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Multiscale Machine Learning Prediction of the Glass Transition Zone in Thermoset Polymers

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RESEARCH HIGHLIGHTS

- Glass transition modeled as a continuous temperature-dependent zone, not a single Tg
- Introduced triple-scale fingerprinting (micro, meso, macro)
- Compared SVR, GP, and ANN models on 204 thermoset polymers
- ANN selected as best model based on multi-metric evaluation
- Validated against three new polymer classes beyond training data

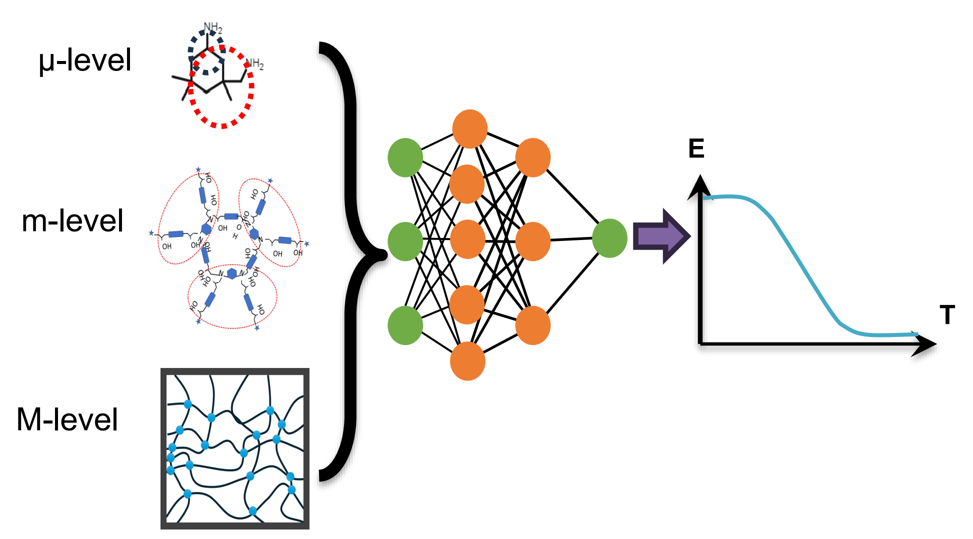

Figure 1: (a) Diagram of the three multiscale features

STATEMENT OF THEORY AND DEFINITIONS

The glass transition zone is characterized by four parameters:

- Onset temperature (T_L): beginning of modulus decay
- Endset temperature (T_H): completion of transition
- Glassy modulus (E_g): stiffness in the glassy state
- Rubbery modulus (E_r): stiffness in the rubbery state

