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Remarks on Special Issue on Computational Science:
Potential and Possibilities of Computational Science on Steel Product Development

New steel products are developed naturally for actual use in the market. Therefore, when discussing the properties of such developed products, it is important to focus on their use and expected performance as a final product or a component.

Widely varied characteristics are required for a final product or a part; in the case where the properties of steel play a decisive role in the product characteristics, the manufacturing conditions of steel are designed and devised such that the required properties are incorporated in it by optimizing the alloy chemistry and controlling the microstructure characteristics, including the amount and size of each microstructure and precipitate particle, their shapes, hardness, distribution, and crystal orientation. The control of microstructure, or micrometallurgy, is generally discussed through the following two approaches.

One is to clarify how steel properties (strength, deformation behavior, toughness, ductility, etc.) change depending on its microstructure and which microstructure is effective in improving individual property. The other approach is to define the manufacturing processes to obtain such a microstructure; in other words, an approach to identify a metallurgical route for controlling the alloy chemistry of steel and its thermo-mechanical treatment conditions so as to tailor the microstructure of steel to a desired state. It is possible to manufacture and supply steel products that meet the market requirements only when these two approaches work effectively in a synchronized manner.

Thus, an important function of microstructure is to translate steel users' requirements into the technical language used by steel producers. While the steelmaking industry of Japan, in the modern sense of the word, completed 150 years in 2007, the understanding of the function of microstructure as the translator between the market requirement and steel manufacturing technology is about to enter into a new stage. When considering the features such as strength characteristics and deformation behavior, we notice that there have been many findings in the effects of different microstructures and vast information has been accumulated regarding the roles played by microstructural units of ferrite and other microstructures of steel. However, little is known about how local deformation behavior of microstructures continuously leads to macroscopic deformation of steel. To understand the translating function of the microstructure of *steel, it is indispensable to grasp the microscopic state of the material two- or three-dimensionally, for example, to confirm experimentally the local strain and stress states during deformation.*

However, it is not always easy to experimentally collect all relevant information. Furthermore, the two- or three-dimensional construction of the microstructure obtained through industrial thermo-mechanical treatment is often insufficient as optimum materials' properties. It is therefore difficult to fully understand the translation function of microstructure and to study optimum microstructures that bring about desired properties and the process to obtain them only through experimental approaches. It is computational science that offers an additional freedom to experimental approaches. Computational science has brought a clearer aspect of translation function of microstructure in combination with experimental approaches.

As stated, in-use properties of steel are combined with manufacturing process control technology with microstructure as the translator. When plastic deformation is considered to be important in the market, it is possible to use the translation function of microstructure to improve the properties of the material if we well understand how microscopic deformation behavior governs macroscopic deformation of the material. Here, it is necessary to deal with the impact of microscopic inhomogeneity on macroscopic deformation behavior of steel. In addition, it is necessary to quantitatively treat microscopic deformation; stress or strain concentration; and the formation and growth of voids as a result considering the movement, pile-up, and structure changes of dislocations. The use of numerical operations applying the finite element method and the phase-field method for clarifying these phenomena has been expanding. Such operations are expected to be powerful in clarifying the optimum microstructure through the virtual assessment of the effect of microstructural factors on the macroscopic behavior of deformation and failure.

Computational science is expected to further contribute largely to establish process conditions for obtaining optimum microstructures. In steel manufacturing processes, the materials undergo large temperature changes within a comparatively short period. Therefore, thermal equilibrium is not always attained. For this reason, it is essential to accurately understand the kinetics of reactions that are characteristic to the formation of different microstructures while taking stand on thermodynamics. The study of the kinetics of phase transformation and precipitation, which have been eagerly pursued since the 1950s, is based on the assumption of reactions on fixed-shape interfaces in a uniform field. As a consequence, it can only express the aspects of microstructure required for individual use. In this relation, the phase-field method mentioned above is expected to be effective in reproducing the complicated shapes and dispersion of microstructures. In addition, the first-principle calculation and other approaches are expected to be useful in quantitative discussion about, for example, the true nature of interface energy and the influence of alloy elements, and segregation, which have been treated as adjustable unknown parameters.

The numerical prediction of microstructural evolution has mainly been discussed two-dimensionally; however, if it is possible to directly deal with three-dimensional reactions, it will be possible to reproduce microstructural aspects that govern the properties of steel and to model *nucleation and growth of each transformation product in a more physical manner. To bring such quantitative reproduction of microstructures into reality, many problems need to be solved. One such problem is how to consider the structural and chemical non-uniformities and their development during reactions, the effects of shape factor, and the competition of nucleation and growth of each transformation product. However, once such a framework is systematically established, it will be possible to identify metallurgical routes to obtain a desired microstructure, and by selecting the most viable process from among possible routes, we will be able to produce the products that the market demands without having to rely excessively on trial and error.*

Thus, the evolution of computational science will make it possible to construct sizes, types of crystal, crystal orientations, shapes of each component with various solute elements, and distribution of precipitates in a three-dimensional space of a virtual steel manufacturing process set up in a computer, and also bring the material to an optimum state through evaluation of its performance under supposed conditions of actual use. It is very important to experimentally confirm the predicted results of computational science in a virtual space. The rapidly advancing physical analysis technologies using high-energy beams, such as direct three-dimensional measurement of microstructure, crystal orientation, and atomic-scale structural analysis, are expected to play important roles in this field of experimental verification.

Three- or four-dimensional (with a time axis) observation and analysis are aggressively pursued also in Japan through activities carried out in various groups such as the forums of the Iron & Steel Institute of Japan (ISIJ). Elaborate databases are being compiled for such application, and joint studies with overseas research groups and institutes are under way. The present technologies and findings in the field of computational science are being collected by ISIJ committees and other organizations; as a result, the understanding and control of steel microstructure are rapidly changing from two- to three-dimensional.

As stated, microstructural observation technology and computational science are likely to significantly change the conventional manner of steel material development. To make this happen, it is important to continue elaborating constituent technologies such as establishing more realistic expressions of phenomena, introducing new mathematical expressions and calculation methods, and specifying new microstructural aspects in three-dimensional space. Computational science that connects the market and steel manufacturing processes by the translation function of microstructure is expected to play an important role in detailed understanding, new development, and improvement of steel products.