Inverse design of the composition of thermally and electrically conductive polymer composite by multi-objective optimization

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Polymer composite materials are widely used in automobiles, aircraft, and communication devices. The discovery of polymer composites with mechanical, thermal, and electrical properties suitable for specific products is an important task in current R&D. In many studies, after developing a model for predicting individual properties, it was general to filter the polymer composite material composition with a range of satisfactory properties based on this model. In this study, a compositional reverse engineering model of a polymer composite material that satisfies the target values of electrical/thermal/mechanical properties was developed. The previously developed physical property prediction model was used by the XGBoost method, and the optimization process was performed to find a configuration that satisfies the target property by applying NSGA-Ⅲ and Variational autoencoder. In addition, by applying a cost function that can satisfy various target values, it is optimized close to the target property. The developed model will be an alternative that can reduce the time and cost required to develop a composite material with desired electrical/thermal properties.