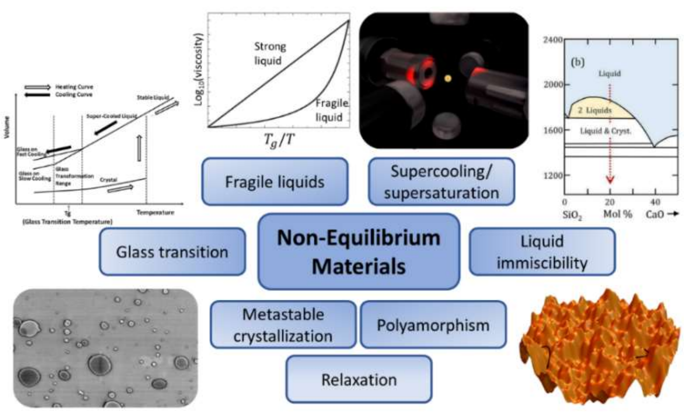

Fig. 1. Topic areas recommended for research on non-equilibrium materials. (Image refs.: A-E)

Within these areas, there are pressing scientific questions where control of fluid motion and sedimentation can enable pioneering research. The use of models to both develop and test ideas and ultimately to establish predictive capabilities is an essential adjunct to the main experimental campaigns.

Glasses can be formed from all classes of materials [7-9]. Changes in thermophysical and thermochemical properties (*e.g*. viscosity, density, heat capacity), structural evolution, and energetics differ significantly among materials - polymerized and unpolymerized ionic liquids, semiconductors, metals, and organic molecules. A unified model of glass formation encompassing these diverse materials will be a major step forward in understanding the vitrification process. Toward this goal, measurements on supercooled liquids as they cool and form glass are important to answer questions about the mechanisms of vitrification. Understanding the extent to which glass forming behavior can be predicted from liquid properties and structure will help to guide the focus of experimental research efforts to improve functional glass properties. In soft materials, molecular conformality can be affected by fluid flow-induced stresses. Understanding how this influences the stability of glasses and their properties can help to improve pharmaceutical and food processing and development of functional soft materials. Glasses formed in a wide range of extreme thermal and chemical conditions occur throughout the Universe. Characterization of natural glass and amorphous materials is needed to evaluate them as resources. Studying the effects and behavior of radiation (*e.g*. cosmic rays) on glasses is important for development of reliable, long range flight hardware.

Fragile liquids exhibit varying degrees of non-Arrhenian behavior in the *lg. viscosity-inverse temperature* relationship [10,11]. The majority of liquids are fragile and many can form glass. These liquids provide a rich area for development of new non-equilibrium products in all classes of materials. Unveiling the temperature and composition dependence of viscosity, density and structure of supercooled liquids above the glass transition temperature is essential to understanding fragile liquids. The Stokes-Einstein relationship accurately relates viscosity and diffusion in some liquids but not others. Exploring the underlying differences between these cases can give valuable insight into structural evolution during processing and expected relaxation mechanisms. Some liquids can undergo strong-fragile transitions. A mechanistic understanding of this transition can provide the basis for developing new materials. For example, fragile liquids often require high cooling rates to avoid crystallization. Understanding effects of microgravity on the critical cooling rates for vitrification of fragile liquids made from heavy metal fluorides/chalcogenides (*e.g*., ZBLAN) is needed to produce high quality optical products from these materials. Thermal processing could be used to develop “fictive temperature gradients” to spatially tailor glass properties. Gradients form in many additive manufacturing processes, so it is essential to understand how these are affected by flows driven by diffusion, convection, and/or surface tension.

