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Science-informed materials discovery via computational materials engineering: Multi-scale multi-physics modelling

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Abstract

Additive manufacturing (AM) is a promising, emerging, designable materials processing method used for fabricating complex three-dimensional geometries with multi-material and compositionally/functionally graded structure required for various future engineering applications. Fusion-based AM which melts materials-by-materials and layer-by-layer using prescribed scanning path could offer precise dimensional control and designable microstructure and site-specific property. The challenge lies in process control; melt flow dynamics, materials mixing, and composition change during the multi-material AM process. The composition-process design is vital for predicting laser power-time-temperature processing window and final quality. This talk will focus on computational additive manufacturing enabled materials discovery and the development of a holistic computational AM framework to enable multi-material AM for engineering, especially, discovery of new materials and processing route for biomedical application. A high-fidelity multi-physics multi-scale modelling approach for accurate tracking of surface shape, thermo-capillary dynamics and vaporisation is developed and used to search for new materials with processable conditions to have desired micro/nanostructure and controllable property. The computational materials engineering framework serves as a science-based tool to enable materials discovery with precise processing route using multi-material AM.

Keywords:

Multi-material additive manufacturing Materials discovery Computational materials engineering