Approach for process design solving invers problem by deep learning for nanoimprint process

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Introduction

Deep learning is applied in many technical fields, including the nanofabrication process. In nanoimprinting, more efficient and lower defective process are demanded even if unknown materials or geometries. Those have been approached with the huge of experiments, simulation analysis, experience, and another comprehensive knowledge. We have been demonstrated application of deep learning for nanoimprinting process for prediction of the nanoimprinted results or support for process and material design [1]. In deep learning, the main function is to predict and determine the results under given process conditions by learning many examples. However, proposing a process to achieve the desired outcome, i.e., solving an inverse problem, has not been well demonstrated. For example, in thermal nanoimprinting, there is no system that automatically suggests press pressures and temperatures to obtain the desired pattern height and fill rate.

In this paper, we newly propose the use of deep learning to suggest process conditions for obtaining a given result, rather than using deep learning to predict the nanoimprinted result, as shown in Figure 1.

Procedure to solve inverse problem

In deep learning, the weight coefficients between the nodes of the network are determined in the process of learning the results under various conditions. This process requires a lot of computational power. However, once determined, the coefficients of the network are fixed. Predicting the results when conditions change is done by a simple four-way calculation, and the computation time is extremely fast. Here, a large number of process condition items are divided into fine cases, and the results are calculated in large quantities on a matrix. Of course, the same thing can be done using high-precision simulation, but the cost of computation is by far the cheapest with deep learning.

The relationship between "factors" and "results" obtained by deep learning in this way is stored in a matrix. From this matrix, several process conditions can be proposed by searching for "factors" that satisfy the required "result. In other words, the inverse problem has been solved.

Case study

We try to find the relationship between press pressure and pattern aspect ratio to satisfy the desired values of pattern height and induced strain after nanoimprinting. To obtain the learning data, numerical simulation is performed for various configurations. Figure 2 shows example of the learning data by simulation work. Nanoimprinted resin shape and strain distribution are simulated for varying pattern aspect ratio and resist film thickness.

Figure 3 shows a superimposed plot of the relationship between predicted pattern height and distortion from the training results, with the pattern height and induced strain predicted by varying the conditions in various conditions. In this example, the aspect ratio of the pattern (abscissa) and the relative press pressure (ordinate) to the material modulus are shown to yield results with a height greater than 60% and a strain less than 150%. The dark area where both overlap is the condition for a intended result.

As described above, a process design support system using deep learning in nanoimprinting was obtained.

References:

[1] Y. Hirai, et al., Nanomaterials, 12, 2571(2022).



Fig. 1. Schematics of usage of deep learning.



Fig. 2. Example of the learning data by simulation work.

(Nanoimprinted resin shape and strain distribution are simulated for varying pattern aspect ratio and resist film thickness.)



Fig. 3. Results of the proposed condition map for intended results.