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Comparing nanoindentation and macroscale yield stress in polypropylene

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ABSTRACT

Understanding the yielding of semicrystalline polymers such as isotactic polypropylene (iPP) remains challenging due to morphology-dependent deformation mechanisms and the sensitivity of yield stress to temperature, strain rate, and loading mode. Here, yield stress is measured across macro- (tensile, compression) and micro-scales (nanoindentation) over a range of temperatures and strain rates. Nanoindentation-derived yield stresses obtained using the expanding cavity model agree closely with compression measurements, confirming the dominance of compressive fields, while Tabor-derived values correlate with tensile maximum stress. To rationalize the observed temperature and rate dependences, three theoretical frameworks—Eyring's model, crystal plasticity, and the lamellar cluster model—are comparatively evaluated. The Eyring model captures the logarithmic strain-rate sensitivity and thermal softening but lacks structural specificity; the crystal plasticity model provides a slip-based interpretation with improved agreement at elevated temperatures; and the lamellar cluster model differentiates deformation modes, accounting for the convergence of compression and indentation yields. The combined experimental–modeling analysis demonstrates the utility of nanoindentation for localized yield assessment and highlights the model-dependent nature of structural interpretation in semicrystalline polymers.

Keywords: Nanoindentation; polypropylene; yield stress; strain rate; thermo-mechanical modeling.

INTRODUCTION

Isotactic polypropylene (iPP) is one of the most widely used semicrystalline thermoplastics due to its excellent chemical resistance, processability, and mechanical performance [1-3]. Understanding its yielding behavior is critical for predicting performance under mechanical loading [4]. However, its complex morphology of crystalline lamellae embedded in an amorphous matrix, results in a nonlinear viscoplastic response that challenges the accurate determination of yield stress [5, 6]. Traditionally, the 0.2% offset method is used in uniaxial tensile tests to define yield stress in polymers. While convenient, this approach can underestimate the actual yield point in semicrystalline systems like iPP, where plastic

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deformation begins gradually. Alternative methods, such as the maximum stress in tensile curves or compression yield points, provide complementary information but are not standardized.

Depth-sensing nanoindentation with spherical indenters has emerged as a powerful technique to probe local yielding at small scales [7-10]. Yield stress can be estimated from indentation data using analytical models such as Tabor's relation, which correlates hardness (H) and yield stress (σ_y) as $\sigma_y = \frac{H}{3}$ [11] or via the expanding cavity model (ECM) [12] based on Johnson's foundational work [13], which models plastic flow beneath an indenter as the expansion of a spherical cavity. These approaches enable comparison between indentation- and bulk-derived yield stresses. The seminal work by Oliver and Pharr [7] established a widely accepted framework for determining hardness and elastic modulus from instrumented indentation, which remains foundational in the field. More recently, comprehensive reviews, including that by Pshyk et al. [10], have underscored nanoindentation's expanding role in characterizing viscoelastic and plastic deformation in polymers. Nevertheless, the comparability of indentation-derived yield stresses with those obtained from macroscopic mechanical testing remains insufficiently explored for semicrystalline polymers such as iPP.

Temperature and strain rate play a critical role in governing the viscoplastic behavior of iPP [14]. Beyond empirical relations, several micromechanical models have been developed to rationalize the temperature and strain-rate sensitivity of polymer yielding. Thermally activated processes—such as chain segment mobility, crystalline slip, and inter-lamellar shear—compete during yielding [14]. The Eyring model treat yielding as a thermally activated process, predicting that yield stress decreases with temperature and increases logarithmically with strain rate [15]. Crystal plasticity models attribute yielding in semicrystalline polymers to dislocation slip within lamella, linking morphology to mechanical response [16, 17]. The Lamellar Cluster model considers collective deformation of lamella stacks, with the cluster exponent (n) reflecting inter-lamellar constraint and tie-chain [18, 19]. Takayanagi et al.'s work [18] first applied the lamellar cluster model to PP morphology and yield behavior, later extended by Nitta and Takayanagi [19] with model fittings to mechanical data. Experimental studies have demonstrated that Ree–Eyring type models can successfully describe the rate-dependent yield behavior of iPP across wide strain-rate ranges and temperature windows [20]. Moreover, the introduction of morphological parameters into these models has significantly improved their predictive capacity, especially for polymers with complex semicrystalline microstructures [21].

