# Multimodal Deep Learning for Novel Informatics of Composite Materials

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## Abstract

We proposed a pioneering data-centric method for complex materials, namely multimodal deep learning. Our method used multiple generative deep learning models of images and spectra to represent physical or chemical structures of complex materials and used for predicting properties. The proposed method was demonstrated on acrylate polymer composites with ten compositions and eight properties, and applied to find optimal compositions under conflicting multiple properties.

## 1. Introduction

In response to the increasing and changing demand for materials and their manufacturing processes, data-centric methodology has gained much attention. Traditional data-centric methods have primarily focused on molecular descriptors based on elements, chemical bonds, neighborhood associations, and electronic interactions for the discovery of molecules, inorganics, and crystals. However, these methods rely on a precise definition of material structure by elements and chemical bonds, which limits their applicability to complex materials. As a result, most materials in our daily lives, such as plastics, rubber, metal alloys, and wood, face significant challenges in applying data-centric methods. This study proposes an innovative technique, namely multimodal deep learning, to overcome the traditional limitations of data-centric methods. This approach integrates multiple complementary data to obtain more comprehensive information, which is similar to human cognition with five sensory organs. Our idea is to implement (1) multiple generative deep learning of characterization data (images, spectra, etc.) to represent the physical or chemical structures of materials, and (2) an integrated deep learning model to predict properties from multiple sources (Fig. 1A). The effectiveness of our proposed multimodal deep learning was demonstrated on polymer composites consisting of ten compositions of matrices, additives, fillers, and eight mechanical, thermal, and electrical properties.

## 2. Experiment

In this study, acrylate polymer composites were prepared using five acrylate monomers as matrices, two curing additives, and three particulate or fibrous fillers. These materials were mixed using a rotary mixer and cured at 100 °C for 60 min to produce polymer composite sheets with a thickness of 1 mm. A total of 80 samples with different compositions were prepared and their optical microscope images, infrared spectra, Raman spectra were measured for input information of physical or chemical structures. The target properties for prediction were Young's modulus, tensile strength, elongation at break, storage modulus, loss tangent, density, glass transition temperature (Tg), and surface electrical resistivity.

## 3. Results and discussion

To represent the physical or chemical structures of polymer composites, a conditional generative adversarial network with an architecture of BigGAN was introduced. As shown in Fig. 1B, the optical microscope image and infrared spectrum generated by the generative model were very close to those of real measurements. For example, distinct particle and fiber structures were observed in the images, and the absorption peaks were exhibited in the spectra. Thus, the generative model was shown to be effective in representing the physical and chemical structures of complex materials.

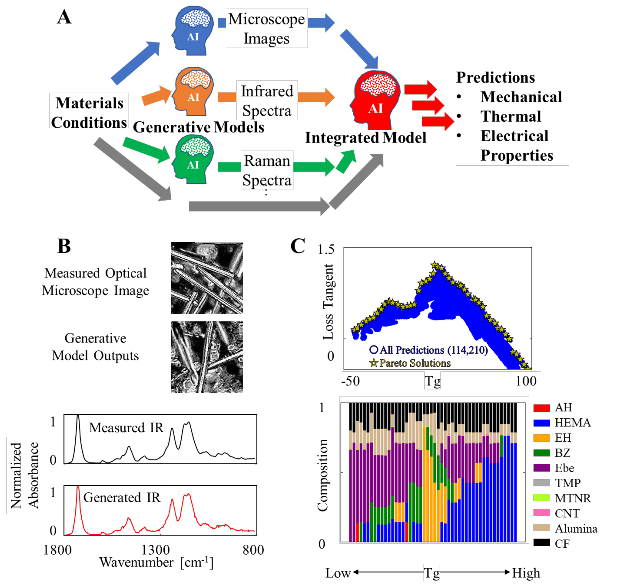


Fig. 1 (A) Schematic of the proposed multimodal deep learning, (B) Constructed generative models for images and spectra. (C) Predictions of properties of polymer composites and their optimal compositional solutions.

By applying multimodal deep learning with the inputs from the generative models, we predicted eight properties of polymer composites. In this article, the comparison of the predicted Tg with the loss tangent was presented (Fig. 1C). An interesting result was observed in the shape of the upper boundary of the predicted values due to the up and down trend. To analyze the precise information, the optimal composition under the upper boundary was extracted and visualized. As the target Tg increased, the optimal composition of the Ebe matrix gradually changed, but the EH matrix was dominant at a certain Tg. This might be due to the conflicting effect of the crosslinking network of soft Ebe and monofunctional EH matrix monomers. Through such predictions using multimodal deep learning, we can identify complex relationships of materials and properties.

## 4. Conclusions

We have developed multimodal deep learning to address the challenge of predicting various properties of complex materials. By combining multiple sources of complementary information and integrating them into a single model, our model effectively predicted various mechanical, thermal, and electrical properties of polymer composites. We believe that our proposed multimodal deep learning will accelerate AI-driven material and process development in various fields of complex materials.

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