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Peridynamic Modelling of Process-Dependent Material Strength in Additive Manufacturing

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ABSTRACT

Additive Manufacturing (AM) processes create complex, process-dependent material properties during printing that cannot be measured in advance and are governed by parameters, such as tool path, temperature history and cooling conditions. A Peridynamics (PD) correspondence framework is presented for simulating the entire AM process chain—printing, cooling and mechanical loading—to predict the resulting material strength. Polymer crystallisation of Polyether Ether Ketone (PEEK) captured via a dual-kinetic model is implemented as a subroutine compatible with the Abaqus HETVAL interface; the resulting crystallinity governs the local nodal stiffness. Thermo-mechanical coupling with convective heat transfer is handled within the PD correspondence formulation. A matrix-based quasi-static solver is coupled with an explicit velocity-Verlet integrator for the fracture phase to eliminate the Courant–Friedrichs–Lewy (CFL) bottleneck of purely dynamic integration. The framework is validated on PEEK dogbone specimens (ASTM D638) for four environment temperatures, demonstrating qualitatively correct crack initiation and propagation and a speedup exceeding two orders of magnitude over a fully dynamic reference computation.

1 | Introduction

Extrusion-based Additive Manufacturing (AM), and in particular fused filament fabrication, enables the production of geometrically complex polymer components without moulds or extensive tooling and is increasingly used for small-batch manufacturing and functional prototypes [1, 2]. A fundamental challenge is that the relevant material properties are not present before production but are created during the printing process itself [3]. Local crystallinity, void fraction and interfacial bonding quality all depend on the thermal history experienced by each deposited bead, which in turn is controlled by nozzle temperature, deposition speed, layer height and ambient conditions. The close material–process–component interaction leads to non-negligible

scatter in mechanical performance even between nominally identical specimens, as visible in the experimental stress–strain curves in Figure 1. Representative pre-process testing to determine strength is therefore not straightforward, and probabilistic process simulation is needed to capture the variability [5].

For semi-crystalline polymers such as Polyether Ether Ketone (PEEK), the degree of crystallisation is the key microstructural quantity linking process history to mechanical performance. It depends strongly on the local cooling rate and directly controls stiffness, tensile strength and fracture mode, as demonstrated by Yang et al. [4] and illustrated in Figure 2: specimens with low crystallinity deform plastically before fracture, whereas highly crystalline specimens fail in a brittle manner—a contrast that

Abbreviations: AM, additive manufacturing; CFL, Courant–Friedrichs–Lewy; FEM, finite element method; NOSB, non-ordinary state-based; PD, peridynamics; PEEK, polyether ether ketone; ZEM, zero-energy mode.

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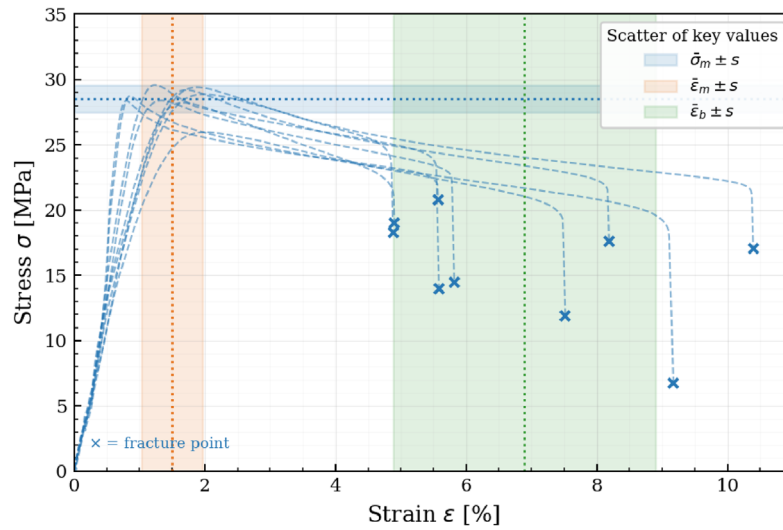


FIGURE 1 | Experimentally measured stress–strain curves of PLA dogbone specimens ($n = 9$, DIN EN ISO 527-1, dashed lines). Shaded bands indicate the $\pm 1\sigma$ scatter of three characteristic values: stress at maximum $\bar{\sigma}_m \pm s$ (blue horizontal band), strain at maximum $\bar{\epsilon}_m \pm s$ (orange vertical band) and strain at break $\bar{\epsilon}_b \pm s$ (green vertical band); dotted lines mark the respective means. Crosses (x) denote individual fracture points. The large scatter in fracture strain (coefficient of variation $\approx 29\%$) reflects process-induced variability in local void fraction and interfacial bonding quality.