Recent investigations have also shed light on how deformation and flow induce crystallographic reorganization at multiple scales. Sharaf et al. [22] recently provided direct evidence of structural evolution from the single-spherulite to the lamellar and chain level during deformation of iPP, offering valuable insights into the physical basis of strain-induced yield mechanisms. These findings underscore the importance of considering both structural and thermomechanical factors when comparing yield stress values obtained from different testing techniques. Yet, their relative predictive capabilities have

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not been systematically benchmarked against experimental data obtained from tests at multiple length scales and loading modes.

In this study, we systematically compare yield stress values obtained from uniaxial tensile, compression, and nanoindentation tests on isotactic polypropylene across a wide range of temperatures and strain rates. The consistency between tensile-, compression-, and nanoindentation-derived yield stresses is critically examined, and the applicability of established constitutive models is discussed as a framework for interpreting scale- and constraint-dependent yielding in semicrystalline polypropylene. This work provides new insights into how deformation constraint and testing scale influence the measured yield response and offers experimentally validated guidance for the interpretation of micro- and macro-scale mechanical data. Among the examined models, the lamellar cluster model is quantitatively fitted to the experimental data, whereas the Eyring and crystal plasticity models are used to rationalize observed temperature- and rate-dependent trends.

EXPERIMENTAL

Materials

An isotactic polypropylene (iPP) homopolymer (Grade 080, Imam Khomeini Petrochemical Complex) was used. The material exhibits a melt flow index of 12 g/10 min (230 °C/2.16 kg), a density of 0.905 g/cm³, and a crystallinity of approximately 34%.

Characterization Methods

Tensile and compression tests were conducted using an INSTRON 5567 universal testing machine in accordance with ASTM D638 (tensile) and ASTM D695 (compression). Mechanical tests were conducted at room temperature (20 °C) as well as at elevated temperatures of 40°C, 60°C, and 80 C. For each temperature, tests were performed at nominal strain rate of 0.1 s^{-1}. The strain rate was kept constant when comparing results across different temperatures. Prior to testing, specimens were equilibrated at the target temperature for 10 min to ensure thermal stability throughout the gauge section. The temperature range of 20–80°C was selected to represent the practically relevant deformation regimes of iPP, while avoiding the onset of thermal softening and heat distortion that could complicate accurate yield stress determination. The lower bound (20°C) corresponds to room-temperature performance, which is most relevant for structural applications, whereas the upper bound (80°C) approaches the thermomechanical transition region of semicrystalline polypropylene. This range allows reliable evaluation of the temperature dependence of yield stress while maintaining the structural integrity of the specimens during both nanoindentation and macroscopic mechanical testing. Stress-strain curves were obtained from the load-displacement data using the initial cross-sectional area and gauge length. For each condition, a minimum of five specimens was tested, and mean values are reported.

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Spherical nanoindentation was performed using a UMIS nanoindenter (CSIRO, Australia) equipped with a diamond spherical indenter of 20 µm radius. The instrument was fitted with a calibrated electromagnetic force actuator and a load cell with a maximum load capacity of 1 N and a force resolution better than 1 µN. Displacement was measured using a capacitive sensor with nanometer resolution. A load–hold–unload protocol was used to capture viscoplastic behavior. Load-displacement data were analyzed via Oliver-Pharr method to obtain hardness and indentation modulus. Yield stress was estimated using Tabor's relation [11] and the expanding cavity model (ECM) with Johnson's framework [13]. Ten indentations were performed per condition, spaced 25 µm apart to avoid plastic zone overlap. Outliers exceeding ±2σ from the mean were discarded. Similar to the tensile and compression tests, the indentation testing carried out at different temperatures and strain rates. Figure 1 shows schematically spherical nanoindentation.

