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WHY IS THIS RELEVANT?

Re-entrant auxetic structures exhibit a negative Poisson's ratio and are particularly attractive for applications requiring high energy absorption, damping capacity and resistance to impact. Their unconventional deformation mechanism arises from the progressive rotation and opening of the re-entrant unit cells, which causes the structure to expand laterally under tensile loading. However, this behaviour is highly sensitive to the actual geometry of the manufactured lattice. Small deviations in thickness, node position, re-entrant angle or cell connectivity may modify the intended deformation mechanism and lead to significant differences between the nominal and experimental mechanical response.

The fabrication of these structures by Fused Filament Fabrication (FFF) using PEEK is especially challenging because of the high processing temperatures involved. The differences between extrusion, build-chamber and build-plate temperatures generate steep thermal gradients, non-uniform cooling and material shrinkage. These phenomena promote the accumulation of residual stresses, which may lead to distortion, dimensional inaccuracies and changes in the expected mechanical behaviour. Numerical simulation therefore provides a valuable tool for predicting critical thermal conditions and defining strategies to reduce manufacturing-induced stresses before experimental production.

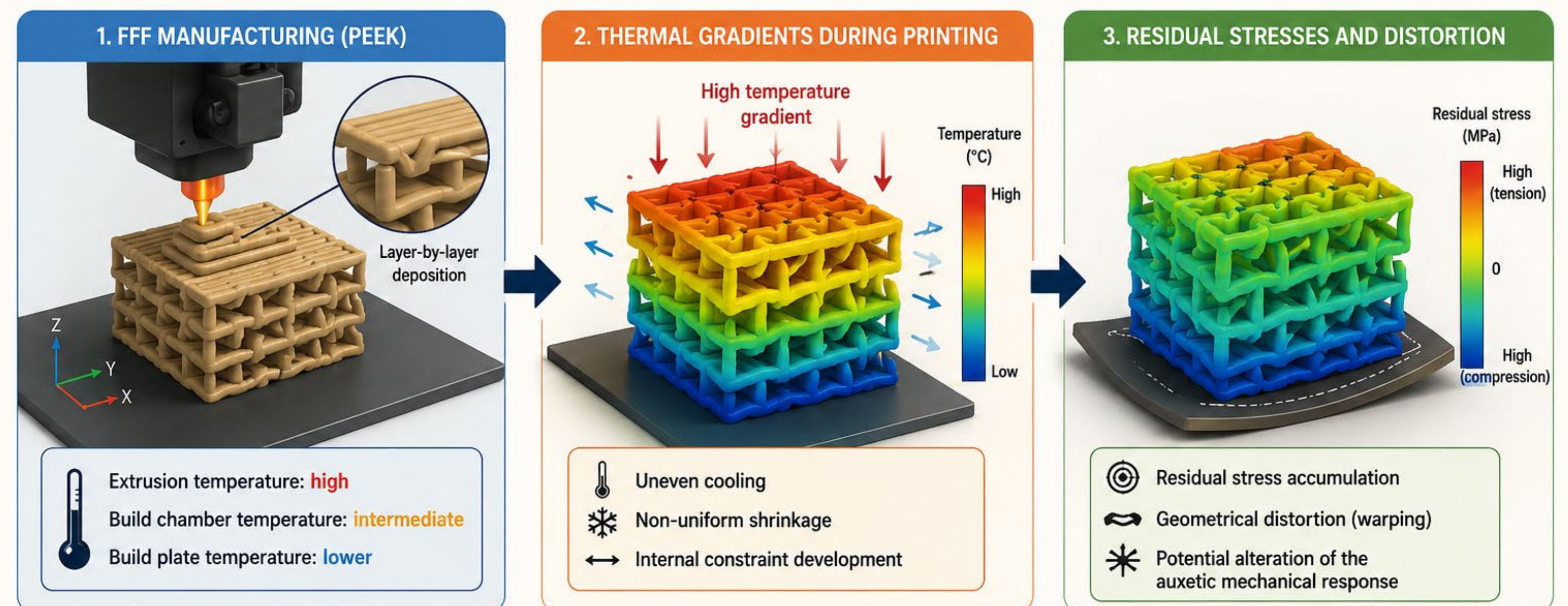


Fig 1. Schematic representation of the thermo-mechanical origin of residual stresses in FFF-manufactured re-entrant PEEK auxetic structures: layer-by-layer deposition, thermal gradient development, and subsequent residual stress accumulation and geometrical distortion.

