Gravitational Effects on Rapid Solidification of Metal Powders for On/Off-Earth Additive Manufacturing

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Rapid solidification of metal powders (RSMP) is the key material process in many metal additive manufacturing (MAM) techniques such as selective laser melting, electron beam melting, and direct powder deposition. Solidification, as the initial stage of MAM materials joining process controls microstructures formation and evolution; i.e. miniatures such as grains and voids that determine final material properties and dimensional accuracy. Thus, understanding and predicting microstructures during RSMP opens an opportunity for quality control and property optimization of additively manufactured metals. Such capabilities require a real-time measurement tool for on the fly monitoring of RSMP microstructures during MAM, which is not currently available; in fact, this is one of the main obstacles for widespread industrial acceptance of MAM despite its huge potential to revolutionize traditional metal manufacturing technologies. We propose to establish a predictive and quantitative computational framework and tool for RSMP and verify/validate the computational tool using on-earth microstructural characterizations for MAM process. We will use this computational tool as a virtual RSMP laboratory with realtime microstructures monitoring to investigate microstructural evolutions under (1) different MAM processing parameters such as laser power and hatching speed for advancing on-earth MAM and (2) different gravitational forces such as Mars’s gravity and microgravity for exploring off-earth MAM possibilities.

The proposed computational framework for RSMP will be able to predict (1) powder compacting, an indicator of dimensional accuracy, as a function of powder size, powder shape, and gravity; thus, it will be able to simulate ~100,000 powders and more, (2) microstructural evolution as a function of MAM processing parameters and gravity; thus, it will act on micrometer length scale and millisecond time scale, (3) quantitative metrics in order to verify/validate the framework with experiments; thus, it will be directly connected to nano scale predictive computational models (molecular dynamics, MD). We propose to initially apply the proposed computational model to study RSMP of titanium powders, given its lightweight and widespread use in as implants and high temperature environments. This stems from the interest of the local industry in Memphis area that includes biodevice companies such as Smith & Nephew, Wright Medical, Microport, and Medtronic, aircraft maintenance requirements in FedEx, and NASA’s interest in lightweight structures. However, the created knowledge can be easily generalizable to study RSPM of other metal powders. A local original equipment manufacturer (Surface Dynamics) for our local biodevice companies will provide additively manufactured titanium samples for the experimental validations/verifications; see the attached letter of collaboration. Computed tomography scans (CT-Scans) of the samples for dimensional accuracy will be conducted at FedEx TechConnect facility; see the attached letter of collaboration. Microstructure characterizations of the samples will be conducted at Integrated Microscopy Center on University of Memphis’s campus.
The main difficulty in computational modeling of microstructural evolutions comes from dealing with the separating interfaces between two different microscopic regions; e.g., interfaces between the solid particles and the liquid matrix or interfaces between different grains at solid particles. PFM is one of the most computationally effective models to deal with interfaces during microstructural evolution [1]; newer class of PFMs such as phasefield crystals also offer nanoscale resolutions (Asadi et al. [2, 3]). PFM and PFC treat the interfaces as diffusive areas and considers a thickness for each interface [4-6]; this allows smooth transitions of variables and produces non-zero gradients of variables at the interfaces. Although PFM and PFC connected to lower-scale computational models such as molecular dynamics (MD) [7], has the potential to predict the solidification microstructure of metals; these models act on diffusive time scale (long time), making them unable to capture critical microstructural evolutions during RSPM that occurs at lower time scale. Therefore, we will use another approach called dissipative particle dynamics (DPD) [8, 9] based on modified-embedded atom method (MEAM) formulation of MD [10-12] and coarse-graining approaches. DPD model increases the length scale of MD from nanometers to micrometers and its time scale from nanoseconds to milliseconds making it suitable for simulations of RSMP of metal powders during MAM. Two DMP models will be derived; one for microstructure prediction and one for powder compacting studies. Both DMP models will be quantified based on MD simulations and will be verified/validated based on experiments. The schematic of the proposed modeling framework is shown at Figure 1. Once the modeling framework is validated/verified, it will be used in a series of simulations to study off-earth RSMP of metal powders. These results will be compared to their on-earth counterparts to determine the possible challenges for off-earth MAM.

Figure 1: The schematics of the proposed work to study RSMP of metal powders. DMP stands for dissipative molecular dynamics model.