

Development of Material Search Technology using Kriging model

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Abstract

Manufacturers over the last decade have tackled the important issues of speeding up and improving quality of product development in an extremely changeable and globalizing world market. Effective use of analysis led design is indispensable in order to solve these issues. Design exploration based on optimization technology using computer simulation is very important to shorten the design period. Therefore, many optimization methodologies have been proposed in the mechanical engineering field. On the other hand, characteristic values such as the diffusion coefficient in a material can be predicted by developing molecular dynamic simulation for searching materials. However, a lot of simulations for possible materials are necessary to determine the target material. These iterative simulations consume a lot of time.

Therefore, authors have developed material searching technology using optimization technique in order to speed up material design. In optimization technology, a response surface method has been proposed as methodology for shortening optimization time instead of experiments and simulations. We have employed the response surface method for material search. There are several response surface models such as quadratic function, artificial neural network etc. We employed Kriging model which is widely used in the last decade. Kriging model yields high accuracy for the approximation of global space containing non-linearity. We searched a target material using Kriging model with fewer sample points. Procedure for searching materials is shown in Fig. 1. Here, response values are characteristic values and design variables are material physical property such as lattice constant.

The effectiveness of the proposed technology is demonstrated by applying it to the material searching of electrode filter. It is necessary to choose electrode filter which doesn't produce air bubbles caused by diffusion. It is said that materials of electrode filter having small value of self-diffusion coefficient at interface do not produce air bubbles. Therefore, we search a material which minimizes self-diffusion coefficient. We choose 31 kinds of element as target materials. We selected lattice constant, melting point and cohesion energy as design variables, and self-diffusion as objective function. Figure 2 shows scatter diagram in design space obtained by Step 5 in Fig. 1. Next sampling point is chosen by selecting material near minimum self-diffusion coefficient from the scatter diagram. Target materials had been chosen by molecular dynamics simulation for all possible materials in the past. However, we have been able to confine the search of the target material to 10 molecular dynamics simulations using the proposed procedure. It is found that the propose technology reduced the material searching time by 70% compared with that for previous methods.

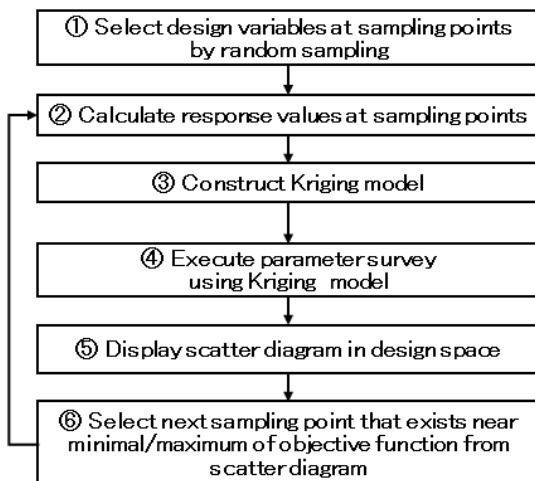


Figure 1. Procedure for material search

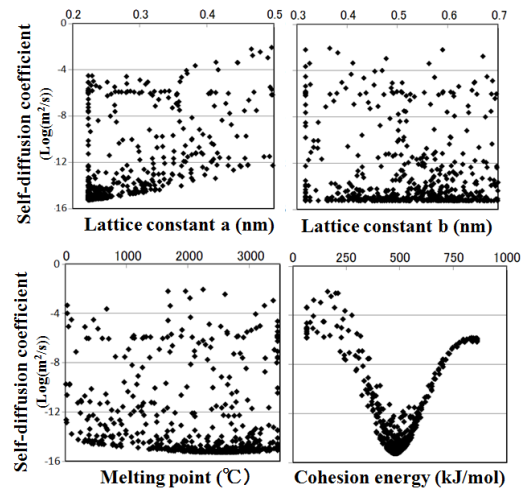


Figure 2. Scatter diagram