AI-Enhanced Hybrid Modeling for Optimizing Polymeric Yarn Manufacturing Processes

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Creating reliable models for synthetic textiles manufacturing process is challenging due to the inherent complexity of polymers and the diversity of manufacturing conditions. Traditional atomistic models, while accurate at the molecular level, are computationally demanding and difficult to scale [1]. On the other hand, machine learning models often struggle to generalize beyond training data, particularly in accurately capturing the physical properties of polymers [2,3]. This research addresses these limitations by introducing a hybrid modeling framework that combines atomistic simulations, surrogate models, and machine learning techniques. The approach leverages the strengths of each method to achieve enhanced predictive accuracy and adaptability in real-time manufacturing conditions.

The primary objective of this study is to accurately model the stress-strain behavior and tenacity of synthetic yarns made of polymers as a function of material composition and process control variables, which include, melting and cooling temperatures, extruder pump pressure, and spinning godets speed. By linking these variables to microstructural properties such as crystallinity and polymeric chains orientation, the proposed model aims to optimize melt spinning manufacturing processes for improved yarn strength and consistency.

The first component of the hybrid approach is a coarse-grained molecular dynamics (CGMD) model, implemented using LAMMPS [4] and Python for data analysis. The CGMD model reduces computational complexity while maintaining accuracy by representing polymeric chains as simplified particles. This approach captures essential features of molecular interactions and links crystallinity and orientation to the mechanical properties of the yarn. Figure 1 shows a graphical representation of the coarse-grained model.

To generate initial configurations, periodic microstructures with alternating crystalline and amorphous domains were created using the Interphase Monte Carlo (IMC) method, as described in [5]. The amorphous phase was modeled using a random walk technique, ensuring realistic distribution of non-crystalline chains. The generated initial configuration was subsequently equilibrated using simulations in the NPT ensemble to obtain a realistic initial condition, in terms of structure and density. Finally, these configurations were subjected to stress simulations to generate the stress strain curves. An example of the generated curves is shown in Figure 2.

To enable real-time predictions, a surrogate model was developed to approximate the behavior of the atomistic model. The input and output of the reduced model are the same than those of the atomistic one: crystallinity and polymeric chains orientation as inputs, and mechanical properties such as maximum stress, elongation, and tenacity as outputs. This reduced model uses Principal Component Analysis (PCA) to minimize the dimensionality of input and output variables while preserving critical features. A Radial Basis Function (RBF) network, implemented using Scikit-Learn, maps the transformed inputs to the corresponding outputs, predicting properties such as maximum stress, elongation, and tenacity. The surrogate model significantly reduces computational requirements while maintaining predictive accuracy. To train the surrogate model, a parametric set of physical simulations was performed, followed by machine learning fitting to capture the underlying relationships.

The final component is a dense neural network model developed in PyTorch, designed to directly link manufacturing variables to mechanical properties. The process begins with an experimental dataset providing process variables (u_{exp}) and measured mechanical properties (y_{exp}). Figure 3 illustrates this hybrid modeling framework that integrates three key elements:

- Neural Network 1 (NN_1) transforms process variables into microstructural features.
- Neural Network 2 (NN_2) maps these features to mechanical properties.
- A surrogate physical model generates secondary predictions for comparison.

Three loss functions ensure accuracy and consistency:

- Empirical Loss aligns predictions with experimental data.
- Physical Loss ensures consistency with the surrogate model.
- Constraint Loss enforces domain-specific physical rules.

The total loss function optimizes the hybrid framework to balance experimental and physical accuracy.

Preliminary validation indicates the hybrid model improves stress-strain predictions by 25% compared to traditional atomistic and standalone machine learning approaches.

The resulting hybrid tool provides real-time predictions of the mechanical performance based on

current process conditions. It integrates insights from both molecular dynamics and empirical data, providing a holistic predictive solution. The model successfully links process control variables to both the tenacity and mechanical properties of the yarn, providing a valuable tool for optimizing manufacturing conditions.

In summary, this study demonstrates a novel hybrid modeling framework that combines atomistic simulations, surrogate modeling, and neural networks to address the challenges of synthetic yarn manufacturing. By leveraging the strengths of these techniques, the model offers real-time, accurate predictions of mechanical properties based on process variables. This approach has the potential to transform process control and material optimization in polymer manufacturing.

Future work will focus on expanding the model applicability to other polymer systems and incorporating additional experimental data to improve robustness. Validation in industrial settings will further assess its scalability and impact on manufacturing efficiency.

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References

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Figures

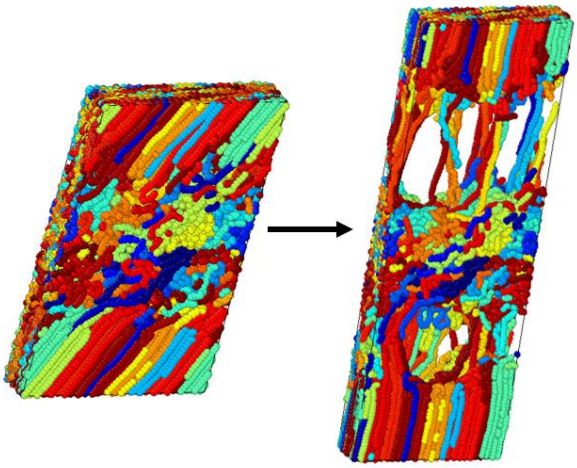

Figure 1. Atomistic tensile test

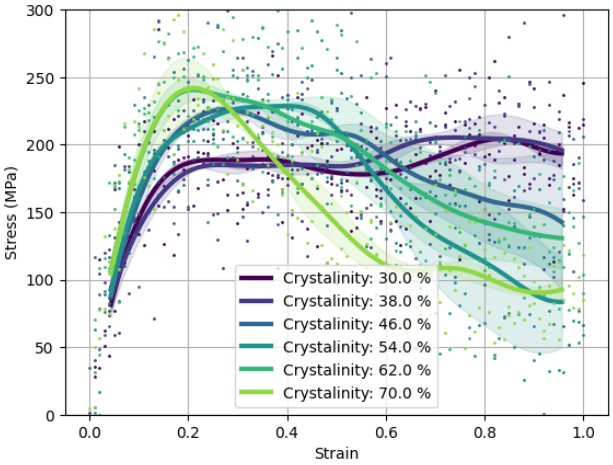

Figure 2. Stress strain curve obtained with the coarse-grained toolkit

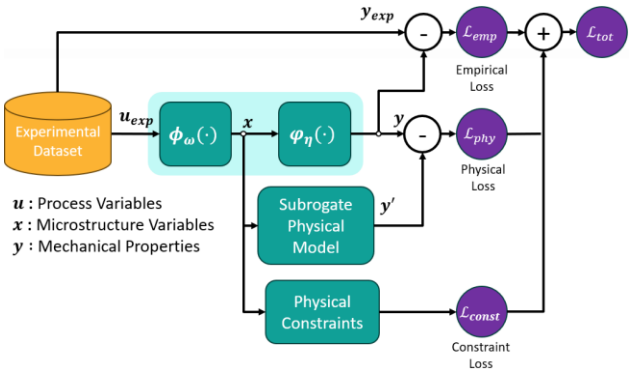

Figure 3. Hybrid modelling methodology proposed.