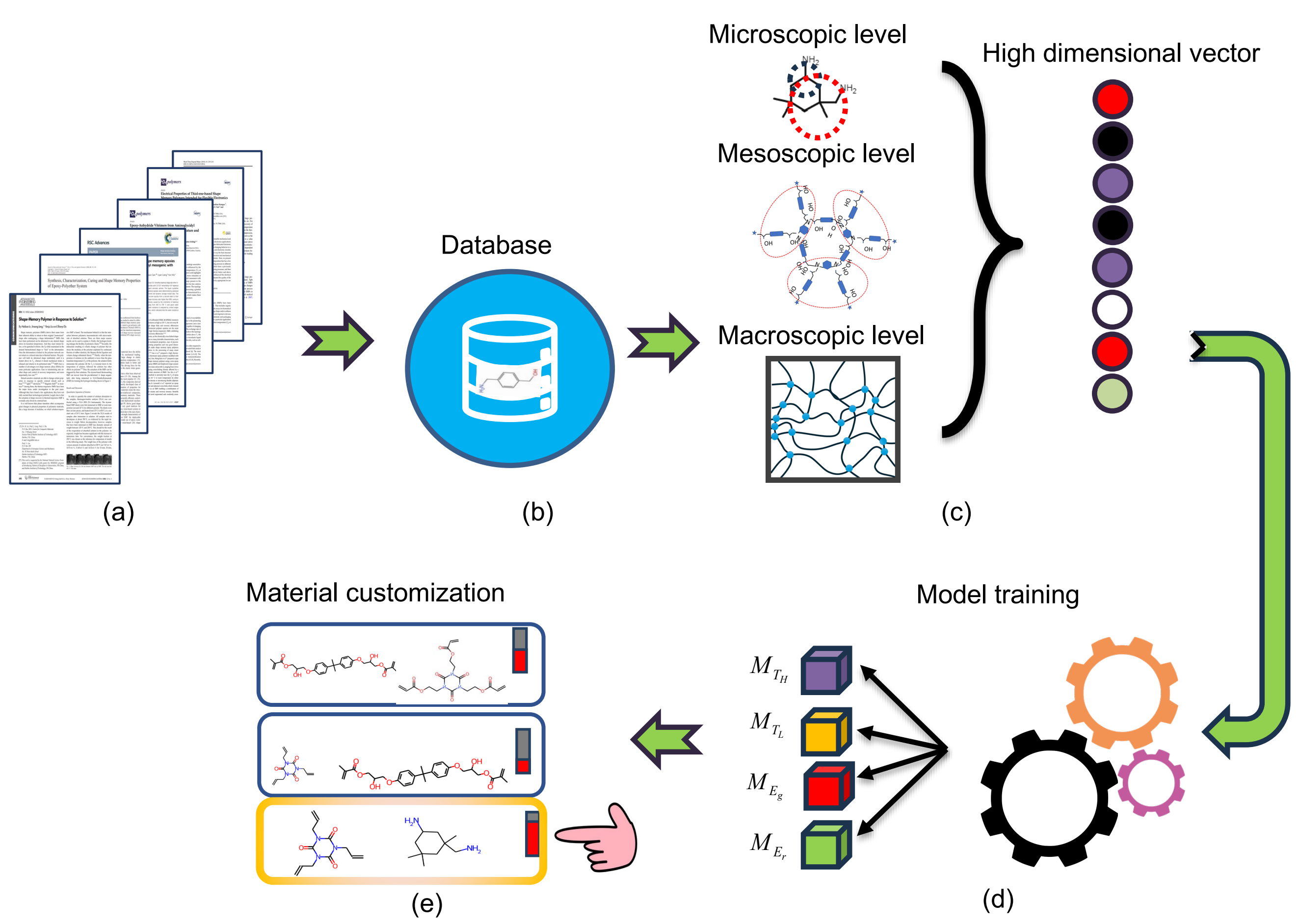

Figure 2: Framework of polymer customization

ABSTRACT

The glass transition governs the thermomechanical behavior of polymers, yet accurately predicting this process remains challenging. This work presents a multiscale machine learning framework to model the entire glass transition zone of thermoset polymers by integrating microscopic, mesoscopic, and macroscopic features. SVR, GP, and ANN models were trained and evaluated on thermoset polymer data.. The ANN demonstrated the highest predictive accuracy and was validated on new polymer classes, confirming strong generalization. This approach provides a practical, data-driven tool for predicting and tailoring thermoset polymer performance.

METHODOLOGY

- A dataset of 204 thermoset shape memory polymers was used for model development.
- Polymer structures were encoded using multiscale feature engineering (microscopic level, mesoscopic level, macroscopic level.
- Three supervised learning models were trained and compared: support vector regression (SVR), Gaussian process regression (GP), and artificial neural networks (ANN) to predict the four Tg parameters.

