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# Computational Materials Science

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## Preface to the special issue ‘Additive Manufacturing’

With the ability to overcome deficiencies of current manufacturing techniques, additive manufacturing (AM) otherwise known as 3D printing is gaining widespread usage in aerospace, medical, energy, automotive, consumer products, and other industries. AM has been used for rapid prototyping for several decades, but with continuing improvements in hardware and software, we now use it to manufacture parts that could not be easily and economically made before. Examples include intricate metallic parts with fine and closely spaced features, customized components such as patient-specific medical implants, components with internal cooling channels, parts with site-specific chemical composition and properties, lattice structures and truss networks with optimized strength to weight ratios. The AM process has a short lead time, and we can now print many parts as a single unit that previously required assembly. The same equipment can produce very different parts, especially legacy parts for which the supply chains no longer exist. The recent available data on machine sales and the number of patents granted suggest the continued growth of AM in the foreseeable future.

In AM metals are deposited layer-upon-layer to make three-dimensional structures of common alloys such as steels, nickel, titanium, and aluminum alloys. There are several variants of AM depending on the types of the power source and the feedstock, but two main techniques, powder bed fusion, and directed energy deposition are commonly used. AM is a relatively new process and it faces many scientific, technological, and commercial problems [1]. Of the 5,500 commercial alloys, only a handful are now routinely printed. The quality of 3D printed parts is often affected by the formation of common defects such as porosity, lack of fusion, and cracking [2]. These defects significantly degrade the mechanical properties and serviceability of the parts and lead to part rejection in extreme cases. Mitigation of defects to improve part quality is often performed by trial-and-error of the process variable adjustment. The complexity of the AM processes, the high costs of equipment and feedstock make the use of the current trial and error technique expensive and time-consuming. In addition, models can correlate process variables with the product attributes. As a result, when a model is adequately tested and validated, its use before printing can reduce the parameter space, save time and money, and improve quality [3].

Improving microstructure, properties, and serviceability of parts will require a framework that uses the theories of metallurgy with the emerging tools of mechanistic, statistical, and machine learning tools [3,4]. Connections between process variables and the geometry, composition, microstructure, mechanical properties, and defects for a given alloy based on scientific principles via modeling can expedite progress in this important area. The papers in this special issue provide

examples of recent progress in this area. For example, heat transfer and fluid flow models [5–10] are used to predict temperature and velocity fields, molten pool shape, and size. Examples of modeling of solidification structure [11], common defects such as cracking [12] and porosity [13,14], evolution of residual stresses [15] and mechanical response of parts [16] are also included in the special issue. In addition, the special issue provides examples of applications of data-driven techniques such as machine learning for reducing defects [17] and controlling mechanical properties [18]. Clearly significant progress has been made in diverse areas. It should be recognized that work in this important area is just beginning. If the time taken for modeling other important manufacturing processes such as welding and casting provides any indication of the efforts needed, AM will require sustained research and development over many decades.

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