Karlstad Applied Analysis Seminar (2020)

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Numerical and multiscale materials modelling of formation and effects of material defects

Abstract

Material manufacturing processes result in a variety of defects at different spatial scales across different respective material hierarchies and substructures. These defects are the result of various physical mechanisms associated with solidification, forming and deformation and extrusion processes, to name a few. The role of these defects is of great interest as they have a profound and fundamental role in the resulting material behavior, or in more macroscopic terms, the associated engineering material and product properties. In current work we focus on defects, their formation mechanisms and their role on material behavior particularly at the scale of material nano- and microstructure. The approach is primarily computational, i.e., we present a range of multiscale materials modeling associated methods to tackle the respective physics across a range of materials, from metallic alloys to thin films and hard materials all the way to composite microstructures. We briefly review the multiscale computational paradigm and subsequently focus on use cases. Firstly, we assess microstructure and defect formation mechanisms in solidification, particularly related to metal additive manufacturing. Secondly, we assess the role of dislocation substructures and microstructural defects with an eye on implications to metal plasticity and fatigue strength by way of crystal plasticity and micromechanical modeling. Lastly, we address defects both in hard material and polymer-based carbon fiber reinforced composites. Additionally, we discuss and present some recent progress with data-driven

methods, i.e., concepts and examples how to utilize machine/deep learning methods in better exploiting the physics- based model derived defect evolution data for design, inference and constrained optimization purposes.