Process and material design using hybrid machine learning for direct thermal nanoimprint

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Thermal nanoimprinting provides direct nanofabrication of a wide variety of materials. The results of the process, such as the shape, are determined by the mechanical properties of the material, such as its elastic modulus, the process conditions, such as temperature and pressure, and the geometric conditions, such as the size of the mold pattern. When using a new material or shape, the nanoimprinted is predicted by simulation based on the mechanical properties of the material, and experimentally confirm the process conditions.

In case of a change in material or modification of required profile, an amount of measurement of material property and experiments are required to design the revised processes. However, sometimes it is difficult to measure mechanical properties or additional experiments are restricted.

In this work, we have proposed a hybrid machine learning system that presents the optimum materials and process conditions for direct nanoimprint. In nanoimprint process, few report has been published to predict pattern defects[1], but process and material design has not yet approached.

Figure 1 shows schematics of the hybrid machine learning systems. Machine learning based on experiments is performed under limited experimental conditions. On the other hand, based on the simulation results under various conditions, machine learning is performed to supplements the experimental learning results which does not handled in the experiments under some assumptions and approximation. As a result, processing results for unknown properties of materials could be predicted and we can get suggested materials and process condition.

We applied actual process design as follows. For instance, PVA (Polyvinyl Alcohol), a water-soluble resin, has been used as a disposable mold and sacrificial layer. However, when PVA is heated over 150°C, its water solubility is impaired. To solve the problem, we newly try to lower the pressing temperature by mixing Glycol into PVA. However, there is no information to confirm the molding temperature and needs large amount of experiment for optimize the concentration of Glycol and process temperature.

The thermal characteristics of the elastic modulus of the resin was approximated to be acrylic resin, noting that the thermal characteristics of the elastic modulus shows almost similar characteristics after the glass transition temperature of the resin. We also noted that the pattern profile after imprint was determined in a normalized form by the ratio of press pressure to the modulus of elasticity of the resin and the geometric dimension ratio of the mold pattern [2].

By learning the results of a small number of experiments under constant pressure condition and varying both the press temperature and PVA concentration, we can predict the results at a constant press pressure as demonstrated in Fig.2 (a). On the other hand, by learning of the simulation results in which the relative pressing pressure and relative shape are varied, we can predict the molding results for different pressing pressures as demonstrated in Fig.2 (b).

Based on these two predictions, the system can, for example, suggest the PVA concentration, press temperature, and press pressure to obtain the desired molding results. It is also possible to predict the outcome of a decision under specific conditions. Figure 2 shows comparison with experiments and predictions of the pattern height in various pressures, temperatures under 10% PVA contain resin. The hybrid learning successfully predicts the experimental results even for unknown characteristic of resin property.

References

[1] T. Akter and S. Desai, Materials and Design 160, p836 (2018).

[2] Y. Hirai, et al., J. Vac. Sci. Technol. B 22, p3288 (2006).

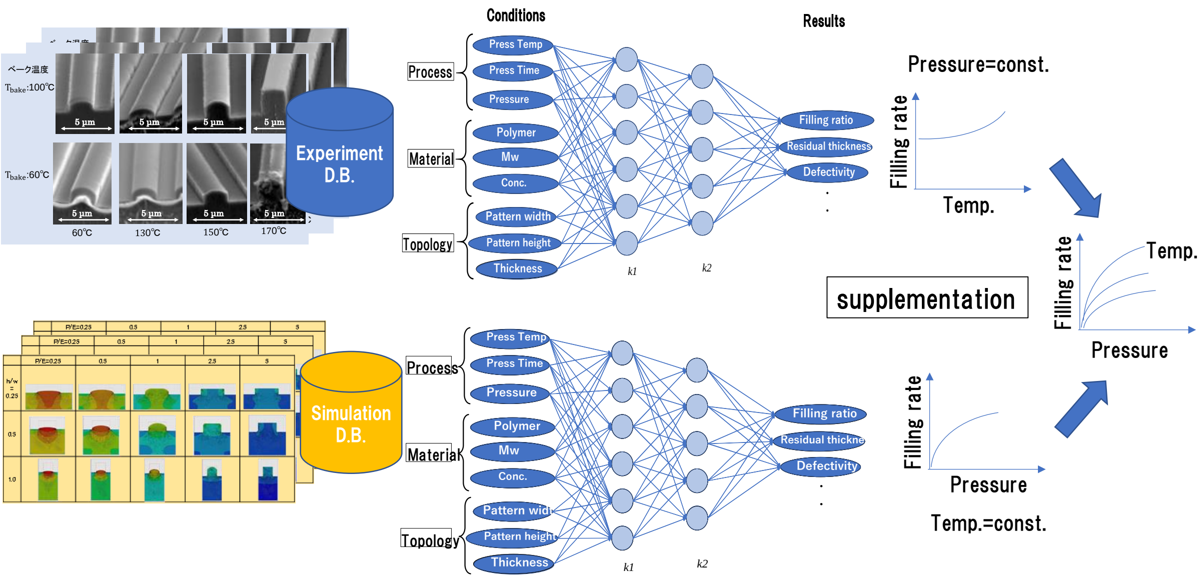
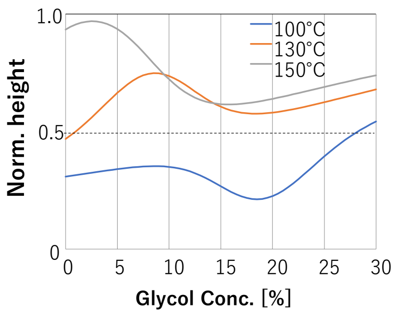
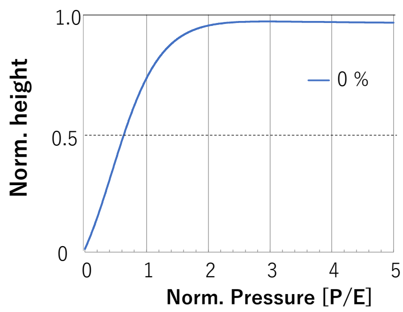


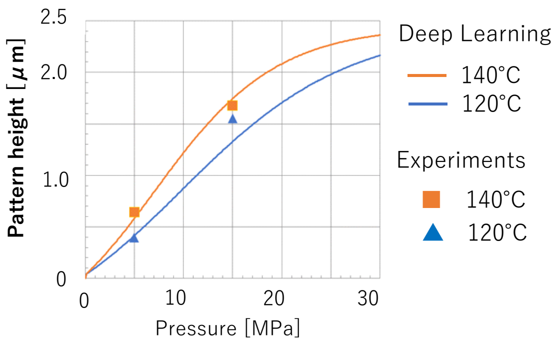
Fig.1. Schematics of the shrinkage and correction models



a) Experimental learning under constant pressure



b) Simulation learning without Glycol



c) Comparison with the experimental results (Not learning data) of predicted pattern height under various pressure and temperature at Glycol concentration=10%
(lines: machine learning, ■ and▲:experiments)

Fig.2. Proposal of Glycol concentration and process conditions for PVA direct imprint process.