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Further development of a simulation model for the description of the crystallization kinetics of semi-crystalline thermoplastics

Felix Winkelmann, Dr. Robert Hein
German Aerospace Center

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Additive Manufacturing

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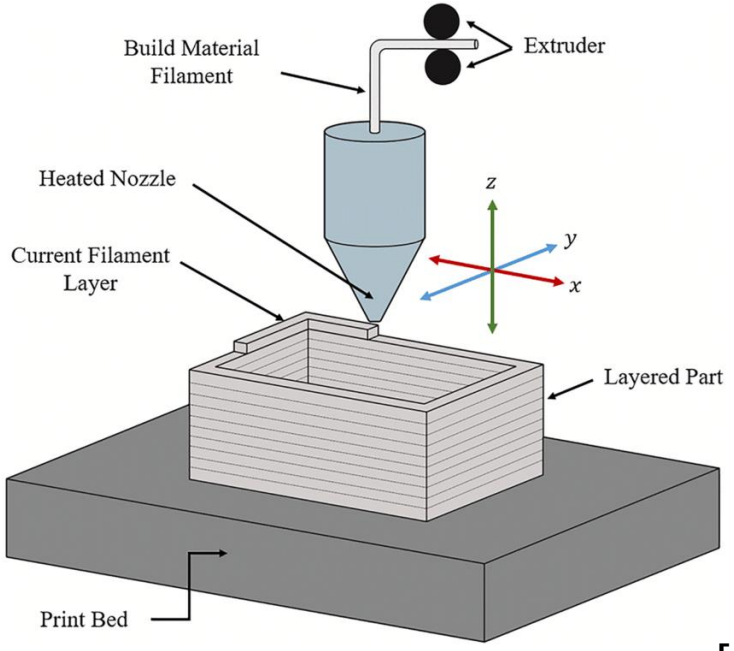
Motivation - Additive Extrusion

- Additive extrusion processes enables qick manufacturing of complex structures without moulds
- Many process parameters influence the final properties
- Process simulations can help to predict the properties and evaluate the process parameters



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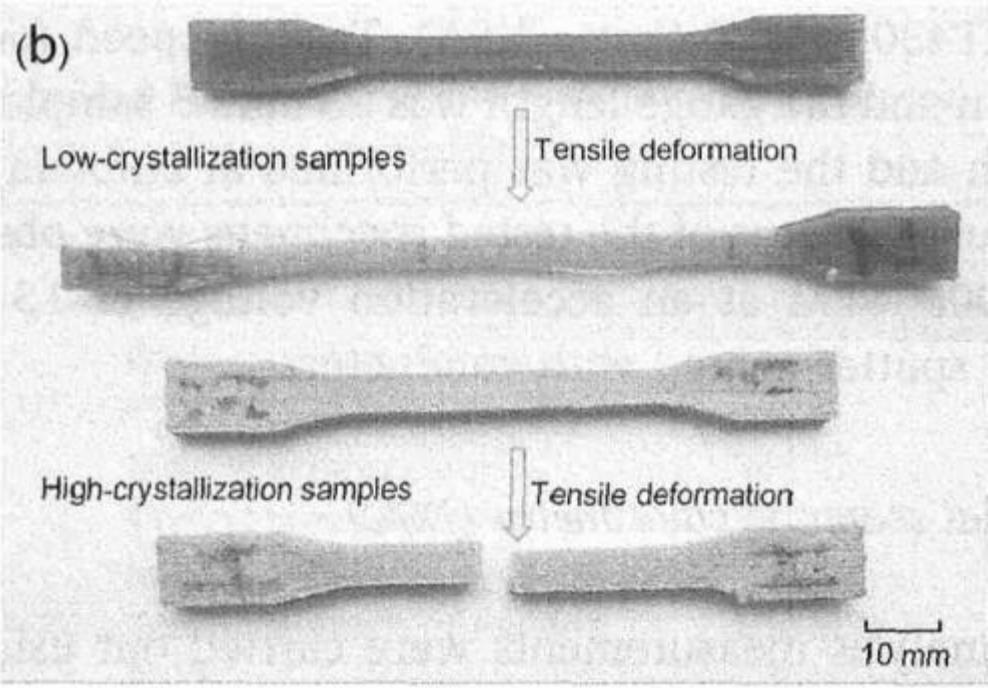
Motivation - Crystallization