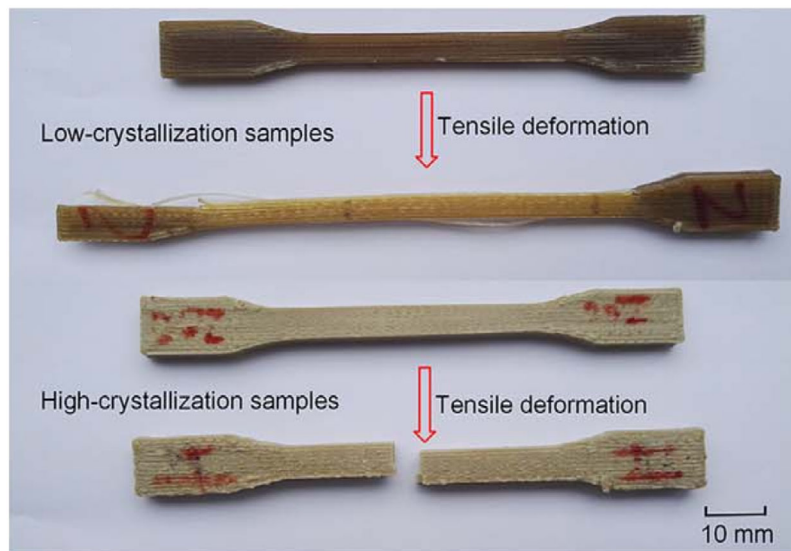


FIGURE 2 | Influence of crystallisation degree on failure mode of printed PEEK specimens under tension [4]. Low-crystallisation samples (top pair) exhibit ductile deformation with large strains prior to failure; high-crystallisation samples (bottom pair) fail in a brittle manner with little prior deformation.

any predictive framework must reproduce. Similar crystallisation effects have been studied with Peridynamics (PD) in the context of soft polymer curing [6], and preliminary process simulations within PeriLab were first presented in [7].

PD [8] is an attractive framework for this problem for three reasons. Firstly, it replaces the classical divergence operator with a non-local integral, so the governing equation remains valid even at discontinuities and crack initiation and propagation emerge naturally without crack-tracking algorithms, remeshing or stress-intensity factors; a bond-level failure criterion triggers bond breakage, and the macroscopic crack path emerges from

the collective bond failure [9, 10]. Secondly, the material-point discretisation [11] allows the computational mesh to be generated automatically from the printer G-code, avoiding the tedious tool-path alignment required in commercial Finite Element Method (FEM)-based AM tools [3]. Thirdly, the open-source framework PeriLab [13, 14] integrates thermal, thermo-mechanical, additive and damage models in a single Julia-based code that can be installed and extended without the overhead associated with older Fortran-based codes such as Peridigm [15].

A key computational challenge in quasi-static AM simulation with PD is the explicit velocity-Verlet integrator. Although it is

stable, parallelisable and the standard choice in the PD community [12], its Courant–Friedrichs–Lewy (CFL) stability condition forces time steps governed by the highest eigenfrequency of the system, while the actual loading rate is orders of magnitude slower. In the present PEEK dogbone case, more than 99% of the 10 h total runtime is spent before any damage occurs. To overcome this bottleneck, the quasi-static loading phase is handled by assembling and solving the linearised PD stiffness matrix [16–18], with the velocity-Verlet integrator taking over only after damage initiates.

The following sections describe the PD correspondence formulation including stiffness assembly and Zero-Energy Mode (ZEM) stabilisation (Section 2), the thermo-mechanical coupling and crystallisation model (Section 3) and the simulation setup and results (Section 4).

2 | Peridynamic Correspondence Formulation

PD was introduced by Silling [8], as a reformulation of classical elasticity theory for problems with discontinuities and long-range forces. The governing equation is the balance of momentum expressed as an integro-differential equation [9]:

$$\int_{\mathcal{H}} (\mathbf{T}(\mathbf{x}, t) - \mathbf{T}(\mathbf{x}', t)) dV_{\mathbf{x}'} + \mathbf{b} = \rho \ddot{\mathbf{u}}. \quad (1)$$

Here, $\mathcal{H}$ is the spherical horizon neighbourhood of radius δ centred at $\mathbf{x}$; $\mathbf{T}$ is the vector force-density state encoding the force that bond $\mathbf{x}' - \mathbf{x}$ exerts; $\mathbf{b}$ is the body-force density; ρ is the mass density; and $\ddot{\mathbf{u}}$ is the acceleration. Because no spatial derivative of $\mathbf{u}$ appears in Equation (1), the equation admits solutions with jump discontinuities—the fundamental reason PD can simulate crack propagation without additional crack-tracking algorithms. In the discrete material-point method [11], the integral is replaced by a sum over neighbour points j within the horizon, and damage is introduced by permanently removing bonds that violate a failure criterion.

Three classes of PD models exist in order of increasing generality: bond-based, ordinary state-based and the Non-ordinary State-Based (NOSB) correspondence formulation [9, 12]. The latter allows arbitrary classical constitutive models to be embedded directly into the PD framework and is therefore used here. For each material point, i the shape tensor

$$\mathbf{D}_i = \sum_{j \in \mathcal{H}_i} \omega_{ij} V_j \mathbf{X}_{ij} \otimes \mathbf{X}_{ij} \quad (2)$$

characterises the reference-configuration geometry, with undeformed bond vector $\mathbf{X}_{ij} = \mathbf{x}_j - \mathbf{x}_i$, neighbour volume V_j and influence function ω_{ij} . Near boundaries or in regions with broken bonds $\mathbf{D}_i$ may become ill-conditioned; the Moore–Penrose pseudoinverse $\mathbf{D}_i^+$ is then used to maintain numerical stability [16]. The non-local deformation gradient is computed as