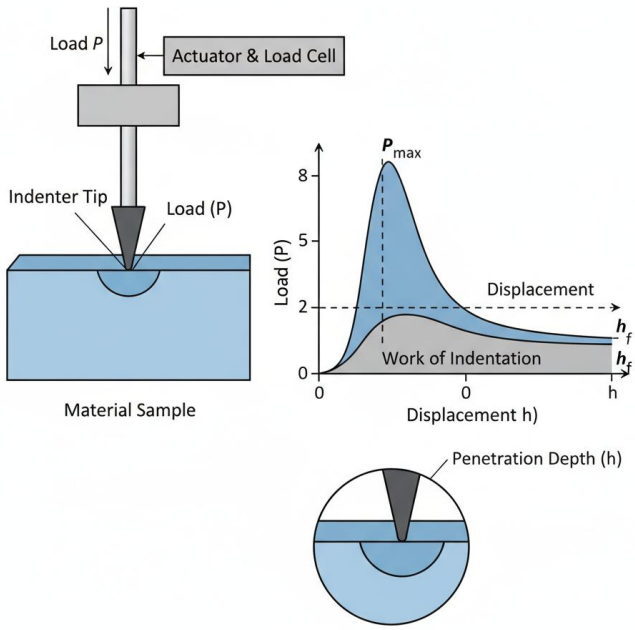

Figure 1. Schematic illustration of spherical nanoindentation on isotactic polypropylene (iPP). The indenter tip (radius = 20 µm) creates a localized deformation zone on the sample surface. Indents are spaced 25 µm apart to prevent plastic zone overlap. Elastic and plastic regions beneath the indenter are illustrated, consistent with Tabor and Expanding Cavity Model analysis.

MODELING

Several analytical and micromechanical models were employed to interpret yield stress: Tabor's relation [11] relates indentation hardness to tensile yield stress as $\sigma_y = \frac{H}{3}$. Based on Johnson's formulation [13], expanding cavity model (ECM) relates mean contact pressure (P_m) to yield stress [12]:

$$\frac{P_m}{\sigma_y} = C = A + B\ln(Z)$$

where A and B are constants and Z is a dimensionless parameter depending on the $\frac{\sigma_y}{E}$ $\frac{\sigma_y}{E}$ratio indenter geometry.

Eyring model describes yielding as a thermally activated rate process [15]:

$$\sigma_y = \frac{2}{V^*}\left[\Delta H + kT.\ln\frac{\dot{\varepsilon}_y}{\dot{\varepsilon}_0}\right]$$

where ΔH is the activation enthalpy, V^* the activation volume, k the Boltzmann constant, and $\dot{\varepsilon}_y$ the applied strain rate. This model captures the temperature and rate dependence of yielding, which is particularly relevant in polymer deformation.

The thermally activated crystal plasticity model is used here to rationalize the temperature dependence of yielding by associating macroscopic yielding with dislocation-like slip within crystalline lamellae. In semicrystalline polymers, plastic deformation of the crystalline phase occurs through thermally activated crystal slip and lattice shear processes involving chain segments, rather than through classical metallic dislocations. Accordingly, the "dislocation" terminology adopted in the model is non-literal and represents lamellar shear, chain slip, and interlamellar deformation within the polymer crystal lattice. In the present work, the crystal plasticity model is employed in a phenomenological manner to compare the temperature-dependent yield stress with the Eyring-type activation analysis. The yield stress can be expressed in the form [17]:

$$\sigma_y = \frac{K(T,\varepsilon)}{2\pi}\exp\left[-\left(\frac{2\pi\Delta G_a(T)}{L_s K(T,\varepsilon) b_v^2}+1\right)\right]$$

where ΔG_a is the activation energy for crystal slip, L_s is the stem length, and b_v represents an effective Burgers vector associated with chain-segment motion within the crystalline lamellae. In this formulation, K is an effective stiffness factor that incorporates crystallographic and geometric contributions to lamellar shear; it is not equivalent to the macroscopic shear or Young's modulus. The parameters b_v and L_s are taken in the effective crystal-plasticity sense, an effective crystallographic slip distance associated with chain-segment motion in the lamellae, consistent with prior polymer crystal plasticity frameworks and do not represent classical metallic dislocation quantities. This formulation is used here for interpretive comparison and is not calibrated as a full constitutive model.

