The Materials Genome Initiative and Additively Manufactured Metals: New Computational Tools and the Central Role of Materials Data

The classical method for designing materials to achieve certain performance goals involves a laborious procedure wherein intuition drives the design of a material that is then created and tested. In most cases, the performance goals are not achieved, and this costly procedure is repeated. By integrating data, computations, and artificial intelligence it is possible to break this expensive cycle and bring innovative new materials to the marketplace faster and at a lesser expense. The materials design process requires links between processing conditions and the resulting microstructure. We illustrate an approach to coupling the processing conditions of additive manufacturing (AM) to microstructure. A phase field model has been developed that follows the evolution of thousands of grains in three dimensions as a heat source propagates along a surface at the high rates seen during AM. Through this approach it is possible to determine the effects of the solidification conditions, the weld pool geometry, and multiple passes of the heat source on the resulting grain morphology.