Supercooling and supersaturation are frequently means by which a system enters non-equilibrium. The degree to which this occurs depends on avoiding nucleation of new phases. Supercooling/supersaturation is essential to form glass from liquid precursors. Containerless processing can enable deep supercooling/supersaturation of liquids by eliminating extrinsic heterogenous nucleation [12-14]. This process enables investigation of supercooled liquids and often formation of glass or amorphous materials that cannot be made by other methods. Levitation techniques can help to reveal the structural pathways through a variety of cooling routes [4]. These “extreme” glasses can serve as benchmarks for glass discovery. Understanding the ways that thermophysical properties and structure of liquids change as a function of supercooling will help to support models of liquids. For example, correlation of melt and solution properties and structure with process parameters can provide needed data for machine learning based design of functional materials. Understanding how the properties of supercooled/supersaturated molecular liquids behave in response to fluid flow is important for development of non-equilibrium phases in soft materials. Terrestrially, practical issues of fluid motion and dissolved gases affect the degree to which liquids can be supercooled. In microgravity, supersaturation of dissolved gases in “quiescent” liquids can be explored and exploited to develop new structural materials. Freeze casting can transform polymeric aqueous solutions and colloidal suspensions into complex hierarchical glassy and composite materials, such as those mimicking nacre and other bio-inspired materials with superior mechanical behavior and other unique properties [15, 16]. Controlled freezing experiments in a microgravity environment combined with multiscale modeling provides a powerful means to develop a fundamental understanding of the combined effects of fluid flow on complex reorganization of non-equilibrium matter.

Fluid immiscibility, or phase separation, results in formation of coexisting liquids with different chemical composition and usually different density [17]. In addition to diffusion, the morphology of such mixtures depends on convective transport and density driven sedimentation. Inhomogeneities or phase separation may be useful if they can be introduced into a liquid or glass in a controlled manner to develop periodic differences in density, composition, refractive index or hardness. The degree to which fluid motion affects phase separation and the morphology of resulting products will be crucial for space-based materials processing. Understanding how phase separation affects the stability of glasses that are prone to surface (interface) crystallization is needed for future *in-situ* resource utilization. The behavior of dissolved and exsolved gases can also result in two phase mixtures. Flow and buoyancy can move gas bubbles in liquids, and the magnitude of motion affects the ability to remove unwanted gases (fining). Precise measurements of diffusion coefficients can play a significant role in developing realistic models of convective dissolution processes, such as those in CO_2 sequestration techniques [18].

Polyamorphism is the transformation of an amorphous phase into a different phase with the same chemical composition and different density (High and Low Density Amorphous, HDA and LDA) [19]. New high performance optical glasses can be explored with better knowledge of how polyamorphism is related to glass formation, fragile-strong transitions and incongruent phase separation. Investigation of the properties, structure and energetics of HDA/LDA phases *in-situ* can provide data on complex systems undergoing metastable transformations.

Metastable Crystallization frequently occurs from a vapor or a liquid *via* formation of nanosized and often disordered nuclei, or phases with different structure from the stable bulk form [20]. The crystallization pathway typically proceeds *via* metastable phases with incremental changes in structure and free energy occurring until the most stable product forms. Kinetic stabilization of novel metastable materials can be enabled by understanding the thermodynamics of phases at the nanoscale. Thermodynamics and kinetics of crystallization are both relevant to glass and glass ceramics production. Morphological instability can result from positive feedback between diffusional gradients and interface motion during processes such as solidification, electrodeposition and precipitation. Avoidance of natural convection is essential to investigate and characterize these phenomena that will be important in space based materials processing and fabrication. Quantifying the energy released when supercooled liquids and metastable materials crystallize is important for modeling heat transfer and hydrodynamics of deep space environments.

Relaxation decreases the free energy of a non-equilibrium state, usually *via* activated processes that transition between minima in the energy landscape. When a glass is “trapped” in a low energy state, it may persist indefinitely due to large activation barriers [21, 22]. Understanding the origins of primary and secondary relaxation modes will help guide discovery of more stable non-equilibrium phases. This is important in both hard and soft matter glasses where different degrees of stability occur. Flow can affect relaxation, particularly in molecular liquids where conformality changes can alter non-equilibrium processes and kinetics. Shear-induced flows and mechanical excitations of the liquid change chemical trajectories through the energetic landscape, resulting in unexpected reaction selectivity [23-25].