Lamellar cluster model considers deformation of lamellar clusters through bending of tie molecules, with yield stress given by [19]:

$$\sigma_y = n\sqrt{2E_0 U_y}$$

where n is a morphology-dependent constant and U_y the yield energy derived from stress–strain data. In the lamellar cluster model, the parameter E_0 represents the effective elastic modulus of a lamellar cluster, incorporating contributions from crystalline lamellae and the surrounding constrained

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amorphous regions. Since E_0 is not directly measurable, it was estimated from the experimentally determined Young's modulus obtained from the initial linear elastic region of the tensile stress–strain response. This approach is consistent with previous implementations of the lamellar cluster model for semicrystalline polypropylene and related polymers, where the small-strain elastic response is governed by the cooperative deformation of lamellae and constrained amorphous regions and can be reasonably approximated by the macroscopic Young's modulus [19]. The resulting E_0 lies within the range reported in the literature for iPP with comparable crystallinity, ensuring physical consistency of the fitted model parameters. The parameter E_0 was treated as a material constant and fixed to the tensile Young's modulus (1.8–1.9 GPa) for all deformation modes. Compression and indentation moduli were not used to estimate E_0, as they are influenced by geometric constraint and hydrostatic stress components and therefore do not reflect the intrinsic elastic stiffness of the lamellar cluster assumed in the model. These models form the theoretical basis for interpreting the results presented in Results and Discussion section.

RESULTS AND DISCUSSION

All mechanical and indentation parameters used in the analyses were extracted from the experimental data and are reported explicitly in tabulated form (Tables 1-3).

Effect of temperature on yield stress

Tables 1-2 and Figure 2 present the temperature dependence of yield stress as measured via tensile testing (0.2% offset and maximum stress), compression testing, and nanoindentation using Tabor's relation and ECM. Yield stresses estimated via ECM from nanoindentation align closely with compressive yield stress values, consistent with shared compressive stress fields and findings from indentation of similar semicrystalline systems under hydrostatic loading conditions [12]. Tabor's model produces values that closely match the tensile maximum stress, confirming its applicability to semicrystalline polymers and consistent with previous hardness-yield correlations in polymers [23]. As temperature increases, all measured yield stresses decline in a manner indicative of thermally activated deformation mechanisms, in line with Eyring-type behavior observed in iPP [14]. The 0.2% offset method yields lower values, particularly at elevated temperatures, due to its sensitivity to early viscoplastic flow and its tendency to underestimate yield in semicrystalline polymers. At near-melting temperatures, yield stress approaches zero, indicating the progressive breakdown of crystalline domains that provide structural resistance, as also observed in PP [24].

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Table 1. Yield stress of iPP obtained from tensile and compression tests at different temperatures and strain rates.

Temperature		Strain rate (s^{-1})	Tensile yield stress (0.2% offset) (MPa)	Tensile max stress (MPa)	Compression yield stress (MPa)
(ºC)	(K)				
20	293	10^{-3}	16.4	28.5	49.4
20	293	10^{-2}	18	31.6	51.8
20	293	10^{-1}	20.0	34.8	59.1
40	313	10^{-1}	17.1	29.7	51.9
60	333	10^{-1}	10.6	21.5	38.3
80	353	10^{-1}	6.9	15.9	30.1

*Standard deviations were within ±5% unless otherwise stated.

Table 2. Nanoindentation-derived mechanical properties of isotactic polypropylene.

Temperature (ºC)	Indentation modulus, E (GPa)	Hardness, H (MPa)	Yield stress from ECM, σ_y (MPa)	Yield stress from Tabor, σ_y (MPa)
20	2.6	110.7	53.8	36.9
40	20.1	93.9	41.5	31.3
60	13.1	79.2	38.0	26.4
80	11.2	63	29.0	21.0

*Spherical nanoindentation results obtained using a 20 µm radius diamond indenter. Indentation modulus and hardness were determined using the Oliver–Pharr method, while yield stress was estimated from the expanding cavity model (ECM). Reported values represent the average of ten indentations per condition.

