Aligning molecular and structural dynamics in fused deposition modelling: Novel routes to tailor product functionalities

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Additive manufacturing, often referred to as 3D printing, is a rapid developing technology. Products are created layer by layer, rendering extraordinary dimensional flexibility and control in fabrication of complex geometries. Via a variety of 3D printing technologies, niche products of high added value are entering automotive, aerospace, defense, art and medical industries [1]. However, from economical perspective reservations rise due to mismatched expectations in production speed and functional product quality; the Achilles heel of 3D printing. Low production speed and disappointing product quality are particularly evident for materials of thermoplastic origin that are processed via fused deposition modeling (FDM).

FDM relies on the facile processability of thermoplastics, whereby material is extruded and shaped in liquid state, after which the new shape preserved upon solidification. However, thermoplastics differ from other materials classes such as ceramics and metals since covalent bonds and subsequent connectivity of elementary building blocks into large individual macromolecules can slow down the molecular mobility significantly [2]. In addition to the common time scales of layer build-up and temperature changes also those of conformational rearrangements (like crystallization), intermolecular diffusion during shaping need to be taken into account and balanced in case of FDM with macromolecules, as depicted in Figure 1 (a).

In this study the local structural effects of (mis-)aligned timescales are mapped for polylactides via systematic variations in judiciously chosen molecular parameters. Polylactides varying in molar mass and enantiomeric purity, and consequently different fusion and crystallization dynamics, serve as model. Results indicate that complex heat management that deviates as function of build height and print speed lead to layer-specific inhomogeneity in degree of fusion, crystallization, crystallographic composition, thermodynamic and thus geometrical instability (Figure 1(a) and (b)). The molecular understanding of the dynamics of fusion, crystallization, print strategy, coupled with the use of additives (reinforcing phases, nucleating agents and blending strategies to promote fusion) provide opportunities to exploit, position and direct local structure induced functionalities.

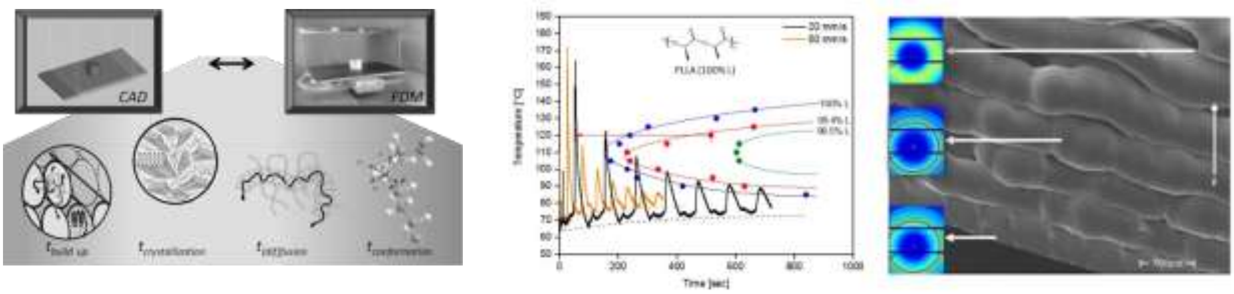

Figure 1: (a) Illustration of timescales relevant for FDM; (b) Temperature profiles for different print speeds overlaid by the isothermal crystallization half-times of polylactides with varying L-enantiomeric purity, illustrate timescales of printing, crystallization; (c) Inhomogeneity in crystallization as a result of printing.

References:

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