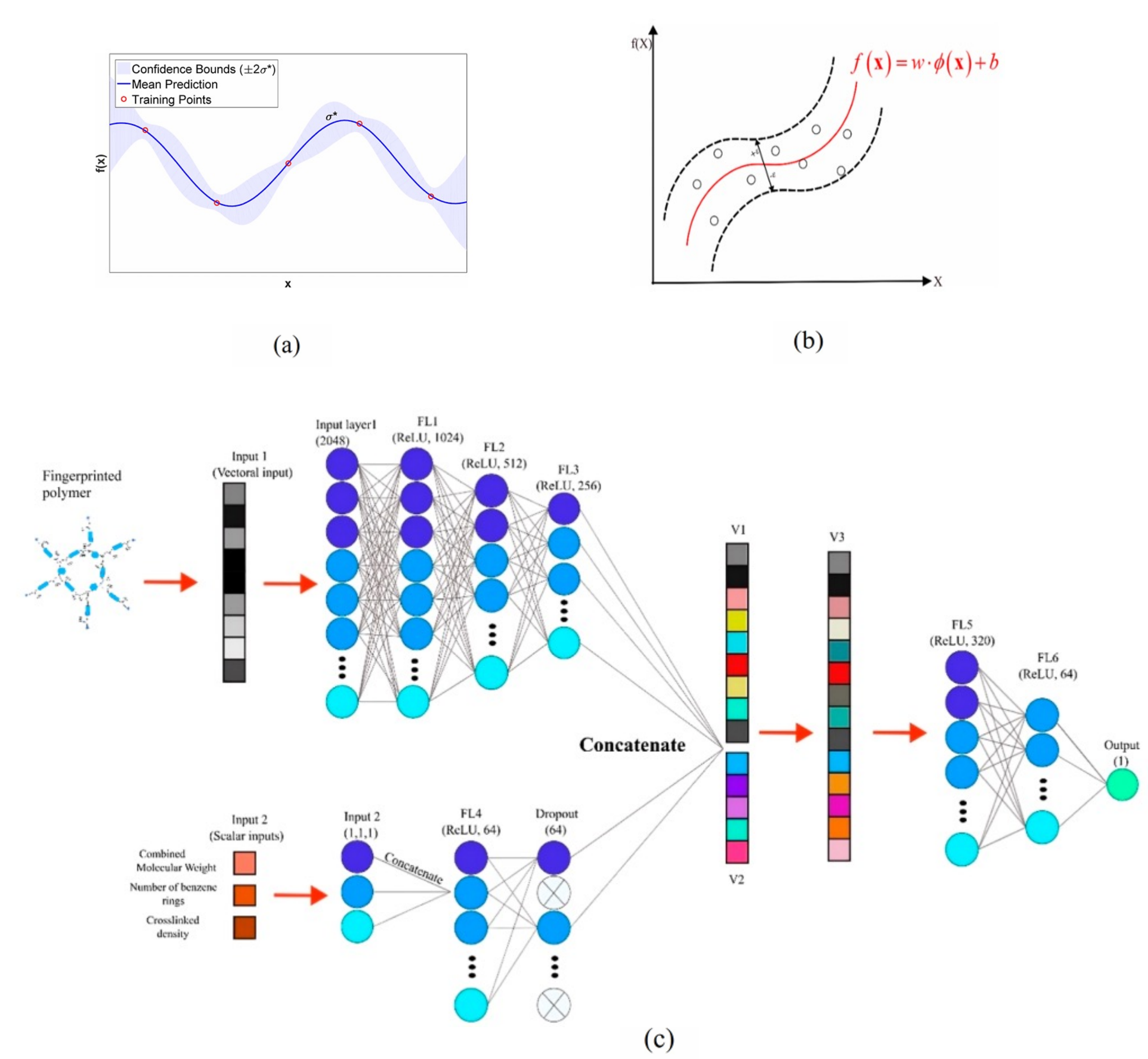

Figure 3: (a) Schematic diagram for GP model (b) Conceptual illustration for SVR algorithm, (c) Architecture for the newly designed ANN models

RESULTS

The comparative performance of ANN, SVR, and GP models across onset temperature, endset temperature, rubbery modulus, and glassy modulus is summarized below. The ANN demonstrates consistently higher predictive accuracy and lower error across all parameters, particularly in capturing nonlinear modulus behavior within the transition zone.

Table 1. Summary of ANN Results for the Four Models

Metric	Endset (Train)	Endset (Test)	Onset (Train)	Onset (Test)	Rubbery (Train)	Rubbery (Test)	Glassy (Train)	Glassy (Test)
R^2	0.97	0.82	0.94	0.81	1.0	0.97	0.96	0.9
PCP (%)	100	100	99.39	100	96.93	63.41	95.09	85.37
MAPE (%)	1.24	3.07	1.68	2.9	3.63	22.06	6.65	11.69
MAE	4.94	11.67	5.88	10.14	0.74	2.63	0.11	0.24

Table 2. Summary of SVR Results for the Four Models

Metric	Endset (Train)	Endset (Test)	Onset (Train)	Onset (Test)	Rubbery (Train)	Rubbery (Test)	Glassy (Train)	Glassy (Test)
R^2	0.83	0.83	0.86	0.86	0.38	0.57	0.4	0.45
PCP (%)	100	100	100	100	63.8	43.9	41.72	46.34
MAPE (%)	3	4	3	3	51.0	181.0	37.0	33.0
MAE	11.64	14.79	10.23	11.71	6.76	7.31	0.54	0.58

Table 3. Summary of GP Results for the Four Models

Metric	Endset (Train)	Endset (Test)	Onset (Train)	Onset (Test)	Rubbery (Train)	Rubbery (Test)	Glassy (Train)	Glassy (Test)
R^2	0.94	0.82	0.94	0.8	0.99	0.8	0.88	0.81
PCP (%)	100	97.56	100	97.56	87.12	39.02	88.34	80.49
MAPE (%)	2.08	3.34	2	3.47	11.46	50.6	12.34	14.73
MAE	8.06	12.41	7.61	11.74	1.12	5.8	0.2085	0.3

CONCLUSION

- Glass transition was successfully predicted as a continuous zone
- ANN identified as most robust and reliable model
- Validated on three new polymer classes
- Provides fast alternative to computationally intensive simulations
- Supports data-driven thermoset polymer design

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