*Standard deviations were within ±5% unless otherwise stated

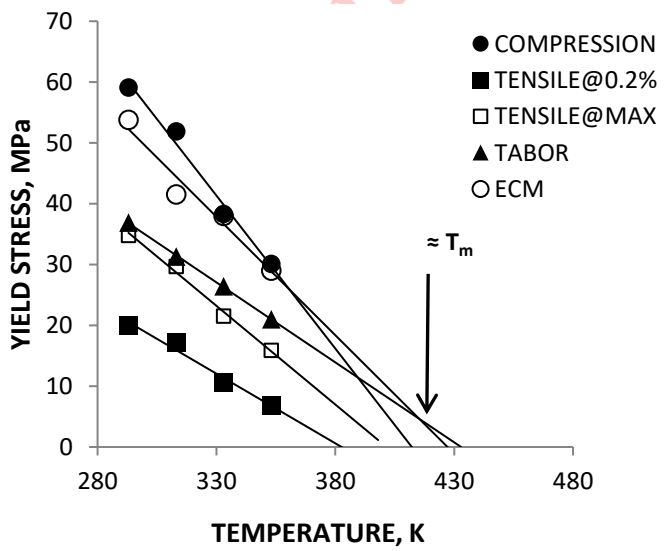

Figure 2. Temperature dependence of yield stress in isotactic polypropylene measured via tensile testing (0.2% offset and maximum stress), compression, and nanoindentation methods (Tabor's relation and expanding cavity model).

This progressive reduction underscores the critical role of crystalline lamella in controlling yields. As temperature rises, interlamellar tie chains gain mobility and lamella undergo partial melting, reducing effective load transfer across crystalline-amorphous interfaces.

Consequently, the dominant deformation mechanism transition from shear-dominated yielding to viscous flow. This transition is especially evident in the deviation of the 0.2% offset yield stress, which reflects early onset of local viscoplastic deformation. Such sensitivity highlights why the offset method is less reliable for semicrystalline polymers than the maximum-stress definition.

Effect of strain rate on yield stress

The effect of strain rate on yield stress is shown in Table 1 and Figure 3. As expected, higher strain rates result in increased yield stress across all testing methods. Nanoindentation (ECM) and compression continue to display strong agreement, reinforcing the consistency of indentation-based yield estimates at high loading rates. This observation aligns with recent findings demonstrating that strain-rate sensitivity measured via nanoindentation matches that of bulk-scale tests—even up to rates of ~10^4 s^{-1}—supporting the validity of indentation under dynamic loading conditions [25].

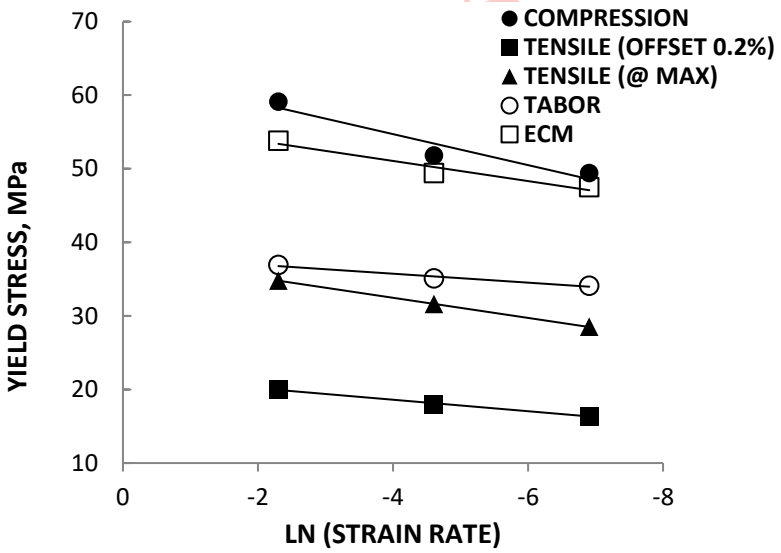

Figure 3. Effect of strain rate on yield stress in isotactic polypropylene determined by uniaxial tensile, compression, and nanoindentation (ECM and Tabor) methods at room temperature, illustrating the rate sensitivity and inter-method comparison.

Tabor-derived yield values again follow the trend of tensile maximum stress, whereas the 0.2% offset stress remains significantly lower. These results confirm the robustness of indentation techniques for probing local yielding, especially when macroscale testing is impractical due to sample size or rate constraints [12].

The observed strain-rate dependence is consistent with a thermally activated flow description commonly employed for semicrystalline polymers, such as the Eyring framework; however, direct mechanistic verification of chain-segment relaxation was not examined in the present study. The strong correlation between ECM-based indentation and bulk compression data suggests that the local stress state under indentation mimics the hydrostatic compression component, explaining their agreement. By contrast, the larger discrepancy with tensile offset values reflects the greater contribution of dilatational processes (e.g. cavitation or craze initiation) under tensile loading, which are less activated in indentation.

These findings reaffirm the importance of using well-calibrated models when interpreting indentation data. Advanced analysis techniques, including those reviewed by Pshyk et al. [10], can further refine yield stress determination by accounting for time-dependent deformation and material heterogeneity.

