Performance Prediction Technology for Rubber Materials Utilizing Machine Learning

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Abstract

Various rubber components are used in electrical products. To identify rubber components that can be applied to products from among the many varieties available, multiple performance evaluation tests need to be conducted, which requires an enormous amount of time. Therefore, to improve the efficiency of performance evaluation tests for rubber components, we examined performance prediction technology for rubber components using a regression model trained via machine learning on component performance and analytical data(1). In this study, by utilizing computer-based virtual experiments, including Finite Element Method (FEM) analyses, for collecting training data, we reduced training-data collection time to one-tenth of that required for repeated physical experiments. The developed model was able to predict the nonlinear load–displacement relationship of rubber components with an average accuracy of 84%.

1. Introduction

In recent years, advances in machine learning have enabled faster and more efficient development of materials, and higher-performance materials are expected to be commercialized in shorter time frames. For materials users such as Mitsubishi Electric, it will be important to quickly find and utilize materials that can be applied to their own products. As such, we are developing technology that uses machine learning to predict the performance of resin-based materials such as plastics and rubber, as well as components made from these materials. Because resin-based materials have drawbacks such as rapid degradation under environmental condition, a variety of time-consuming performance evaluation tests are needed before being applied in products. If the performance of resin-based materials and components can be estimated, it becomes possible to prevent rework due to evaluation test failures and to narrow down the candidates for testing, thereby improving the efficiency of performance evaluation.

This paper outlines the development of performance prediction technology for rubber components that contributes to such efficiency in performance evaluations.

2. Investigations to Improve Efficiency of Training Data Collection

This chapter outlines the investigations carried out to improve the efficiency of training data collection.

2.1 Collection of training data leveraging virtual experiments on a computer

A feature of this development is that the training data required for machine learning were collected through computer-based virtual experiments. An overview is shown in Fig. 1. The performance of rubber materials is known to be influenced by micro-structure, such as the degree of dispersion of carbon black mixed in as a reinforcing material(2)(3), and we examined extracting features from Transmission Electron microscopy (TEM) images to use as explanatory variables. However, prototyping materials, evaluating performance, and acquiring TEM images require an enormous amount of time. Therefore, using CAD, we created a model that represents TEM images, and we extracted features related to the micro-structure from this model. Furthermore, we calculated the performance of rubber components to use target variable by FEM analysis.

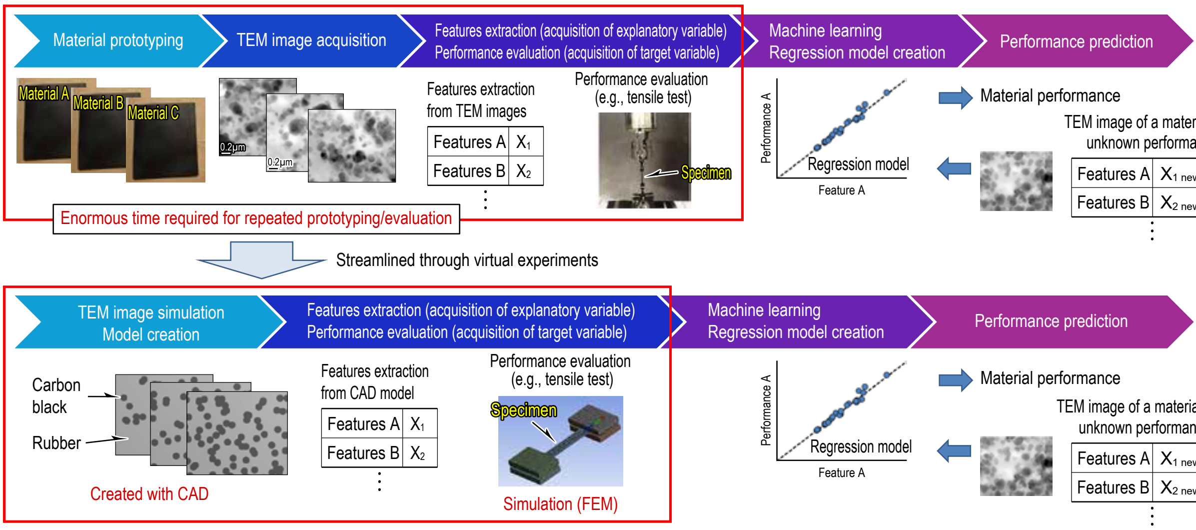

Fig. 1 Overview of the performance prediction technology for rubber components

2.1.1 Creation of a CAD model simulating TEM images and extraction of explanatory variables

An overview of the CAD-created model that simulates TEM images is shown in Fig. 2. The model was created by randomly placing circles to represent carbon black on a 2D plane. It is known that at the interface between the carbon black mixed into the rubber and the rubber matrix, there exists a middle layer with higher elasticity than the rubber[4], and a model of this middle layer was created in a similar manner. In this paper, we created 100 models in which the number and diameter of circles varied, and from each model we extracted features such as the fraction of area occupied by carbon black.

