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Accelerating alloy design for Additive Manufacturing: A modelling perspective

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Abstract

Alloy design has accelerated over the last couple of decades through Integrated Computational Materials Engineering (ICME), that systematises the use of materials modelling to understand chemistry-process-structure-property correlations. With the advent of Additive Manufacturing (AM) in recent years, there has been greater focus on adapting the ICME tools for alloy design by taking into account the effect of the unique process conditions of AM on the microstructure and properties.

In powder-bed-based AM techniques, each layer of metallic powder is spread out and selectively melted by a laser or electron beam, thereby building up a part layer-by-layer. Due to the rapid cooling rates and high thermal gradients involved, several key issues come up while designing materials for metal AM. Firstly, defects such as cracks and porosity may form easily, which deteriorate the printability of alloys. Next, rapid solidification conditions influence the phase formation and segregation. Finally, the structure is typically made up of large, columnar grains. Elaborating on these four key aspects of printability, segregation, phase formation, and grain structure control, we present the existing knowledge and modelling approaches to tackle them, what works and does not work for AM, the new directions that we have taken, and finally the opportunities that are available. Examples from different alloy classes such as steels and Ni-base superalloys demonstrate the pathway to accelerate alloy design for metal AM through ICME.

Overall, we show that ICME tools have to account for or be adapted to account for rapid solidification effects and multicomponent interactions in order to be used reliably for alloy design for metal AM. Advancements in these areas are crucial for more widespread adoption of metal AM technology.

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Durga Ananthanarayanan is a researcher at the Department of Materials Science and Engineering, KTH Royal Institute of Technology, Stockholm, Sweden. She attempts to unravel the connection that is forged between processing of materials and microstructures through fiddling with Gibbs energies and partial differential equations. Her current research focus is on alloy design for metal additive manufacturing using computational thermodynamics and kinetics. Previously, she worked as a Research Scientist at GE Research, Bangalore, India, wherein she applied materials modelling to optimise casting and additive manufacturing of Ni-base superalloys. She graduated from KU Leuven, Belgium, in 2015 with a PhD focused on the development of a phase-field model coupling mechanical and chemical effects to simulate microstructural evolution during solid-state phase transformation.

Zoom link: https://arizona.zoom.us/j/86328470857