Predicting the Stress-Strain behaviour of isotactic Polypropylene (iPP) by using Molecular Dynamics and Neural Networks

Mikel Irigoyen[1], Héctor Lobato[2], Aitor Arriaga[2], Aizeti Burgoa[2], Jose Javier Egurrola[2], Fernando Ruipérez[3], Jon M. Matxain[4],
[1] POLYMAT and Department of Polymers and Advanced Materials: Physics, Chemistry and Technology, Faculty of Chemistry, Univesidad del Pais Vasco/Euskal Herriko Univertsitatea UPV/EHU, Donostia-San Sebastián 20018, Spain
[2] Leartiker S. Coop, Xemein etorbidea 12 A, Markina-Xemein, Spain
[3] POLYMAT and Physical Chemistry Department, Faculty of Pharmacy, University of the Basque Country UPV/EHU, 01006 Vitoria – Gasteiz, Spain
[4] Department of Polymers and Advanced Materials: Physics, Chemistry and Technology, Faculty of Chemistry, Univesidad del Pais Vasco/Euskal Herriko Univertsitatea UPV/EHU, Donostia-San Sebastián 20018, Spain and Donostia International Physics Center (DIPC), Paseo Manuel Lardizábal 4, 20018, Donostia−San Sebastian, Spain

mikel.irigoyenu@ehu.eus

The study of semicrystalline polymers' mechanical properties is vital due to their significant role in various industries. For example, isotactic polypropylene (iPP), a semicrystalline polymer, is the second most produced synthetic polymer globally and is widely utilized in products like films, fibers, and plastics. The characteristics of these materials, such as their chemical structure, molecular weight, degree of crystallinity, and molecular alignment, are influenced by the methods and conditions used during their synthesis and processing. [1-3]

Molecular dynamics (MD) simulations have proven effective in capturing the chemical and physical structures of polymers, such as polypropylene (PP), and in modeling their mechanical properties. Prior studies have represented isotactic polypropylene (iPP) using atomistic or united-atom models, which simplify the system by excluding explicit hydrogen atoms. [4,5] Similarly, MD simulations have been employed to study the tensile deformation of polyethylene (PE). [6] This method involved equilibrating the system between strain applications, yielding stress–strain curves closely matching experimental observations. [7]

Artificial intelligence, particularly machine learning, is becoming a powerful tool in scientific research, offering innovative solutions to complex problems by identifying patterns and enabling predictions from large datasets. Artificial neural networks (ANNs) have gained traction in materials science as a robust regression tool for capturing complex correlations between processing conditions, microstructure, and resulting thermo-mechanical properties. [8,9] ANNs, with their flexibility and capacity to model intricate relationships, have shown the ability to effectively describe the complex structure–property correlations of this kind of materials. [10]

In this study, we perform MD simulations of various iPP systems to predict stress–strain behavior, validating our results against experimental data and using different properties such as the molecular weight, the crystallinity and the Hermman's orientation factor to parameterize a constitutive model. Additionally, we apply ANNs to explore structure-property relationships, linking the chemical and physical features of the polymer to the constitutive model parameters that describe its mechanical behavior. Here, we train ANNs on data generated from MD simulations, using experimental data only for validation.

References

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Figures

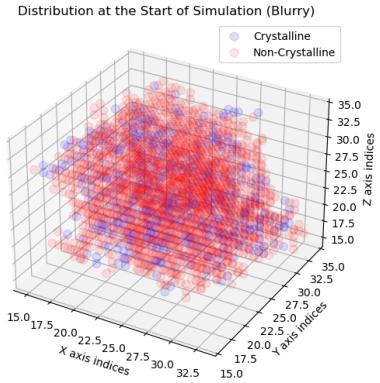

Figure 1. Spatial distribution of crystalline and non-crystalline regions of the simulated iPP.

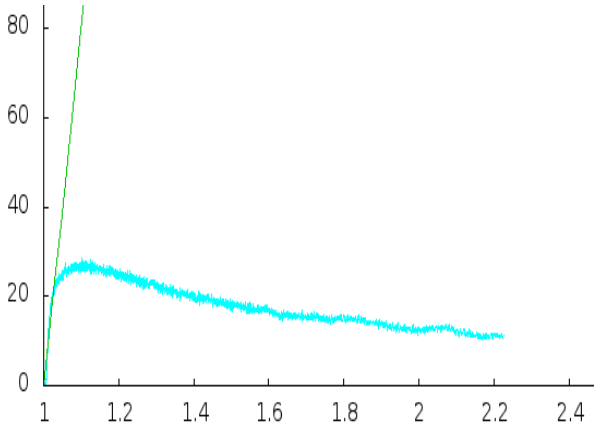

Figure 2. Simulated Stress-Strain curve at 10^8 s^{-1} for iPP calculated by Molecular Dynamics simulations (blue) and linear region (green) for computing Young's modulus