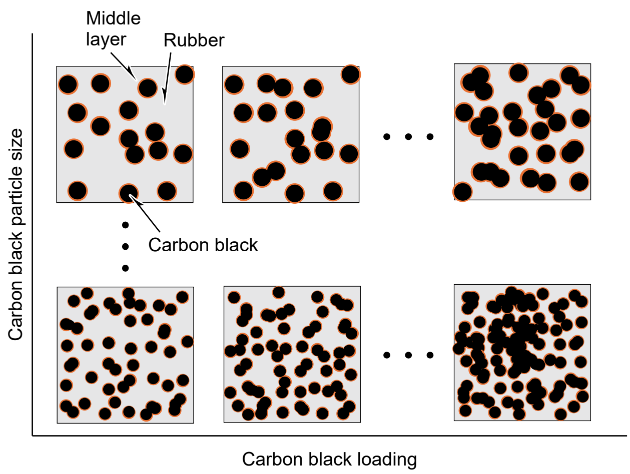

Fig. 2 Overview of CAD-simulated models of TEM images

2.1.2 Acquisition of target variables by FEM

In this paper, we obtained the performance of the target variable of rubber components through FEM analysis. An overview of the FEM analysis is shown in Fig. 3. Component performance can be evaluated using metrics such as the load–displacement relationship, creep deformation, and sealing performance. In this paper, as a simple example, we outline results predicting the load–displacement relationship of a strip specimen. Because the micro-structure such as degree of caebon black dispersion of rubber, affects the performance of macro-scale components, we conducted a Multi-Scale Simulation that couples the properties and behavior of structures at different scales. In the Multi-Scale Simulation, the load–displacement relationship of the strip-shaped component is calculated in FEM analysis 2. The stress–strain relationship required as material property in FEM analysis 2 was obtained by FEM analysis 1 using the CAD model created in section 2.1.1. With this method, differences in material properties arising from differences in the rubber's micro-structure can be reflected in the FEM analysis that simulates macro-scale performance evaluation tests. Note that the elastic modulus values of the rubber, carbon black, and middle layer used in

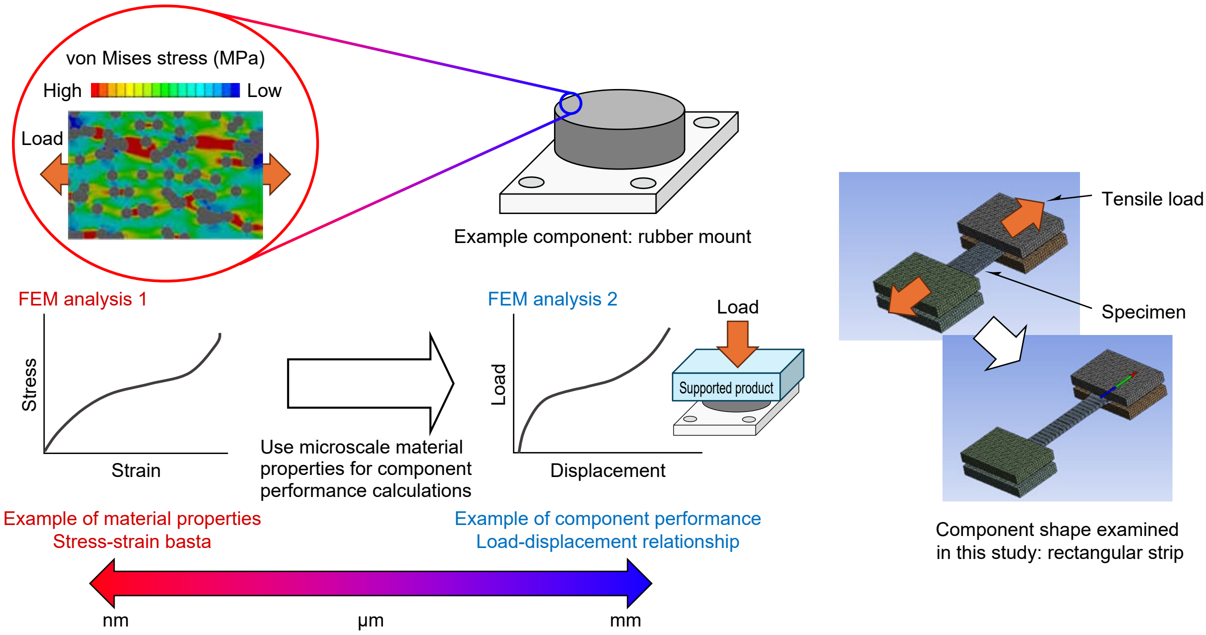

Fig. 3 Overview of the multi-scale simulation and the component shapes examined in this study

FEM analysis 1 were estimated from prototyping and evaluation of rubber without carbon black and from analyses such as Scanning Probe Microscopy (SPM) and Atomic Force Microscope (AFM).