Evaluation of predictive models

To interpret the temperature-dependent yield stress behavior of isotactic polypropylene (iPP), three constitutive models were examined: the Eyring model, the expanding cavity model (ECM), and the lamellar cluster model (LCM). Each offers a complementary framework for correlating macroscopic and indentation-scale deformation mechanisms. The Eyring model relates yield stress to strain rate and temperature through a thermally activated flow process, whereas the ECM describes indentation-induced plasticity by linking mean contact pressure to the material's yield stress. Here, the extracted Eyring parameters are used primarily to quantify rate- and temperature-dependent trends in yielding rather than to deduce specific molecular relaxation mechanisms. In contrast, the LCM explicitly considers the hierarchical deformation resistance of lamellar stacks, thereby bridging semicrystalline morphology and macroscopic yielding.

Table 3 summarizes the activation volumes determined from the Eyring analysis for different deformation modes at room temperature. Activation volumes obtained from localized spherical nanoindentation agree well with those extracted from bulk tensile (evaluated at the maximum stress) and compression tests. This consistency suggests that a similar thermally activated deformation process governs yielding under both localized and macroscopic loading conditions. Because the classical Eyring formulation is defined for the stress at the onset of macroscopic flow (i.e., the maximum tensile stress), deviations observed for the 0.2% offset tensile yield are expected and reflect differences in yield definitions rather than a breakdown of the model.

The extracted activation energies lie in the range 200–250 kJ mol^{-1} (Table 3), which is consistent with values reported for cooperative segmental mobility in semicrystalline polypropylene and related polyolefins. The variation among deformation modes is moderate and reflects the differing stress states

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and mechanical constraints. Nanoindentation exhibits the largest activation energy due to the mixed hydrostatic–deviatoric loading beneath the spherical indenter, whereas compression and tensile (maximum stress) exhibit lower values corresponding to more homogeneous flow. The higher activation energy associated with the 0.2% offset tensile yield arises from the definition of yield prior to the onset of full plastic flow rather than from a change in deformation mechanism.

Table 3. Parameters used in Eyring and lamellar cluster model for isotactic polypropylene.

Test method	Parameter			
	Eyring		Lamellar cluster	
	Activation volume (nm^3)	Activation energy ($kJ\ mol^{-1}$)	n	E_0 (GPa)
Tensile (0.2% offset)	8.97	237	0.82	1.8
Tensile (max)	5.12	201	-	
Compression	3.33	208	0.53	
Nanoindentation (ECM)	5.12	253	0.67	

Overall, these results demonstrate that the Eyring analysis provides a consistent description of temperature- and rate-dependent yielding across deformation modes. The remaining variations are attributed primarily to differences in constraint and stress state rather than to fundamental changes in molecular mechanism. While the classical Eyring model effectively captures the strain-rate and temperature dependence of yield stress—consistent with earlier reports on thermally activated flow in iPP [15, 20]—it does not explicitly incorporate morphological attributes such as crystallinity, lamellar thickness, or orientation. Extended Ree–Eyring or cooperative models, including those validated for bulk polymers and nanocomposites, provide more refined predictions of yield stress as functions of temperature, strain rate, and porosity and have been shown to outperform single-process Eyring approaches [21].

Crystal plasticity models attribute yielding in semicrystalline polymers to thermally activated shear within crystalline lamellae, often described in terms of chain slip and lattice shear. Although the conventional formulation does not yield a closed-form $\sigma_\gamma(T)$ function, the model rationalizes the experimentally observed decrease in yield stress with temperature through an Arrhenius-type reduction in the energy barrier for crystalline slip. Full quantitative calibration requires structural inputs such as lamellar thickness, Burgers vector, crystallite orientation, mobile dislocation density, and phase-partitioned shear moduli, which were not directly measured in the present study; therefore parameter fitting was not attempted.