$$\mathbf{F}_i = \mathbf{I} + \left[\sum_{k \in \mathcal{H}_i} \omega_{ik} V_k \mathbf{U}_{ik} \otimes \mathbf{X}_{ik} \right] \mathbf{D}_i^{-1}, \quad (3)$$

with relative displacement $\mathbf{U}_{ik} = \mathbf{u}_k - \mathbf{u}_i$. Throughout this work, a small-strain (geometrically linear) assumption is adopted. The linearised strain tensor $\boldsymbol{\varepsilon}_i = \frac{1}{2}(\mathbf{F}_i + \mathbf{F}_i^T) - \mathbf{I}$ is passed to a linear-elastic constitutive law $\boldsymbol{\sigma}_i = \mathbf{C}_i : \boldsymbol{\varepsilon}_i$, where $\mathbf{C}_i$ is the fourth-order elasticity tensor. Within the small-strain regime, the distinction between Cauchy and First Piola–Kirchhoff stress is negligible; the bond force-density state is accordingly approximated as [9]

$$\mathbf{T}_{ij} = \omega_{ij} \boldsymbol{\sigma}_i \mathbf{D}_i^{-1} \mathbf{X}_{ij}, \quad (4)$$

and the total PD internal force at node i is

$$\mathbf{F}_i^{\text{pd}} = \sum_{j \in \mathcal{H}_i} (\mathbf{T}_{ij} V_j - \mathbf{T}_{ji} V_i), \quad (5)$$

whose antisymmetric structure guarantees conservation of linear momentum. Damage is modelled by the critical-stretch criterion: bond ij is permanently removed when its stretch exceeds s_c , and the damage index $d_i = 1 - (\sum_j \mu_{ij} V_j) / (\sum_j V_j)$, with bond status $\mu_{ij} \in \{0, 1\}$, quantifies the fraction of failed bonds.

2.1 | Linearised Stiffness Assembly

For quasi-static loading, expressing the linearised PD internal forces as a global stiffness matrix and solving $\mathbf{K}\mathbf{u} = \mathbf{F}_{\text{ext}}$ bypasses the CFL constraint entirely [16–18]. The assembly follows from substituting Equation (3) into Equation (4), and collecting terms in nodal displacements. Defining $\mathbf{B}_{ik} = \mathbf{D}_i^{-1} \mathbf{X}_{ik}$ and the contracted modulus $\mathbf{CB}_{ik} = \mathbf{C}_i : \mathbf{B}_{ik}$, the stiffness block for each triple (i, j, k) with $j, k \in \mathcal{H}_i$ is

$$\mathbf{K}_{ijk}^{\square} = \omega_{ij} \omega_{ik} (\mathbf{X}_{ij}^T \mathbf{D}_i^{-1}) \mathbf{CB}_{ik}, \quad (6)$$

where j is the outer bond index (force direction), and k is the inner neighbour index (deformation gradient). This block is computed once per triple and scattered simultaneously into four positions of the local stiffness block for the cluster $\{i\} \cup \mathcal{H}_i$:

$$\begin{aligned} \mathbf{K}_{ii} &+= +\mathbf{K}_{ijk}^{\square} V_j V_k & \mathbf{K}_{ik} &+= -\mathbf{K}_{ijk}^{\square} V_j V_k \\ \mathbf{K}_{ji} &+= +\mathbf{K}_{ijk}^{\square} V_i V_k & \mathbf{K}_{jk} &+= -\mathbf{K}_{ijk}^{\square} V_i V_k \end{aligned} \quad (7)$$

The top row carries forward contributions (force at i , weighted by V_j) and the bottom row carries backward contributions (force at j , weighted by V_i). For $k = j$ the entries $\mathbf{K}_{ik} = \mathbf{K}_{ij}$ and $\mathbf{K}_{jk} = \mathbf{K}_{jj}$, recovering direct bond coupling as a special case. Assembly cost scales as $\mathcal{O}(|\mathcal{H}|^2)$ per node, and prescribed displacements are enforced by partitioning into free and fixed degrees of freedom, preserving the sparsity structure [16].

2.2 | Zero-Energy Mode Stabilisation

The NOSB correspondence formulation is susceptible to ZEMs—spurious deformation modes that produce no bond force and hence no restoring force in the stiffness matrix, manifesting as checkerboard-like displacement patterns [19, 20]. Following Wan et al. [21], a stabilisation force proportional to the non-affine part of the bond deformation $\mathbf{z}_{ij} = \mathbf{U}_{ij} - \mathbf{F}_i \mathbf{X}_{ij}$ is added; this term vanishes for any affinely deforming neighbourhood and therefore

