Inprovement of Adhesion between NiTi Alloy and Diamond-like Carbon Film by Bayesian Optimization

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About our Study

In this study, we considered optimizing the structure of silicon-incorporated diamond-like carbon (Si-DLC) interlayer using **"Bayesian optimization"**, which is known as one of machine learning, in order to apply fluorine-incorporated DLC (F-DLC) to low blood compatible nickel-titaniumu (NiTi) alloy.

The purpose of this study is evaluating the effectiveness of **Bayesian optimization** for determing optimal structures of interlayers between metallic substrates and F-DLC (**Fig. 1**), and **developing high blood compatible NiTi alloy by improving adhesion properties of F-DLC**.



Fig. 1 The improvement of adhesion by Bayesian optimization





Evaluation of Adhesion on NiTi stent

The one with the highest adhesion (optimized DLC) and lowest adhesion (not optimized DLC) were deposited on the NiTi stents, and after performing the crimp test and the fatigue test, the surface was observed by Scanning Electron Microscope (SEM). As a result, no delamination was observed in the interlayer derived by Bayesian optimization, whereas delamination occurred in the sample in which structure was not optimized (**Fig. 3**).

Therefore, this study shows that adhesion properties between metallic material and DLC thin film can be improved by Bayesian optimization.

Update by Bayesian Optimization

The adhesion properties between NiTi substrates and DLC thin films were evaluated by the scratch test, and the structures of Si-DLC interlayer were updated successively by Bayesian optimization on the obtained data (**Fig. 2**). The critical load increased as the film formation conditions were updated, suggesting that Bayesian optimization was working.

Total of 30 Si-DLC interlayers were produced, and the highest adhesion could be improved to about 53 mN, while the lowest adhesion was about 22 mN.



Fig. 3 Images of after crimp test : (a) not optimized DLC, (b) optimized DLC, and images of after fatigue test : (c) not optimized DLC, (d) optimized DLC