Representative structural parameters for isotactic polypropylene (iPP) relevant to thermally activated crystal plasticity include an effective Burgers vector $b \approx 0.5–0.7$ nm, corresponding to the chain periodicity in the crystallographic slip direction, and a lamellar stem length/lamellar thickness $L_s \approx 10–20$ nm, consistent with small angle X-ray scattering (SAXS) and morphological measurements in

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commercial iPP [26]. Activation energies associated with lamellar shear and chain-segment slip processes have been reported in the range $\Delta G_a \approx 80–200\ \mathrm{kJ\ mol^{-1}}$ [27] . Using these representative values, the crystal plasticity framework predicts that thermal assistance to crystalline slip becomes appreciable at elevated temperatures ($\approx 0.6T_m$), consistent with the experimentally observed reduction in tensile yield stress. In addition, the crystal plasticity interpretation is compatible with the Tabor relation, as indentation-derived yield stresses probe shear-dominated modes that are more sensitive to crystalline lamellae. Such agreement supports the view that crystalline-phase slip contributes more strongly to indentation and high-temperature tensile yielding, whereas amorphous-phase flow dominates at lower temperatures. In the present work, the crystal plasticity model is employed qualitatively to rationalize the temperature sensitivity of yielding and to contextualize the higher activation energies inferred from the Eyring analysis.

Figure 4 presents the fitting of the lamellar cluster model to the yield stress data obtained from (a) compression tests and (b) nanoindentation experiments (ECM-based) for isotactic polypropylene. The model predictions, described in Modeling section, were fitted to the experimental data to extract the lamellar cluster parameter *n*, which quantifies the relative contribution of crystalline and amorphous phases to the yielding process. The fitted *n* values varied with deformation mode (Table 3):

- $n \approx 0.82$ for tensile (0.2% offset) yield stress,
- $n \approx 0.53$ for compression,
- $n \approx 0.67$ for nanoindentation

A sensitivity analysis showed that a ±10% variation in the assumed cluster modulus E_0 resulted in negligible changes in the fitted lamellar cluster parameter n, indicating that the model predictions are robust with respect to reasonable uncertainty in E_0. These differences in *n* reflect the distinct stress states and local deformation mechanisms associated with each testing configuration [18, 19]. The higher *n* value under tensile loading proposes yielding dominated by inter-lamellar slip and lamellar rotation, with limited constraint from the amorphous phase. In contrast, the lower *n* value in compression suggests a more cooperative deformation in which amorphous regions play a greater role in accommodating plastic strain through shear yielding and chain rotation. The intermediate *n* value obtained from nanoindentation corresponds to the mixed hydrostatic–deviatoric stress state beneath the indenter tip.

Overall, these results confirm that the lamellar cluster model effectively captures the deformation behavior of semicrystalline polypropylene across different loading modes. The consistency of the fitted parameters supports the interpretation that temperature- and rate-dependent yielding of iPP arises from hierarchical interactions between crystalline lamellae and the amorphous matrix, modulated by the local stress state and constraint level. This finding agrees with previous reports of $n \approx 0.37$ for iPP [15]. Nevertheless, the model fails to fully capture the tensile maximum stress because of competing deformation mechanisms—crazing and shear yielding—at large strains. Crazing introduces localized dilatational failure, whereas shear yielding governs the overall plastic deformation [28].

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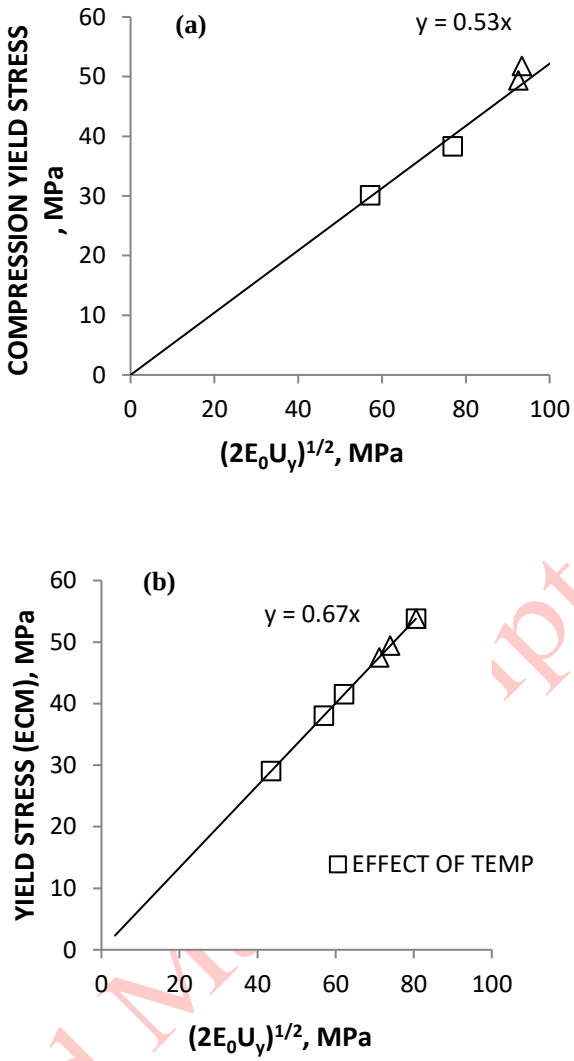

