Materials Integration for Accelerating Research and Development of Structural Materials

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This paper provides a current research trend for “Materials Integration”, which is a concept to accelerate research and development of structural materials by computationally linking among process, structure, property, and performance. The survey is carried out based on the special issue published in February, 2019 in Materials Transactions (Vol. 60, No. 2) and the overviews published in November, 2020 in Materials Transactions (Vol. 61, No. 11). The concept has been embodied in a computer system named MInt (Materials Integration by Network Technology), on which computational modules and workflows are implemented to predict performance from process through microstructure and property. The research works on the system development and the computational materials analyses are briefly introduced, highlighting the rising trend of data-driven research in structural materials. [doi:10.2320/matertrans.MT-M2021135]

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1. Introduction

Process, structure, property, and performance are the key elements in materials science and engineering, and to study relations among them is what material researchers do. Collecting and organizing the relations are necessary to predict performance from process considering structure and property, leading to accelerating the R&D of new innovative materials. Based on this idea, a new concept named Materials Integration (MI) was proposed in the Cross-ministerial Strategic Innovation Promotion Program (SIP) “Structural Materials for Innovation” and the MI systems called MInt (Materials Integration by Network Technology) is being developed in the SIP “Materials Integration for revolutionary design system of structural materials”; here, the SIP projects are supported by Council for Science, Technology and Innovation of the Cabinet Office, Japan.

A special issue was edited in February, 2019, in Materials Transactions (Vol. 60, No. 2) under the title of “Materials Integration”. This was a bundle of contributions that are works following the MI concept. Most of them came from the above-mentioned projects, including performance predictions such as creep, fatigue, and Hydrogen embrittlement and microstructure prediction. Furthermore, another special issue was edited in November, 2020 in Materials Transactions (Vol. 61, No. 11) under the title of “SIP Materials Integration Project”. This consisted of five overviews and a contributing article on microstructure prediction for Ni-base superalloys.

These special issues were designed to clarify the concept of materials integration proposed in the above-mentioned SIP projects and to report on its progress. The first special issue collected contributing papers from the SIP project and the other research works relating to the concept of materials integration. The second special issue consists mainly of overviews by the project members together with a contributing paper from the project.

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2. Concept of Materials Integration and Its System, MInt

The concept of MI is to computationally linking among process, structure, property, and performance. In the MInt system each link is implemented as a module and to connect several modules as a workflow enables us to predict performance from process through structure and property. The workflows can be regarded as accumulations of multiple research achievements; for example, a workflow to predict creep rupture time of a weld joint shown in Fig. 1 consists of the welding simulation, the detection of heat affected zone, and the creep damage simulation. Each research achievement constitutes academic knowledge with content that has been reported as papers and these academic knowledge are digitized as a workflow and stored in the MInt system.

Another characteristic of the MInt system is its extensibility and by adding a new workflow it is possible to handle any kinds of materials problems. In fact, various studies are reported for predicting performances such as fatigue for steels, Al alloys, Mg alloys, and Ti alloys; brittle fracture for steels, hydrogen embrittlement, and so on. Representative efforts on performance prediction are summarized in Ref. 11). The prediction accuracy obtained in these studies was practically reasonable as demonstrated in Fig. 2.

Microstructure prediction is mainly studied using phase field simulation as summarized in Ref. 10). One of the challenges is to apply multi-phase field modeling to simulate the phase transformation of steels in the welding process. In order to evaluate thermodynamic and interfacial parameters that are necessary for the phase field simulation, the molecular dynamic simulation was conducted. The target materials for which the microstructure is predicted by the phase-field method has been expanded to Nickel-based superalloys.

System architecture of MInt was detailed in Ref. 13) and it consists of the microstructure prediction system, the performance prediction system, and the property-space
analysis system as schematically shown in Fig. 3. MInt can include any types of modules such as numerical simulations, experimental data, theories, and empirical laws. It has user-friendly interfaces for designing a workflow, conducting a calculation according to the designed workflow, and visualizing the calculated results.

3. International Benchmark of MInt

International benchmarks for MInt were discussed as shown in Fig. 4. There are several approaches to handle versatile materials problems, and only MInt provides a flexible and automatic method of combining modules to form a workflow to solve a wide variety of materials problems.
This advantage will be further strengthened by the establishment of a function that is useful to solve the inverse problem which has been tackled in the latest SIP project. Another point is that MInt is a tool for in-house development in industry, which is clearly distinct from other initiatives where computational tools are used to provide solutions in the context of outsourced development.

4. Contribution to the Expansion of Data-Driven Research in Structural Materials

Another important achievement is to intensively apply the data science to materials science and engineering in MI as summarized in Ref. 12). The applications can be classified into three groups, as follows. The first group is to apply the Bayesian inference for model selection, which is proved to be useful to examine contributing factors in creep constituent equations,27,28) ferrite transformation kinetics based on dilatometric measurement,29) and the structure-property relationship with a dual-phase microstructure.30) The second group is to utilize data assimilation methods for improving the prediction accuracy of various computational simulations such as phase field modeling31) and welding process analysis.32) Figure 5 shows an example of applying data
assimilation to determine the initial and materials parameters for texture evolution during recrystallization in Al alloys.\textsuperscript{12)}

The third group is to apply machine learning method for the quantitative analysis of microstructures with both of supervised\textsuperscript{13,14)} and unsupervised\textsuperscript{15)} approaches. Besides, the Bayesian optimization has been applied to a gas atomizing process of Nickel-based superalloy powder.\textsuperscript{36)} The data-driven research on structural materials has been boosted in a couple of years and is expected to become more and more active.

5. Application of MInt to the Latest Material Fields

Recent attention has also been paid to additive manufacturing and the latest SIP project covers the additive manufacturing especially for Nickel-based superalloys. The cracking during the selective laser melting process has become a problem and the solidification cracking was treated under the concept of MI using computational simulation.\textsuperscript{37)} Nondestructive testing using acoustic emission has also been applied to the solidification cracking problem.\textsuperscript{38)} The microstructure evaluation was also examined through the phase field simulation.\textsuperscript{14,39)}

6. Summary

In summary, there are growing research activities relating to the concept of MI to apply the computational approaches to the research and development of structural materials. It should be noted that data-driven research is becoming more and more important in this field as summarized in Ref. 40).

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