4. Action Plan, Scope and Costs: This campaign will establish a Science Definition Team (SDT) that will work closely with NASA to advise, recommend and drive the research program. The goal will be to establish a broad-based community in the area of non-equilibrium materials to develop and implement a program of reduced gravity and ground-based research. The research is crosscutting and impacts multiple fundamental and applied areas. The scope of materials and disciplines overlaps major NASA program areas and mission elements. It includes polymerized and unpolymerized ionic liquids, semiconductors, metals, and organic molecules over a range of temperatures and in a variety of chemical and flow conditions. Establishing multi-disciplinary and international teams will leverage resources and maximize the research output. A high-risk/high-payoff component to provide Rapid Access Funding (RAF) in selected areas will accelerate transformational advances identified in the fundamental research [26, 27].

To maximize impact, the research will include both flight- and ground-based components. Flight experiments exploit the unique capabilities available on rockets, orbiters and potentially planetary-based facilities to control gravity level, fluid flow, sedimentation and convection. Augmenting this work with ground-based characterization and experiment development significantly extends the reach and impact in a cost-effective way. Ground-based research will provide a control to isolate effects of gravity and allow detailed characterization and modeling of materials properties and measurements of structure. These goals will be met *via* ground-based use of: (i) specialized NASA facilities (*e.g*. the ground based electrostatic levitator), in some cases with performance upgrades, (ii) specialized university-based facilities for materials characterization, (iii) national user facilities such as the Advanced Photon Source and Spallation Neutron Source to measure atomic structure and dynamics, (iv) powerful computational modeling for analysis and efficient development of experiments and new materials, and (v) collaborative and international research that achieves the diverse range of knowledge and skillsets needed to solve complex problems.

The campaign will be implemented over 10 years at an estimated total cost of *ca*. $120M, as summarized in the table below. It is important to provide sustained funding and avoid de-scoping of selected projects. Four-year projects with renewal options are recommended. Resources will be used to develop and implement a broad research campaign on non-equilibrium materials. A spending profile is proposed that: (i) emphasizes establishing an SDT, program development and flight hardware commissioning in years 1-5, and (ii) experimental research that tapers from ground-based emphasis during years 1-5 to mainly flight-based in years 6-10. Modeling will be funded throughout the campaign. RAF will provide fast-track investment to serve specific mission requirements and/or catalyze realization of transformational products that result from the research campaign. RAF will be available throughout the project. This campaign will provide the “hub” through which the research will be integrated with NASA’s programs.

Program area	**$M,10 Y**	**Main activities**
Program development	1	Establish SDT, build community, workshops (*e.g*. *via* ASGSR)
Ground-based research	25	Flight optimization, structure measurements, characterization
Flight-based research	30	Liquid transport properties, kinetics, diffusion/convection effects
Computer modeling	10	Advanced process-property-structure models
Flight hardware	35	Upgrade successful flight hardware for liquids
RAF	20	Years 1-10, accelerated TRL advancement

*Sustained moderate inflation will decrease the value of the investments. Offsetting funding increases will be required in the future.

Two important elements of the flight program will be use of: (i) containerless techniques, and (ii) high performance light microscopy to study non-equilibrium materials *in-situ*. Flight hardware development is expensive and relatively high risk. Upgrading and/or re-using NASA and international flight hardware designs (*e.g*. the JAXA electrostatic levitation furnace that can uniquely serve non-metals, semiconductors and metals research with upgrades [28]) is an efficient and cost-effective way to build on previous investments, know-how and successes. Soft matter research will benefit from the planned replacement of the NASA Light Microscopy Module [29], enabling investigation of non-equilibrium effects in colloids, particles and phase separating liquids around ambient temperatures. Ideas for upgrading instruments were briefly discussed in the course of developing this paper, for example addition of enhanced instrumentation, imaging, heating and sample environment capabilities to flight- and ground-based hardware. Modeling will accelerate and broaden the transfer of new data to applications, particularly when benchmarks are used for validation [31, 32]. Close connection between experimental research, modeling, and measurements of data will help to ensure a well integrated and high output research program.

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