

論文の内容の要旨

論文題目 Practical applications of sparse modeling to metallurgical problems

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When establishing PSPP relationships of a material using data driven techniques, two modeling routes can be adopted; forward modeling for prediction and inverse modeling for materials discovery. In general, the former is usually not difficult because its relationship is many to one. On the other hand, the latter whose relationship is one to many requires much more effort for at least two reasons: (i) the model parameters may have different values or not consistent with the data, and (ii) discovering the model parameters usually requires the exploration of a huge parameter space. In this study, the research mainly aims to solve inverse problems in materials research especially in case of various properties of metallic materials.

In Chapter 1, the historical background of materials study was briefly introduced on the basis of the four research paradigm with various examples; (i) empirical, (ii) theoretical, (iii) computational, and (iv) machine learning based. current statuses of the application of various modeling techniques are briefly introduced. Then it is emphasized that inverse modeling is an important task not only for designing but also discovering new or improved materials.

In Chapter 2, a data driven modeling methodology called “*sparse modeling*”, which is introduced in this study to solve various inverse problems, are discussed. The basic concept and the mathematical explanation about modeling techniques are given. In addition, their applicability for materials problems are examined with synthetic datasets; (i) a linear problem and (ii) a nonlinear problem. The various modeling criteria is validated with synthetic datasets and their performance are compared under various assumptions.

In Chapter 3, linear model selection techniques such as Akaike information criterion (AIC), Bayesian information criterion (BIC), etc. are applied to identify the important alloying elements which are necessary to predict the Ac3 and Ms phase transformation start temperatures. Their predictive performances are compared to

previously proposed equations and thermodynamic analysis is also conducted.

In Chapter 4, identification of the phase transformation of steel during continuous cooling is performed using the exchange Markov chain Monte Carlo (MCMC) method. The dilatometric experiments which record the volume change during cooling is conducted and the phase transformation kinetics based on JMAK model is fitted to the experimental data. The probability of candidate models is then estimated and the validation is carried out with experimental data and past literature.

In Chapter 5, the viability of establishing low cost surrogate structure-property linkages is investigated using the MKS framework and a Bayesian model selection method. To be specific, the synthetic microstructure dataset is generated and the yield strength is estimated using the crystal plasticity simulation. Then, those microstructure and property relationships are constructed by two-point statistics, principal component analysis, and the Bayesian information criterion. Finally, the model is verified with an independent dataset and its constituent features are interpreted with a morphology reconstruction based on a Monte Carlo algorithm.