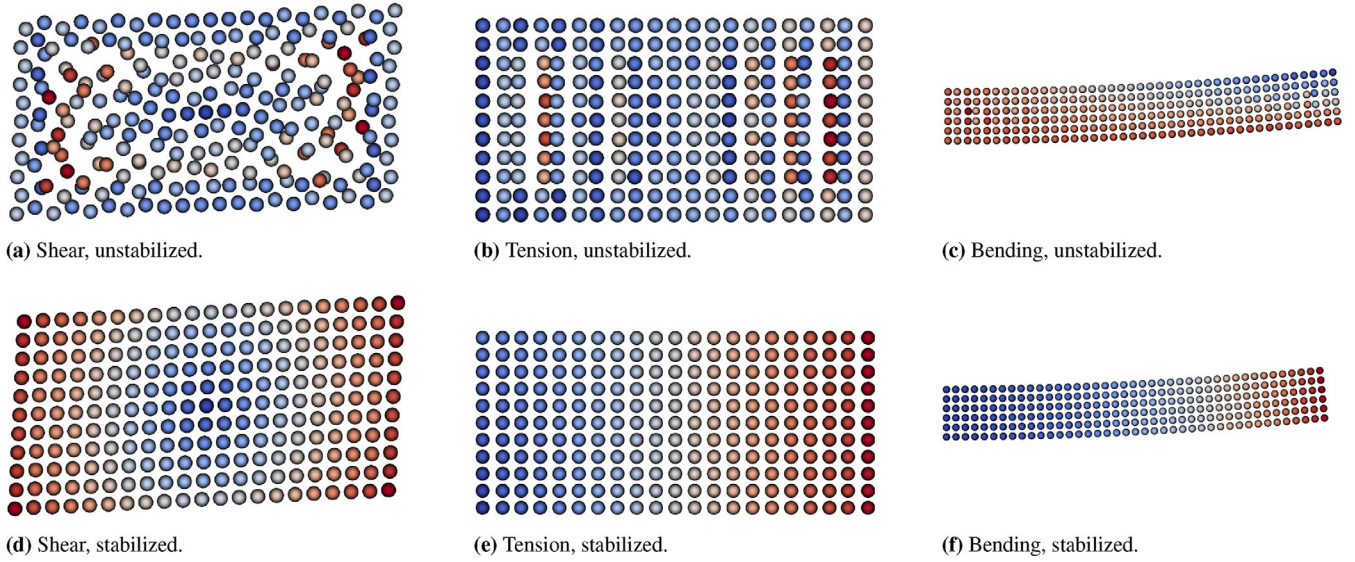


FIGURE 3 | ZEM benchmark [16]. Top row (a–c): without stabilisation—spurious checkerboard modes dominate. Bottom row (d–f): with Wan et al. stabilisation via Equation (11)—correct uniform deformation fields are recovered exactly. Colour indicates relative displacement magnitude.

does not alter the solution for smooth fields while suppressing the spurious modes. Expanding $\mathbf{z}_{ij}$ in nodal displacements and substituting into the stabilisation force $\mathbf{T}_{ij}^S = \omega_{ij} \mathbf{Z}_i \mathbf{z}_{ij}$, the stabilisation contributions follow the same four-position scatter pattern as Equation (7), with

$$\mathbf{Z} = \mathbf{C} : \mathbf{D}^{-1}. \quad (8)$$

The unified scalar prefactor for all $k \in \mathcal{H}_i$ is

$$\begin{aligned} f_{ijk}^{\text{fwd}} &= \omega_{ij} V_j (\delta_{kj} - \omega_{ik} V_k \mathbf{X}_{ik}^T \mathbf{D}_i^{-1} \mathbf{X}_{ij}), \\ f_{ijk}^{\text{bwd}} &= -\omega_{ij} V_i (\delta_{kj} - \omega_{ik} V_k \mathbf{X}_{ik}^T \mathbf{D}_i^{-1} \mathbf{X}_{ij}), \end{aligned} \quad (9)$$

where δ_{kj} is the Kronecker delta. For $k = j$, this gives $f_{ijj}^{\text{fwd}} = \omega_{ij} (1 - \omega_{ij} V_j d_{ij}) V_j$ with $d_{ij} = \mathbf{X}_{ij}^T \mathbf{D}_i^{-1} \mathbf{X}_{ij}$; for $k \neq j$ the Kronecker delta vanishes. The vector $\mathbf{D}_i^{-1} \mathbf{X}_{ij}$ is shared with the correspondence stiffness loop. The stabilisation scatter for all $k \in \mathcal{H}_i$ reads

$$\begin{aligned} \mathbf{K}_{il}^S &+= f_{ijk}^{\text{fwd}} \mathbf{Z}_i & \mathbf{K}_{ik}^S &+= -f_{ijk}^{\text{fwd}} \mathbf{Z}_i \\ \mathbf{K}_{ji}^S &+= f_{ijk}^{\text{bwd}} \mathbf{Z}_i & \mathbf{K}_{jk}^S &+= -f_{ijk}^{\text{bwd}} \mathbf{Z}_i \end{aligned} \quad (10)$$

This single loop over k replaces the previously separate diagonal and cross-term loops and mirrors the structure of Equation (7) exactly. Although correspondence and stabilisation contributions are assembled in a single merged loop in practice, the total stiffness matrix decomposes conceptually as

$$\mathbf{K}_{\text{total}} = \mathbf{K}_{\text{correspondence}} + \mathbf{K}_{\text{stabilization}}, \quad (11)$$

a structure that is confirmed by the benchmark in Figure 3. For the unstabilised case, the points in pure shear and tension cannot be represented correctly. The stabilisation leads to the correct, uniform deformation fields.

TABLE 1 | Material and thermal properties of PEEK used in the three-step AM simulation [3].