- Crystallization influences the mechanical and technical properties of the material
- Degree of crystallization depends on material properties and cooling conditions
- Complex processes during cooling
  - Approach via DSC measurements



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Fitting of DSC data

- Fitting function:

$$X_{vc} = X_{vc\infty}(w_1 F_{\vartheta 1}(k) + w_2 F_{\vartheta 2}(k))$$

$$k(T)_i = I_i = C_{1i} T e^{-\left(\frac{C_{2i}}{T - T_g + T_{add,i}} + \frac{C_{3i}}{T(T_{m,i} - T)^2}\right)}, i = 1,2$$

- Fit 10 curves from DSC measurements with one parameter approach

- Final fitting with genetic algorithm that calculates population from random start values and checks their fitness

Local optimization

Fitting possible but only with good initial values

Fitting several curves in parallel problematic

Global optimization

Fitting works without starting values

Fitting several curves in parallel works

Long fitting times

Alternativ approaches for fitting and calculating the degree of crystallization

Avrami approaches

Simplified Avrami approaches

No successful fits

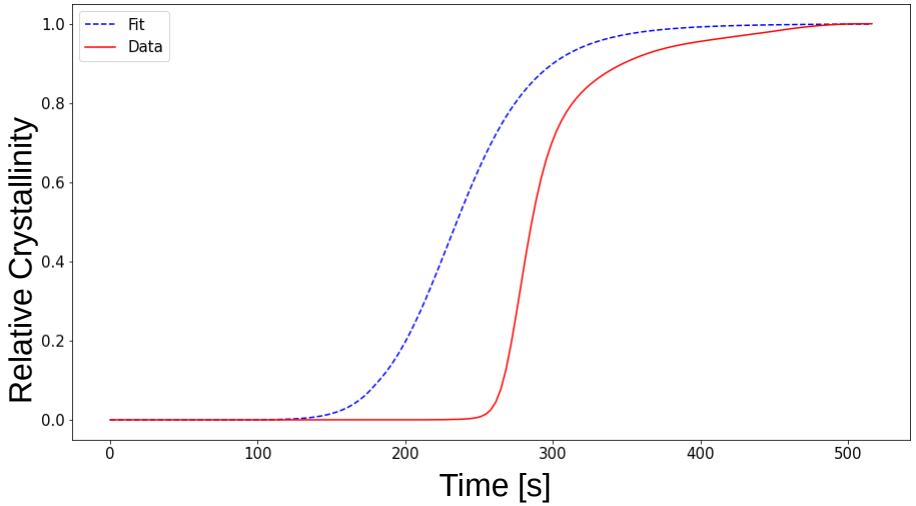
Conclusion

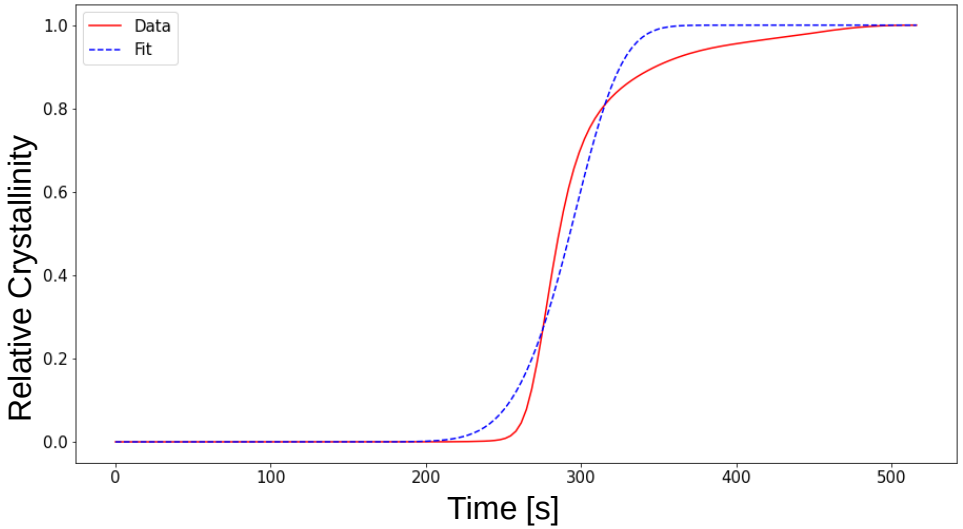
Velisaris and Seferis is used

Nakamura model

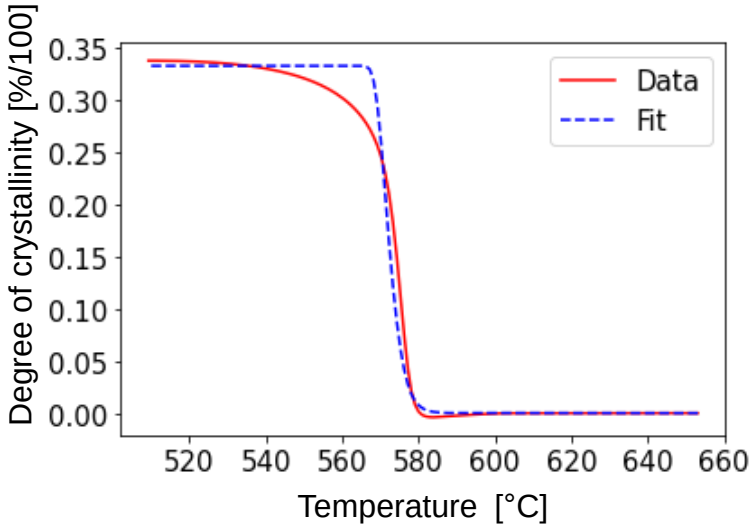
Calculation of the relative degree of crystallization

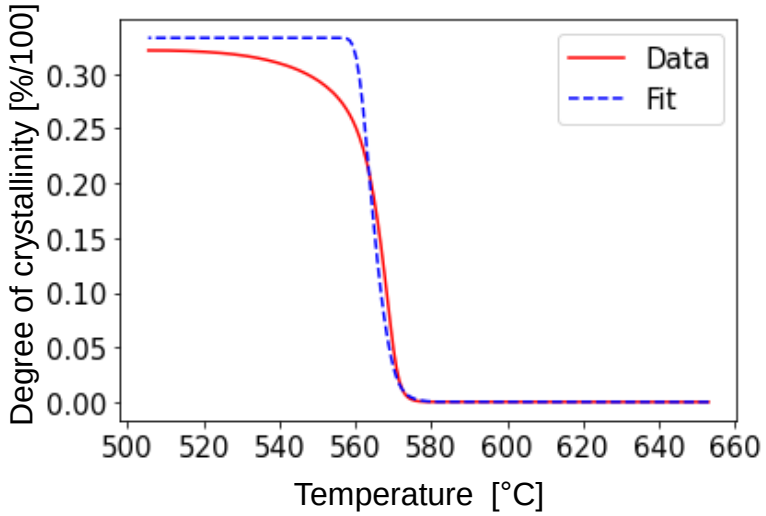
No information on absolute crystallinity