OBJECTIVES & METHODOLOGY

The main objective of this work is to experimentally demonstrate that Digimat-AM® [1] can reliably reproduce the thermo-mechanical behaviour of the FFF manufacturing process for PEEK re-entrant auxetic structures. By comparing numerical predictions with experimentally observed trends, the study aims to validate the capability of the simulation framework to identify the main thermal parameters governing residual stress development during printing.

Once validated, the numerical model is used as a predictive tool to explore and optimize post-deposition thermal treatments. The ultimate goal is to identify a thermal conditioning strategy capable of reducing residual stresses and stress concentrations, thereby improving the thermo-mechanical response, dimensional accuracy and overall reliability of the manufactured auxetic component.

S1 Experimental characterization and Z-PEEK material modelling

A comprehensive experimental characterization of Z-PEEK was first performed to obtain the thermal and thermo-mechanical properties required for numerical process modelling. Dynamic Mechanical Analysis coupled with Digital Image Correlation (DMA-DIC) was used to determine the coefficient of thermal expansion over a temperature range from 20 to 315 °C under a constant load of 100 mN. The methodology was initially validated using aluminium and Grade 2 titanium reference specimens and was subsequently applied to commercial filament and FFF-manufactured Z-PEEK samples printed at 0° and 45° directions.

The non-isothermal crystallization behaviour of Z-PEEK was characterized by Differential Scanning Calorimetry at cooling rates of 1, 2, 5, 10, 15 and 20 °C/min. The experimental crystallinity curves were used to calibrate a Nakamura model coupled with Hoffman-Lauritzen theory. The best agreement between the experimental and numerical results was obtained for an Avrami exponent of $n = 1$. These results, together with the glass-transition temperature, melting and crystallization temperatures, transition enthalpies, thermal stability and complementary mechanical properties, were implemented in Digimat® to generate a representative temperature-dependent material model for Z-PEEK. This previous work is shown in [2]

S2 Cross-validation of the thermal parameter sensitivity

The calibrated material model was transferred to Digimat-AM® to simulate the layer-by-layer manufacture of a re-entrant PEEK auxetic structure. A parametric study was initially performed by varying the chamber and extrusion temperatures while keeping the remaining process parameters constant.

In parallel, an independent Multi-Criteria Decision-Making analysis based on experimental tensile and DMA results had identified the chamber temperature as the processing variable with the greatest influence on the global thermo-mechanical response of FFF-manufactured Z-PEEK. The Digimat-AM® simulations showed the same tendency: changes in chamber temperature produced a greater effect on warpage and internal stress than equivalent changes in extrusion temperature.

This agreement between the experimental MCDM assessment and the numerical sensitivity analysis provided an important cross-validation of the simulation framework. It demonstrated that the model reproduced the dominant process-property relationship observed experimentally and supported its use for the subsequent optimization of the thermal history of the component.

S3 Numerical optimization of residual-stress relief

Once the dominant influence of chamber temperature had been confirmed, the validated material model and thermal parameterization were used to investigate strategies for reducing the residual stresses remaining after deposition. Different post-deposition thermal histories were simulated by modifying the cooling rate, holding temperatures and thermal boundary conditions applied to the printed component.

A reference case without an additional thermal treatment was compared with controlled annealing and cooling cycles. Particular attention was paid to treatments capable of maintaining the component at a sufficiently high temperature to promote stress relaxation while avoiding excessive process duration. One of the evaluated strategies consisted of controlled cooling from 200 to 140 °C at 10 °C/h, followed by heat-source deactivation and natural cooling to room temperature.

The simulated conditions were compared in terms of maximum residual stress, stress localization, field homogeneity and total thermal-treatment time. This second optimization stage was therefore aimed not only at minimizing the internal stresses generated during FFF, but also at identifying a technically effective thermal-conditioning route with a reduced processing time.