Parameter	Symbol	Value
Young's modulus	E	3800 MPa
Poisson's ratio	ν	0.33
Density	ρ	$1240 \times 10^{-12} \text{ tm}^{-3} \text{ m}$
Critical stretch	s_c	0.12
Thermal conductivity	λ	$0.12 \text{ W m}^{-1} \text{ K}^{-1}$
Heat transfer coeff.	κ	$15.0 \times 10^{-3} \text{ t/s}^3 \text{ K}^{-1}$
Print temperature	T_P	653.15 K
Room temperature	T_{RT}	293.15 K
Spec. heat capacity	c_v	$1800 \times 10^6 \text{ mm}^2 / \text{s}^2 \text{ K}^{-1}$

3 | Thermo-Mechanical Coupling and Crystallisation Model

3.1 | Thermal Strains and Stresses

During deposition and cooling, the temperature field evolves continuously, and the associated thermal expansion drives residual stresses that pre-load the structure before the tensile test. Following the standard thermo-mechanical split [3], the total strain is decomposed as $\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}_{\text{mech}} + \boldsymbol{\varepsilon}_{\text{th}}$, with isotropic thermal strain $\boldsymbol{\varepsilon}_{\text{th}} = -\boldsymbol{\alpha} \tau$, where $\tau = T - T_0$ is the temperature increment and $\boldsymbol{\alpha}$ is the thermal expansion coefficient tensor. The thermal stress contribution

$$\boldsymbol{\sigma}_{\text{th}} = -\mathbf{C} : (\boldsymbol{\alpha} \tau) \quad (12)$$

enters $\boldsymbol{\sigma}_i$ through Equation (4) without modifying the PD force assembly, so thermo-mechanical coupling is implemented entirely at the constitutive level.

3.2 | Peridynamic Heat Flux and Surface Detection

The temperature field evolves according to the PD heat-flux formulation derived from Fourier's law [23, 24]:

$$\rho C_v \dot{\tau} = \int_{\mathcal{H}} (\underline{h}(\mathbf{x}, t) \langle \xi \rangle - \underline{h}(\mathbf{x}', t) \langle \xi' \rangle) dV_{\mathbf{x}'} + S_i, \quad (13)$$

where C_v is the specific heat capacity and S_i is a volumetric source or sink. The single-bond flux is $\underline{h}(\xi) = \mathbf{q}^T \mathbf{D}^{-1} \xi$ with $\mathbf{q} = -\lambda \nabla \tau$ and non-local gradient [25]

$$\nabla \tau = \mathbf{D}^{-1} \int_{\mathcal{H}} [\tau(\mathbf{x}') - \tau(\mathbf{x})] \xi \underline{\omega}(\xi) dV_{\mathbf{x}'}. \quad (14)$$

Being first-order in time, Equation (13) admits a stable time step [23]

$$\Delta t < \min_i \left(\frac{(\rho C_v)_i}{\sum_j \frac{\max(\text{eig}(\lambda))}{|\xi_{ij}|} V_j} \right) \quad (15)$$

several orders of magnitude larger than the mechanical CFL step, so the two sub-problems are integrated sequentially with their natural time scales.

Convective exchange enters through $S_i = \kappa(\tau - \tau_{\text{env}})/\Delta$, where κ is the convection coefficient and τ_{env} is the ambient temperature [3]. Since the discretisation is based on material points rather than a conforming mesh, surface nodes are detected dynamically: a material point is flagged as a surface node whenever its actual neighbourhood volume falls below a threshold fraction f_{limit} of the theoretical sphere volume $\frac{4}{3}\pi\delta^3$, and the criterion is updated as new layers are activated during printing [3].

Remark 3.1. The PD heat-flux Equation (13) is first-order in time and involves only the non-local temperature gradient (14), computed via the shape tensor $\mathbf{D}_i$ but without a deformation-gradient approximation. Consequently, the ZEMs that afflict the mechanical NOSB correspondence operator do not arise in the thermal sub-problem, and no analogous stabilisation is required. The two sub-problems are therefore integrated sequentially at their respective natural time scales without additional coupling stabilisation.

3.3 | Crystallisation Kinetics and Stiffness Update

The degree of crystallisation X_{VC} is the central quantity linking the thermal process history to local mechanical properties. It is governed by two competing Avrami-type nucleation-and-growth mechanisms operating at different temperature ranges: a primary mechanism near the melting temperature that forms crystalline lamellae, and a slower secondary mechanism active at lower temperatures that fills in remaining amorphous regions. Following Velisaris & Seferis [3, 6], the combined kinetics read

$$X_{VC} = X_{VC\infty} (w_1 F_{\theta_1}(k) + w_2 F_{\theta_2}(k)), \quad (16)$$

where $X_{VC\infty}$ is the maximum attainable crystallinity, $w_1 + w_2 = 1$ are weighting factors for each mechanism, and $F_{\theta_i}(k)$ are the Avrami kinetic functions evaluated along the local cooling history k (with rate constants k_i following an Arrhenius temperature dependence). Rapid cooling quenches both mechanisms and yields a predominantly amorphous, ductile material; slow cooling activates the secondary mechanism fully and produces a brittle, highly crystalline microstructure consistent with Figure 2.