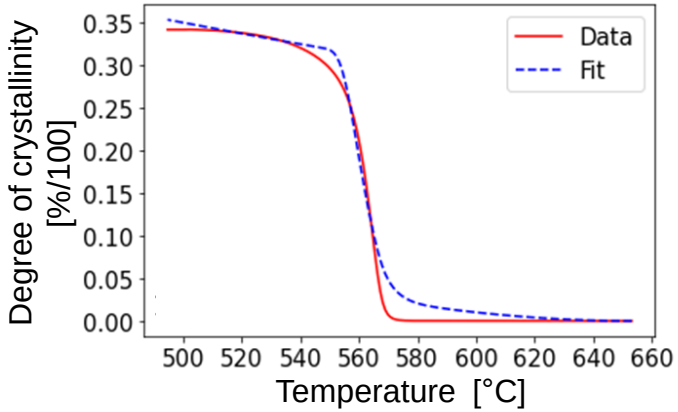


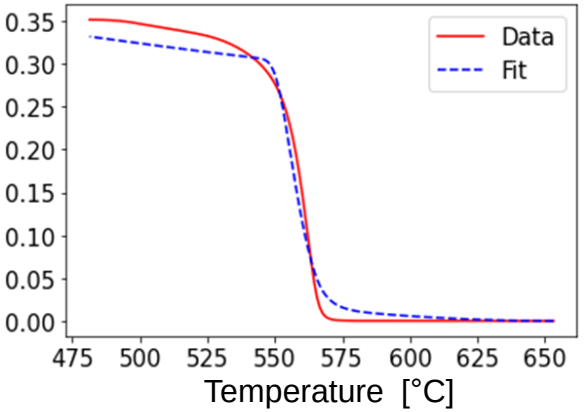


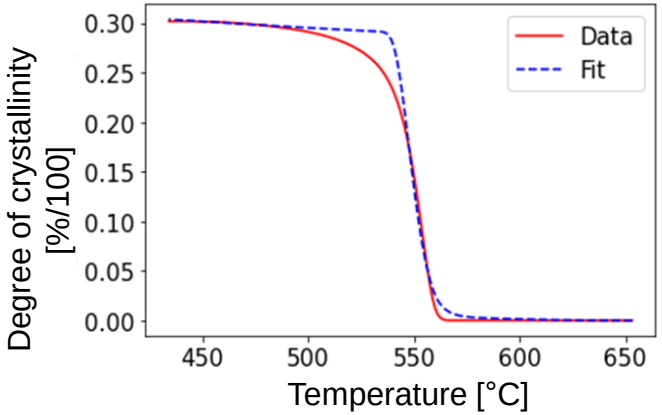
Fit optimization through data selection





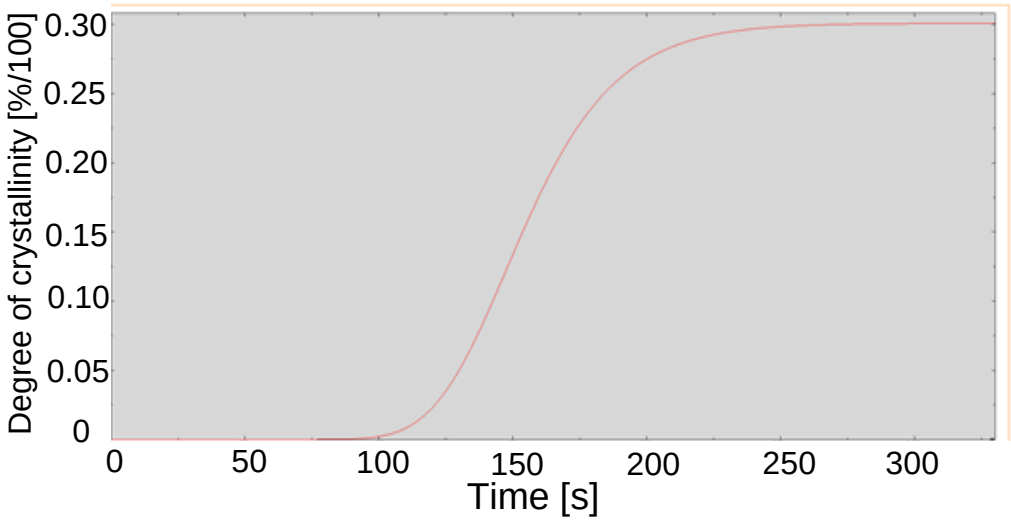


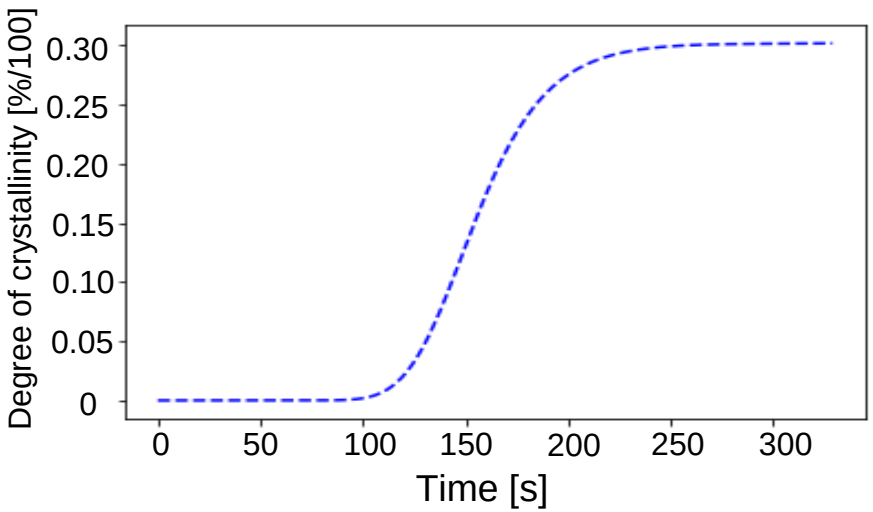