RESULTS

Among the different annealing strategies evaluated through simulation, the most effective thermal profile consisted of gradually reducing the temperature from the build-plate temperature of 200 °C to 120 °C at a controlled cooling rate of 10 °C·h⁻¹. Once 120 °C was reached, the machine was switched off, and the component was allowed to cool naturally to room temperature. This optimized strategy reduced thermal gradients and residual stresses, decreasing the maximum von Mises stress from 154 MPa to 96 MPa, which corresponds to a reduction of 37.7%. These results demonstrate the effectiveness of controlled cooling in improving the structural and dimensional stability of the printed component.

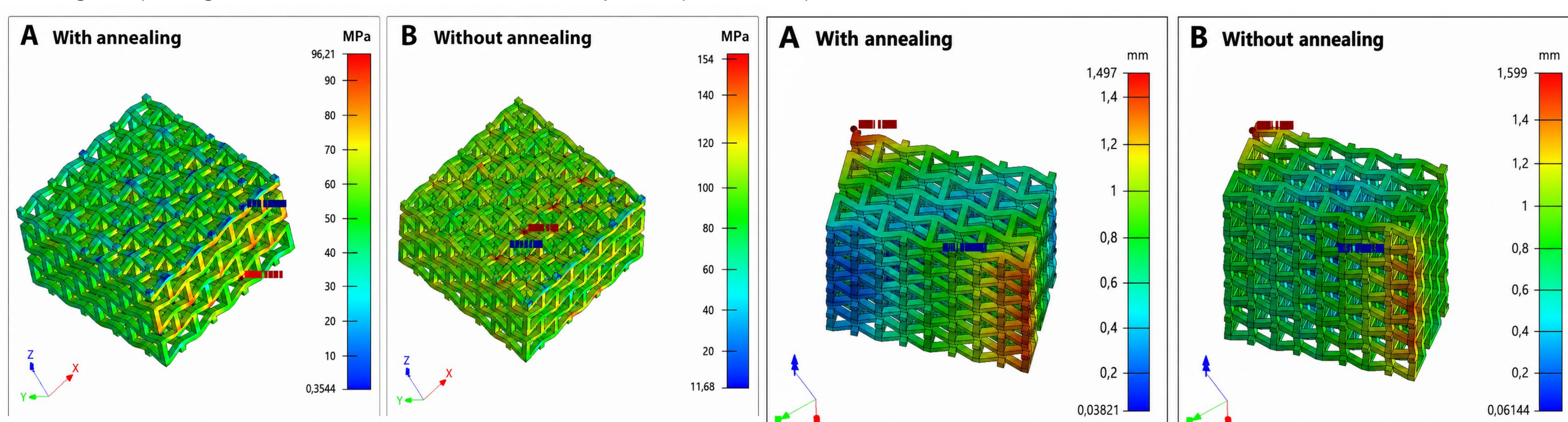


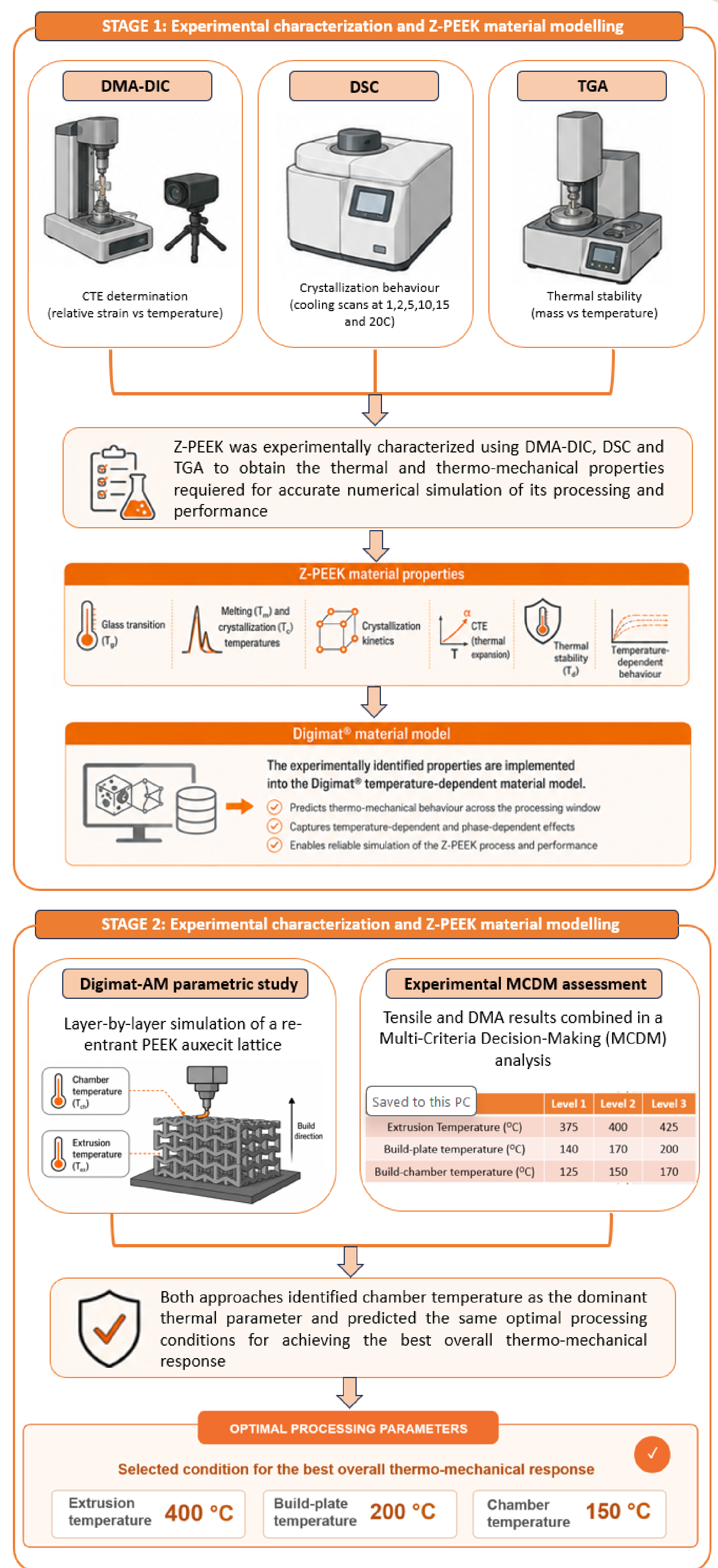
Fig 2. Comparison of the simulated residual von Mises stress distributions and the corresponding total displacement fields for the auxetic structure with and without annealing.

ACKNOWLEDGEMENT:

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REFERENCES:

- Hexagon Manufacturing Intelligence GmbH. *Digimat-AM, Version 2025.2*; Parking 3, 85748 Garching bei München, Germany, 2025
- Solek, C.; Crespo-Sánchez, J.; Fuentes del Toro, S.; Ayllón, J.; Camacho, A. M.; Rodríguez-Hernández, J.; Rodríguez-Prieto, A. Numerical simulation and advanced thermo-mechanical characterization of additively manufactured PEEK 3D-auxetic structures. Companion poster No. 66, 6th International Conference on Materials Design and Applications (MDA 2026), Porto, Portugal, 2-3 July 2026.



CONCLUSIONS

Predictive simulation framework

These results demonstrate the potential of Digimat-AM® as a predictive tool for designing effective thermal treatments, reducing costly experimental trials and improving the dimensional stability and reliability of FFF-manufactured PEEK auxetic components.

Residual-stress reduction

This optimized thermal strategy reduced the maximum residual von Mises stress from 154 to 96 MPa, corresponding to a 37.7% reduction, while also decreasing the associated geometrical displacement.

Dominant thermal parameter

The experimental MCDM assessment and the Digimat-AM® sensitivity analysis independently identified chamber temperature as the dominant thermal parameter governing residual-stress development and geometrical distortion in FFF-manufactured Z-PEEK structures.

Optimized annealing profile

The calibrated temperature-dependent material model enabled the evaluation of different post-deposition thermal histories and the identification of an optimized treatment consisting of controlled cooling from 200 to 120 °C at 10 °C·h⁻¹, followed by passive cooling inside the switched-off machine.

OPTIMAL PROCESSING PARAMETERS

Selected condition for the best overall thermo-mechanical response

Extrusion temperature **400 °C** Build-plate temperature **200 °C** Chamber temperature **150 °C**