The model is implemented using the HETVAL subroutine interface, a standard user-subroutine convention originally introduced by Abaqus for user-defined heat generation. PeriLab calls this interface directly so that existing validated subroutines can be reused without modification [3]; no Abaqus installation is required. The subroutine receives the local temperature history from PeriLab and returns the crystallisation increment per time step. The resulting X_{VC} is mapped to a nodal Young's modulus through a fitting function $E = E(X_{VC})$ [3]; the elasticity tensor $\mathbf{C}$ in Equations (6) and (8) is then recomputed from the updated E so that the stiffness matrix reflects the locally evolving microstructure at every material point and time step.

4 | Simulation Setup and Results

4.1 | Solving Process

The simulation proceeds in two distinct phases. During printing and cooling, the thermal field is advanced explicitly with a velocity-Verlet scheme at each time step, updating the temperature and the crystallisation degree X_{VC} via Equation (16). The time step is governed by the thermal stability condition Equation (15), which is several orders of magnitude larger than the mechanical CFL step, making the coupled thermo-mechanical simulation significantly more efficient than a purely mechanical explicit integration. The resulting nodal Young's modulus $E(X_{VC})$ is used to recompute the elasticity tensor $\mathbf{C}$, from which $\mathbf{K}_{\text{total}}$ from Equation (11) is reassembled. The mechanical response is then obtained by solving $\mathbf{K}_{\text{total}} \mathbf{u} = \mathbf{F}_{\text{ext}}$ via direct factorisation, bypassing the CFL constraint of a fully dynamic integration. No damage evaluation is performed during this phase; the stiffness matrix is updated every step solely to reflect the evolving crystallinity.

Once printing and cooling are complete, the tensile test is simulated by switching to a fully explicit velocity-Verlet integration, which runs until complete specimen fracture. This phase naturally captures crack initiation and propagation without requiring reassembly of $\mathbf{K}_{\text{total}}$, since bond breakage is handled incrementally by the explicit scheme [16]. For the PEEK dogbone case, this hybrid approach reduces total runtime from approximately 10 h to below 5 min without any change in fracture prediction accuracy.

4.2 | Model Setup

All simulations are performed as 2D plane-stress models. The three-step workflow—printing, free cooling and tensile testing—is executed entirely within PeriLab [13, 14]. The material-point mesh is generated automatically from the printer G-code: each point receives an activation time corresponding to when the

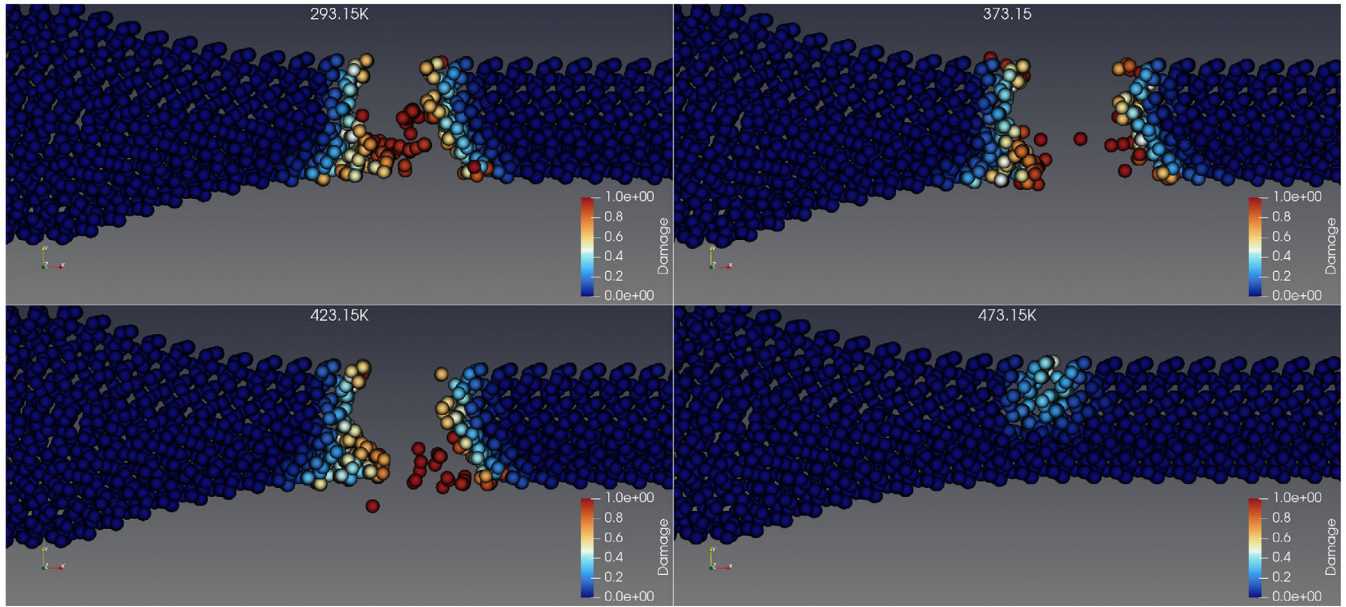


FIGURE 4 | Simulated damage index (0 = intact, 1 = fully broken) at the end of the tensile test for $T_E \in \{293.15 \text{ K}, 373.15 \text{ K}, 423.15 \text{ K}, 473.15 \text{ K}\}$ (left to right, top to bottom). Higher T_E delays crack initiation and broadens the damage zone.