Implementation in Abaqus

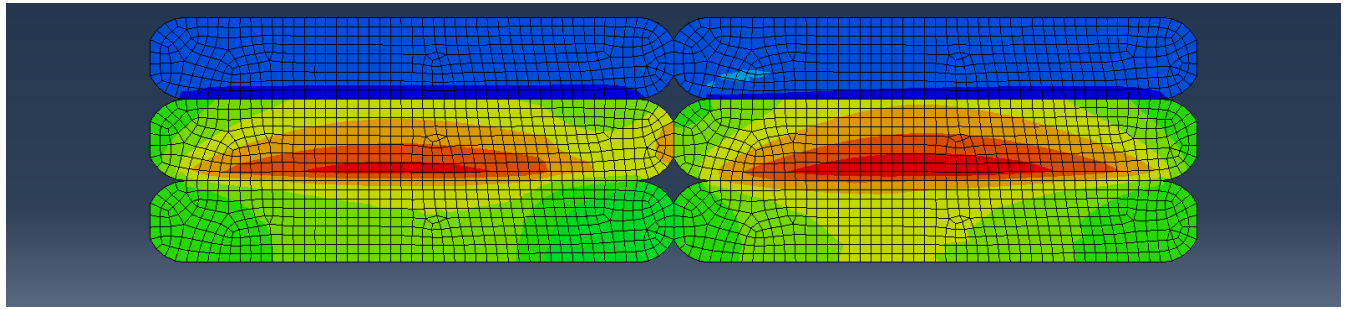
- Model essentially implemented correctly in Fortran (Python / minimal model).
  - Proof by agreement of minimal model and calculations in Python and Octave