2.2 Model training

We performed machine learning using the explanatory variables and the target variable collected in the virtual experiments of sections 2.1.1 and 2.1.2, and built a prediction model. If the training data were collected through actual experiments, it would be expected to take about 50 days; however, in this paper, it was completed in about 5 days. That is, by conducting virtual experiments on a computer, we were able to shorten the collection of training data to one-tenth of the time.

3. Accuracy Verification of the Prediction Model

In Chapter 2, we constructed a prediction model, into which we input features extracted from TEM images of acrylonitrile-butadiene rubber (NBR) with varying carbon black particle size and amount, and predicted the load displacement relationship. The results are shown in Fig. 4. Across all 12 conditions examined in this study, regardless of the particle size or amount of carbon black, the load displacement relationship of the rubber component could be predicted with an average accuracy of 84%. In addition to prediction, machine learning can evaluate the importance of each explanatory variable. Feature-importance analysis showed that carbon black content was the most influential feature, followed by the standard deviation of the contour lengths of the circles used to represent carbon black particles and the spatial dispersion of the centroids of those circles. This result suggested that, for the deformation of rubber components, not only the carbon black content but also the particle size distribution and the degree of dispersion contribute.

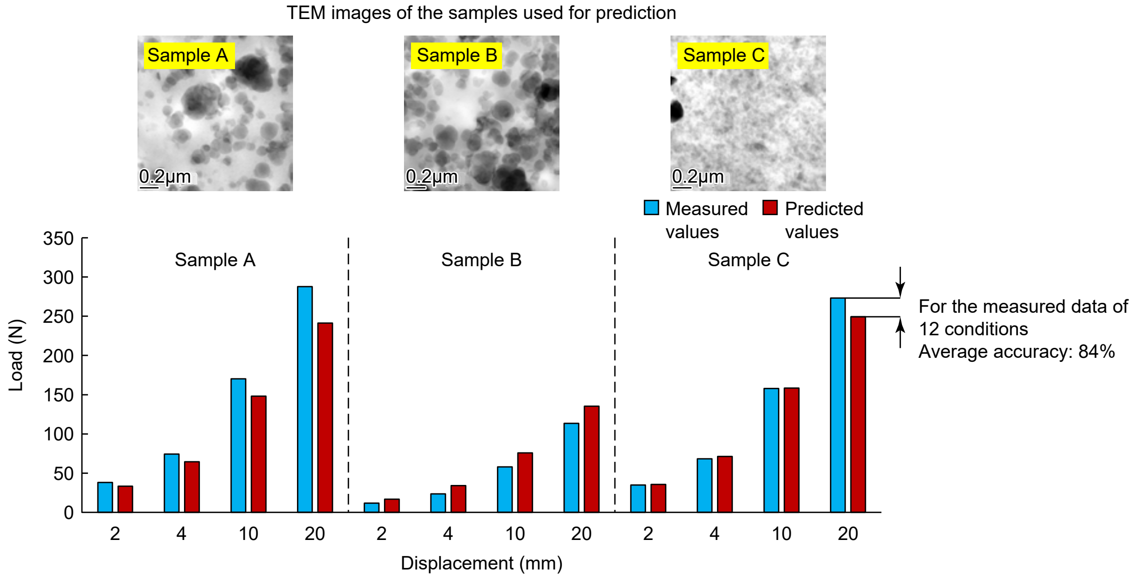

Fig. 4 Results of accuracy verification for the machine learning model

4. Conclusion

Using training data collected from compute-based virtual experiments, we developed a machine learning model that predicts the deformation of rubber components under load. In machine learning, acquiring training data for machine learning is often costly; however, in this paper we established foundational techniques for virtual experiments using CAD and the FEM to enable more efficient data collection, and verified their effectiveness.

Going forward, we will consider developing models capable of predicting various performance characteristics, such as vibration isolation performance, sealing performance and fatigue resistance, using not only features from TEM images, compositional data, and infrared spectral images.

References

(1) Hanawa, Y.: Development of Performance Prediction Technology for Rubber Materials Utilizing FEM and Machine Learning (2), 2023 Annual Meeting of the Society of Rubber Science and Technology, Japan, B-9 (2023)
(2) Nakada, T.: Carbon Black - Focusing on Rubber Reinforcement Performance, Journal of the Carbon Society of Japan, No. 106, 111-120 (1981)
(3) Sakakibara, A., et al.: Improvement of Rubber Properties by Carbon Black, Journal of the Society of Rubber Science and Technology, Japan, 73, No. 7, 385-391 (2000)
(4) Takano, N., et al.: 3D Morphology Analysis and Finite Element Modeling of Nanoparticle-dispersed Materials, Journal of the Society of Materials Science, Japan, 57, No. 5, 423-429 (2008)