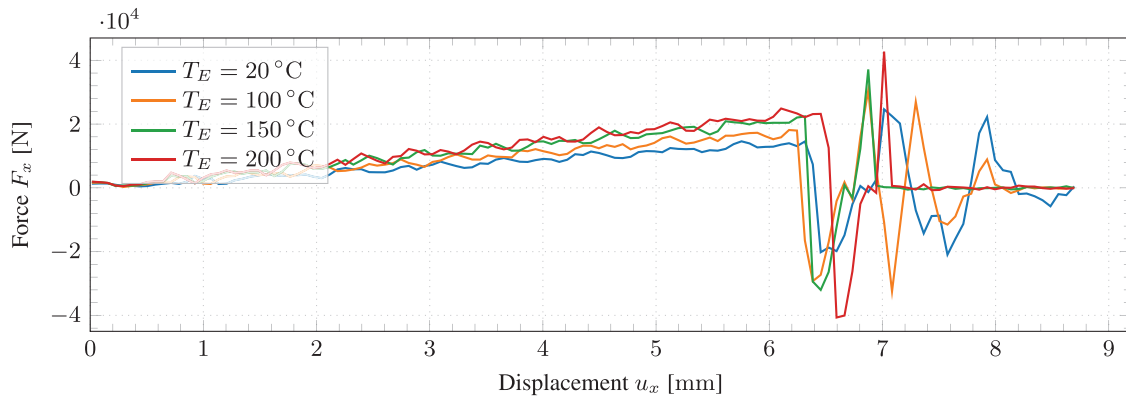


FIGURE 5 | Simulated force–displacement curves for PEEK dogbone specimens cooled to four environment temperatures, T_E . Higher T_E promotes crystallisation, raising stiffness and peak load while reducing ductility. Oscillations arise from the dynamic velocity-Verlet integration and are most pronounced near fracture.

nozzle passes overhead, requiring no manual tool-path alignment [3]. PEEK dogbone specimens (ASTM D638) are printed in 20 layers with a layer height of 0.2 mm. After printing, free convective cooling is simulated at four environment temperatures $T_E \in \{293.15 \text{ K}, 373.15 \text{ K}, 423.15 \text{ K}, 473.15 \text{ K}\}$. The crystallisation subroutine is active throughout, updating $E(X_{VC})$ at every material point and time step. A uniaxial displacement is then applied in the tensile test step. The material and thermal properties are listed in Table 1.

4.3 | Crack Initiation and Propagation

Figure 4 shows the simulated damage field at the end of the tensile test for all four environment temperatures. In all cases, crack initiation occurs at the notch transition of the gauge section,

consistent with experimentally observed failure locations [4]. The crack propagates perpendicular to the loading direction and leads to complete specimen separation. The environment temperature T_E exerts a clear influence: specimens cooled to 293.15 K attain the highest crystallinity, exhibit a sharp and localised crack front and fail at a lower applied displacement, consistent with the brittle fracture mode in Figure 2. Higher T_E values reduce the crystallisation driving force, yield a more diffuse damage zone and shift the critical displacement to larger values, approaching the ductile behaviour observed experimentally [4]. This qualitative trend validates the model's ability to link process conditions to structural failure through the crystallisation kinetics.

Figure 5 shows the simulated force–displacement curves for all four temperatures. Higher T_E promotes crystallisation, increasing stiffness and peak load while reducing ductility. The visible

oscillations are an artefact of the dynamic velocity-Verlet integration and are most pronounced near fracture where inertial effects dominate.

5 | Conclusion

A PD correspondence framework has been presented for simulating the complete AM process chain of PEEK dogbone specimens, encompassing layer-by-layer deposition, thermo-mechanically coupled convective cooling, dual-kinetic crystallisation and uniaxial tensile fracture. Three key contributions work together. Firstly, the Velisaris-Seferis crystallisation model, implemented via the HETVAL subroutine interface, updates the nodal elasticity tensor $\mathbf{C}$ continuously during cooling so that the stiffness matrix reflects the locally evolving microstructure without any manual calibration step. Secondly, ZEM stabilisation via the method of Wan et al. [21], assembled in the same scatter loop as the correspondence stiffness, eliminates spurious deformation modes without problem-specific tuning. Thirdly, the hybrid quasi-static/Verlet strategy reduces total runtime from approximately 10 h to below 5 min—a speedup exceeding 20×—while reproducing the fracture pattern identically. Qualitatively, the simulations capture the experimentally observed transition from ductile to brittle failure with increasing environment temperature, validating the link between process conditions, crystallisation and structural integrity.