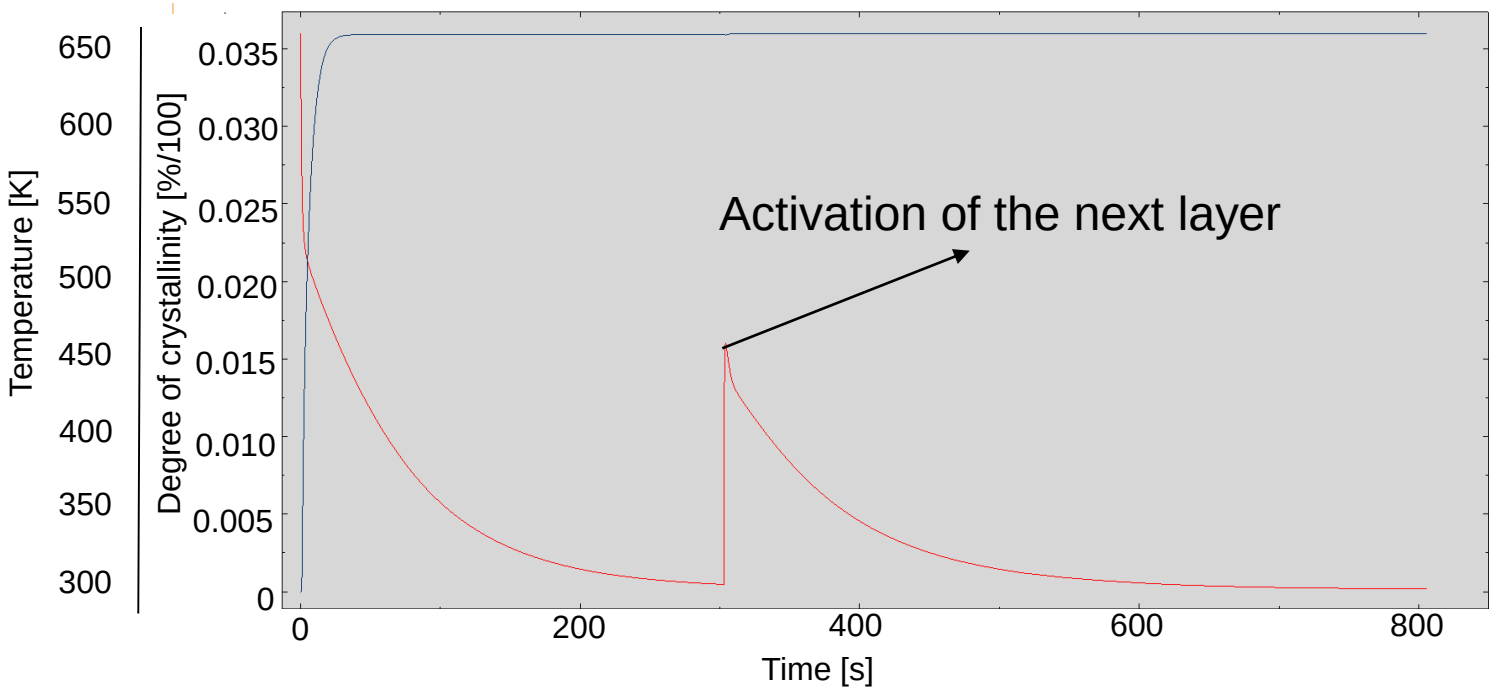




Implementation in Abaqus

- Test with 2D model of a deposition process
  - Bead wise activation





- Calculated degrees of crystallization are very low (between 0.5 and 4 % at standard conditions)
- Data basis of the calculation must be extended

Conclusion and outlook

- Script for the fitting of semi-crystalline thermoplastics works
  - the less variance in the data the better the fit
- Improvement by fitting to expected cooling rates
- Application via fitting script - enter parameters in subroutine - run simulations

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- Flash DSC data fitting still open
- Validation with experiments
- Coupling with AM simulation from Abaqus

Integration in future process simulation

- Crystallization model as a module part of a process simulation
- Future implementation in a toolpath based deposition simulation on part scale

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Thank you for your attention

Felix Winkelmann - German Aerospace Center

Institute of Composite Structures and Adaptive Systems | Structur mechanics | Lilienthalplatz 7 38108 Braunschweig

Phone +49 531 295 1054 | felix.winkelmann@dlr.de

DLR.de

Literature

- [1] https://de.wikipedia.org/wiki/Riesenmammutbaum
- [2] https://www.aim3d.de/materialien/kunststoffe/
- [3] https://www.stratasysdirect.com/technologies/fused-deposition-modeling
- [4] Large-scale 3D printers for additive manufacturing: design considerations and challenges
- [5] Influence of thermal processing conditions in 3D printing on the crystallinity and mechanical properties of PEEK material, Yang,Tian,Li et. al. , Journal of Materials Processing Tech., 2017

Calculation approach and physical basis

- Further development of the Avrami approach for non-isothermal conditions
  - Basic type originates from metallurgy
- Dual kinetic approach to calculate the degree of crystallisation according to Velisaris and Seferis
  - Takes nucleation and growth into account
- 13 parameters are determined by fitting to DSC data (C_{1i}, C_{2i}, C_{3i}, $T_{add,i}$, $T_{m,i}$, n_i, w_1)

Formulas

$$X_{vc} = X_{vc\infty}(w_1 F_{\vartheta 1} + w_2 F_{\vartheta 2})$$

$$F_{\vartheta i} = 1 - e^{\left(-\int_0^t k(T) n_i \tau^{(n_i - 1)}\right)}, i = 1,2$$

$$k(T)_i = I_i = C_{1i} T e^{-\left(\frac{C_{2i}}{T - T_g + T_{add,i}} + \frac{C_{3i}}{T(T_{m,i} - T)^2}\right)}, i = 1,2$$