Figure 4. Fitting of the lamellar cluster model to yield stress data obtained from (a) compression tests and (b) nanoindentation experiments (ECM-based) in isotactic polypropylene.

The divergence between model predictions and experimental data highlights a limitation of the LCM: it assumes lamellae behave as independent clusters with uniform stiffness, whereas in reality, deformation involves cooperative lamellar–amorphous interactions. This suggests the need for hybrid constitutive models that integrate both shear-yield and craze-initiation mechanisms for semicrystalline polymers such as iPP.

The observed variation of the *n* parameter across testing methods also reveals the scale-dependent nature of deformation constraints. The higher *n* from tensile tests indicates greater lamellar rotation and inter-lamellar slip under uniaxial stress, while the lower *n* values from compression and indentation correspond to constrained plastic flow under triaxial stress. This correspondence demonstrates that nanoindentation and bulk tests probe the same fundamental yield mechanisms under different constraint conditions, confirming the robustness of the lamellar cluster model in linking local and macroscopic deformation behavior.

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Recent molecular dynamics (MD) studies further support these experimental interpretations. Li et al. [29] demonstrated that in semicrystalline polymers, chain-segment mobility, interfacial slip, and temperature/strain-rate effects critically govern yield behavior. For isotactic polypropylene and its composites, MD simulations have revealed structural rearrangements—including lamellar slip, chain disentanglement, and tie-chain relaxation—that occur under load and are strongly temperature- and rate-sensitive [30]. These atomistic findings mirror the experimental trends observed in this study: a decrease in yield stress with increasing temperature, and the rate-dependent behavior captured by both nanoindentation and bulk tests.

Although our work operates at the continuum scale, the agreement with MD results underscores the multiscale consistency of the deformation mechanisms. Future research integrating MD simulations with continuum plasticity and morphological modeling could establish a quantitative link between molecular-scale structure, mesoscale lamellar organization, and macroscopic yield response—providing a unified framework for the predictive design of semicrystalline polymers.

CONCLUSION

In this study, yield stress in isotactic polypropylene was investigated across macroscopic (tensile, compression) and microscopic (nanoindentation) scales over a range of temperatures and strain rates. The main findings are as follows:

Yield stresses extracted from nanoindentation via the expanding cavity model (ECM) showed close agreement with compression data, confirming the dominance of compressive fields and validating indentation as a reliable micro-scale technique for semicrystalline polymers. Tabor-based estimates aligned with tensile maximum stresses, illustrating that cross-scale yield correlations are deformation-mode dependent rather than universal.

The temperature and strain-rate dependencies reflect thermally activated chain-segment motion and interlamellar shear within the heterogeneous lamellar morphology. This confirms that yield in semicrystalline polymers is governed by rate-limited cooperative plasticity rather than a unique yield point.

Among the three theoretical frameworks considered, Eyring's model captured the global trends in temperature- and rate-sensitivity but lacked microstructural specificity. The crystal plasticity model performed more accurately at elevated temperatures and low strain rates, consistent with enhanced crystallographic slip and reduced constraint from the amorphous phase. The lamellar cluster model differentiated between deformation modes and highlighted the role of lamellar constraints and local shear, providing morphological interpretation beyond purely phenomenological fitting.

By integrating multi-scale experiments with constitutive models, this work provides a quantitative basis for using nanoindentation as a localized yield probe in semicrystalline polymers and clarifies the limitations and applicability of commonly used yield models. These results offer practical guidance for yield characterization when sample geometry or processing produces spatial heterogeneity, and they

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form a foundation for future studies linking crystalline morphology, temperature-dependent viscoplasticity, and indentation response.

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