Future work will focus on quantitative experimental validation across a broader range of process parameters, incorporation of non-linear material routines via UMAT-compatible interfaces [15], and the extension to full three-dimensional process chains including multi-layer residual stress accumulation

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References

1. J. Shah, B. Snider, T. Clarke, S. Kozutsky, M. Lacki, and A. Hosseini, “Large-Scale 3D Printers for Additive Manufacturing: Design Considerations and Challenges,” *International Journal of Advanced Manufacturing Technology* 104 (2019): 3679–3693.
2. P. K. Penumakala, J. Santo, and A. Thomas, “A Critical Review on the Fused Deposition Modeling of Thermoplastic Polymer Composites,” *Composites Part B: Engineering* 201 (2020): 108336.
3. C. Willberg, J.-T. Hesse, F. Winkelmann, and R. Hein, “Peridynamic Framework to Model Additive Manufacturing Processes,” *Advanced Theory and Simulations* 8 (2025): 2400818.
4. C. Yang, X. Tian, D. Li, Y. Cao, F. Zhao, and C. Shi, “Influence of Thermal Processing Conditions in 3D Printing on the Crystallinity and Mechanical Properties of PEEK Material,” *Journal of Materials Processing Technology* 248 (2017): 1–7.
5. M. Liebis, R. Hein, and T. Wille, “Probabilistic Process Simulation to Predict Process Induced Distortions of a Composite Frame,” *CEAS The Aeronautical Journal* 9 (2018): 545–556.
6. P. Hartmann, C. Weißenfels, and P. Wriggers, “A Curing Model for the Numerical Simulation Within Additive Manufacturing of Soft Polymers Using Peridynamics,” *Computational Particle Mechanics* 8 (2021): 521–539.
7. J.-T. Hesse, C. Willberg, R. Hein, and F. Winkelmann, “Peridynamic Framework to Model Additive Manufacturing Processes,” *PAMM* 23 (2023): e202300033.
8. S. A. Silling, “Reformulation of Elasticity Theory for Discontinuities and Long-Range Forces,” *Journal of the Mechanics and Physics of Solids* 48 (2000): 175–209.
9. S. A. Silling, M. Epton, O. Weckner, J. Xu, and E. Askari, “Peridynamic States and Constitutive Modeling,” *Journal of Elasticity* 88 (2007): 151–184.
10. A. Agwai, I. Guven, and E. Madenci, “Predicting Crack Propagation With Peridynamics: A Comparative Study,” *International Journal of Fracture* 171 (2011): 65–78.
11. S. A. Silling and E. Askari, “A Meshfree Method Based on the Peridynamic Model of Solid Mechanics,” *Computers & Structures* 83 (2005): 1526–1535.
12. F. Bobaru, J. T. Foster, P. H. Geubelle, and S. A. Silling eds., *Handbook of Peridynamic Modeling* (CRC Press, 2016).
13. C. Willberg, J.-T. Hesse, and A. Parnati, “PeriLab – Peridynamic Laboratory,” *SoftwareX* 26 (2024): 101700.
14. J.-T. Hesse and C. Willberg, “Update (v2.0) to PeriLab – Peridynamic Laboratory,” *SoftwareX* 34 (2026): 102644.
15. C. Willberg, et al., “A User Material Interface for the Peridynamic Peridigm Framework,” *SoftwareX* 21 (2023): 101322.
16. C. Willberg and J.-T. Hesse, “Efficient Modeling Strategies Utilizing Stiffness Matrix Formulation for Non-Ordinary State-Based Peridynamics,” *Computers & Structures* 329 (2026): 108301, <https://doi.org/10.1016/j.compstruc.2026.108301>.
17. M. S. Breitenfeld, P. H. Geubelle, O. Weckner, and S. A. Silling, “Non-Ordinary State-Based Peridynamic Analysis of Stationary Crack Problems,” *Computer Methods in Applied Mechanics and Engineering* 272 (2014): 233–250.
18. N. Prakash and R. J. Stewart, “A Multi-Threaded Method to Assemble a Sparse Stiffness Matrix for Quasi-Static Solutions of Linearized Bond-Based Peridynamics,” *Journal of Peridynamics and Nonlocal Modeling* 3 (2021): 113–147.
19. S. A. Silling, “Stability of Peridynamic Correspondence Material Models and Their Particle Discretizations,” *Computer Methods in Applied Mechanics and Engineering* 332 (2017): 42–57.
20. D. Liu, H. Chen, X. Hu, et al., “The Peridynamic Material Correspondence Models: A State-of-the-Art Review on Stabilization Schemes,” *Journal of Peridynamics and Nonlocal Modeling* 7 (2025): 5.
21. J. Wan, Z. Chen, X. Chu, and H. Liu, “Improved Method for Zero-Energy Mode Suppression in Peridynamic Correspondence Model,” *Acta Mechanica Sinica* 35 (2019): 1021–1035.
22. S. Oterkus, E. Madenci, and A. G. Agwai, “Peridynamic Thermal Diffusion,” *Journal of Computational Physics* 265 (2014): 71–96.
23. T. Xue, X. Zhang, and K. K. Tamma, “A Two-Field State-Based Peridynamic Theory for Thermal Contact Problems,” *Journal of Computational Physics* 374 (2018): 1180–1195.
24. M. A. Zeleke and M. B. Ageze, “A Review of Peridynamics (PD) Theory of Diffusion Based Problems,” *Mathematical Problems in Engineering* 2021 (2021): 7782326.
25. X. Gu, Q. Zhang, and E. Madenci, “Refined Bond-Based Peridynamics for Thermal Diffusion,” *Engineering With Computers* 36 (2019): 2557–2587.