

Prediction Models Generation by Machine Learning for Structural Materials Performance by Utilizing the Mi System

Satoshi Minamoto*, Takuya Kadohira, Kaita Ito, Makoto Watanabe and Masahiko Demura

National Institute for Materials Science (NIMS), 1-2-1 Sengen, Tsukuba-city Ibaraki 305-0047, Japan.

*Corresponding Author: Satoshi Minamoto. Email: MINAMOTO.Satoshi@nims.go.jp.

Abstract: The Materials Integration (MI) System is a domestically developed system in the “Cross-ministerial Strategic Innovation Promotion Program” to analyze structural materials performance. The performance on structural materials having complicated inputs/outputs would be solved with the combination of different scientific programs or data from experiment. One of the merits of constructing a combined model (here we call workflow) is that calculations are performed and the data would be stored in the system automatically.

Furthermore, we developed a web application (“MIREA”: MI REgression Analyzer) that enables us to build high versatile prediction models based on machine learning techniques by using the data from workflows. In order to keep affinity with the MI system, unification of data format, connecting MI vocabulary system in order to include metadata required for the models, hyper-parameters tuning in learning process to get proper model, reusability of the models in the MI system, etc. were devised in the MIREA software. Here, we construct prediction models by machine learning techniques with use of workflows consisting of high-precision elemental programs for important issues concerning the performance of structural materials such as fatigue life analysis and creep life analysis. The generated models enable us to reduce time to develop materials having required performance.