Researchers identify breaking point of conducting material

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An improved method to predict the temperature when plastics change from supple to brittle, which could potentially accelerate future development of flexible electronics, was developed by Penn State

College of Engineering researchers.

Next-generation flexible electronics, such as bendable displays and medical implants, will rely on semiconductor materials that are mechanically flexible. Accurate predictions of the temperature when embrittlement occurs, known as the glass transition temperature, is crucial to design conducting polymers that remain flexible at room temperature.

"Previous work to predict the glass transition of polymers relied on complex, multi-parameter models but nevertheless led to poor accuracy," said Enrique Gomez, professor of chemical engineering and principal investigator. "In addition, accurate experimental measurements of the glass transition of conjugated polymers are challenging."

All polymers become brittle when cooled. However, some polymers, such as polystyrene used in Styrofoam cups, become brittle at temperatures higher than room temperature while other polymers, such as polyisoprene used in rubber bands, become brittle at much lower temperatures.

Renxuan Xie, previously a doctoral student at Penn State and now a postdoctoral researcher at the University of California at Santa Barbara, found a way to measure glass transition temperatures by keeping track of the mechanical properties as embrittlement occurs, laying the foundation for understanding the relationship between the glass transition and structure. Follow-up studies then determined the glass transition for 32 different polymers by measuring mechanical properties as a function of temperature.

"This advancement, coupled with data for various polymers in our later studies, revealed a simple relationship between the chemical structure and the glass transition," Gomez said. "Therefore, we can now predict the embrittlement point from the chemical structure."

According to Gomez, this work, reported in a recent issue of *Nature Communications*, allows researchers to predict the glass transition temperature from the chemical structure of conducting polymers before they are synthesized for use in electronics. Most currently used conducting polymers are brittle and inflexible, so this advancement could accelerate the development of flexible electronics.

"Although it sounds simple, we're the first to use the mechanical properties of conducting polymers to measure the glass transition temperature," Gomez said. "We combine the data from many different polymers to derive a simple relationship that predicts the glass transition temperature based on the chemical structure in a more accurate way than previously possible."

Gomez's study was funded by a four-year, $1.75 million grant awarded in 2019 by the National Science Foundation to explore the integration of theory, simulations and experiments to accelerate the development of flexible electronics based on organic compounds. The next steps for this research, Gomez said, are more extensive tests and exploration of practical applications.

"We now want to use our model to design conducting polymers to make ultra-flexible and stretchable electronics," Gomez said. "We also want to push our model to find the limits and see where the model breaks down."

More information: Renxuan Xie et al, Glass transition temperature from the chemical structure of conjugated polymers, *Nature Communications* (2020). DOI: 10.1038/s41467-020-14656-8

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